Parallel Programming … the world beyond mutithreading

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*a made-up company since so many forms require an institution … I like “human learning” not “machine learning”

Disclaimer

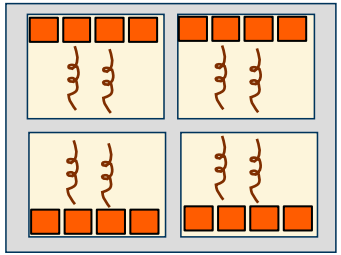
- The views expressed in this talk are those of the speaker.

- If I say something “smart” or worthwhile:
  - Credit goes to the many smart people I work with.

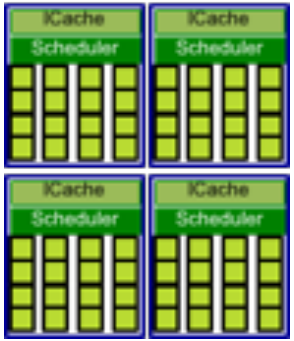
- If I say something stupid…
  - It’s my own fault

For hardware … parallelism is the path to performance

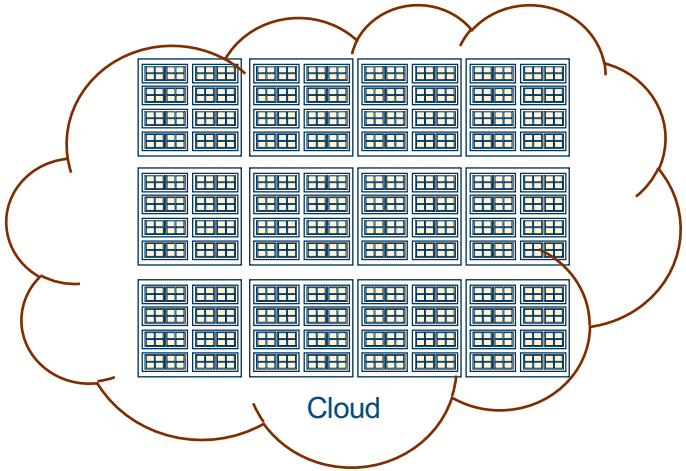
All hardware vendors are in the game … parallelism is ubiquitous so if you care about getting the most from your hardware, you will need to create parallel software.



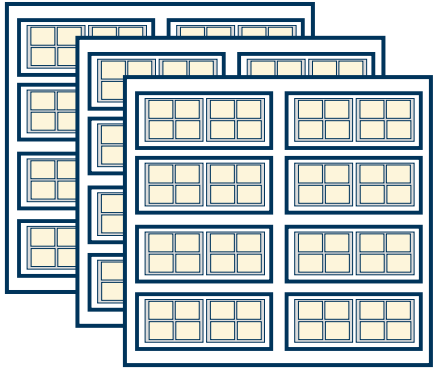
CPU + SIMD/Vector



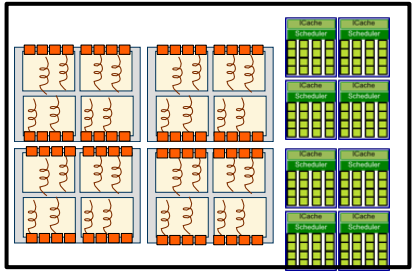
GPU



Cloud



Cluster



Heterogeneous node

Programming for the three major execution models

- In HPC, 3 programming environments dominate … covering the major classes of hardware.
  - **MPI**: distributed memory systems … though it works nicely on shared memory computers.
  - **OpenMP**: Shared memory systems … more recently, GPGPU too.
  - **CUDA**, **OpenCL**, **Sycl**, **OpenACC**, **OpenMP** … : GPU programming (use CUDA if you don't mind locking yourself to a single vendor … it is a really nice programming model)
- Even if you don't plan to spend much time programming with these systems … a well rounded HPC programmer should know what they are and how they work.

Programming for the three major execution models

- In HPC, 3 programming environments dominate … covering the major classes of hardware.
  - **MPI**: distributed memory systems … though it works nicely on shared memory computers.
  - **OpenMP/TBB**: Shared memory systems.

You are all OpenMP and TBB experts and know a great deal about multithreading

You understand GPU programming with CUDA

  - **CUDA**, **OpenCL**, **Sycl**, **OpenACC**, **OpenMP** … : GPU programming (use CUDA if you don't mind locking yourself to a single vendor … it is a really nice programming model)

- Even if you don't plan to spend much time programming with these systems … a well rounded HPC programmer should know what they are and how they work.

Programming for the three major execution models

If you don't know MPI, you aren't really an HPC programmer!

- In HPC, 3 programming environments dominate … covering the major classes of hardware.
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  - **OpenMP/TBB**: Shared memory systems.

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  - **CUDA**, **OpenCL**, **Sycl**, **OpenACC**, **OpenMP** … : GPU programming (use CUDA if you don't mind locking yourself to a single vendor … it is a really nice programming model)

- Even if you don't plan to spend much time programming with these systems … a well rounded HPC programmer should know what they are and how they work.

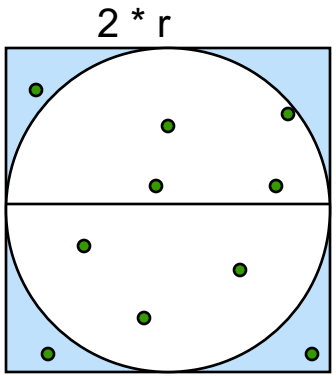
Before we talk about MPI … I have an important topic I need to cover with you.

I'll use OpenMP for this topic, but the ideas we're going to cover apply to every programming model

Exercise: Monte Carlo Calculations

Using random numbers to solve tough problems

- Sample a problem domain to estimate areas, compute probabilities, find optimal values, etc.
- Example: Computing π with a digital dart board:



N= 10	π = 2.8
N=100	π = 3.16
N= 1000	π = 3.148

- Throw darts at the circle/square.
- Chance of falling in circle is proportional to ratio of areas:

  $A_c = r^2 * \pi$

  $A_s = (2*r) * (2*r) = 4 * r^2$

  $P = A_c/A_s = \pi/4$
- Compute π by randomly choosing points; π is four times the fraction that falls in the circle

Parallel Programmers love Monte Carlo algorithms

```
#include "omp.h"
static long num_trials = 10000;
int main ()
{
   long i;      long Ncirc = 0;       double pi, x, y;
   double r = 1.0;   // radius of circle. Side of squrare is 2*r
   seed(0,-r, r);  // The circle and square are centered at the origin
   #pragma omp parallel for private (x, y) reduction (+:Ncirc)
   for(i=0;i<num_trials; i++)
   {
      x = random();         y = random();
      if ( x*x + y*y) <= r*r)   Ncirc++;
    }

    pi = 4.0 * ((double)Ncirc/(double)num_trials);
    printf("\n %d trials, pi is %f \n",num_trials, pi);
}
```

Embarrassingly parallel: the parallelism is so easy its embarrassing.

Add two lines and you have a parallel program.

Random Numbers: Linear Congruential Generator (LCG)

- LCG: Easy to write, cheap to compute, portable, OK quality

```
random_next = (MULTIPLIER  * random_last + ADDEND)% PMOD;
random_last = random_next;
```

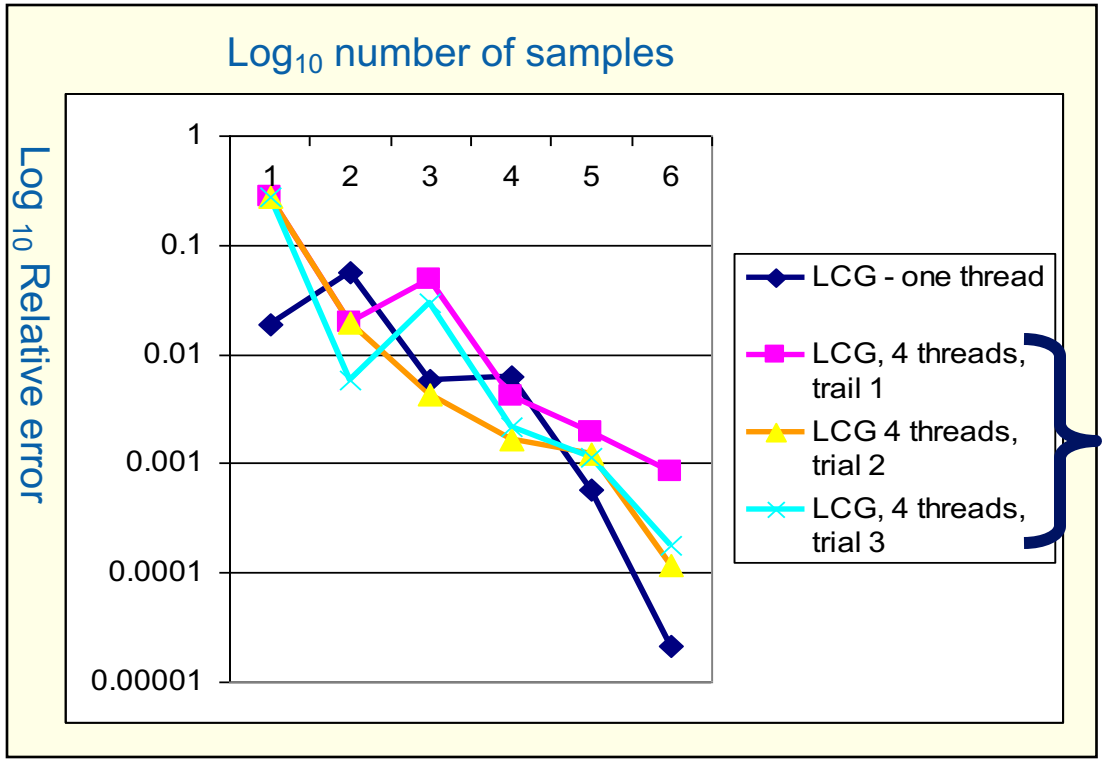
- If you pick the multiplier and addend correctly, LCG has a period of PMOD.
- Picking good LCG parameters is complicated, so look it up (Numerical Recipes is a good source). I used the following:
  - MULTIPLIER = 1366
  - ADDEND = 150889
  - PMOD = 714025

LCG code

```
static long MULTIPLIER  = 1366;
static long ADDEND      = 150889;
static long PMOD        = 714025;
long random_last = 0;
double random ()
{
    long random_next;

    random_next = (MULTIPLIER  * random_last + ADDEND)% PMOD;
    random_last = random_next;

   return  ((double)random_next/(double)PMOD);
}
```

Seed the pseudo random sequence by setting random_last

Running the PI_MC program with LCG generator



Run the same program the same way and get different answers!

That is not acceptable!

Issue: my LCG generator is not threadsafe

Program written using the Intel C/C++ compiler (10.0.659.2005) in Microsoft Visual studio 2005 (8.0.50727.42) and running on a dual-core laptop (Intel T2400 @ 1.83 Ghz with 2 GB RAM) running Microsoft Windows XP.

Data Sharing: Threadprivate

- Makes global data private to a thread
  - Fortran: **COMMON** blocks
  - C: File scope and static variables, static class members
- Different from making them **PRIVATE**
  - with **PRIVATE** global variables are masked.
  - THREADPRIVATE preserves global scope within each thread

Example: Use threadprivate to create a counter for each thread.

```
int counter = 0;
#pragma omp threadprivate(counter)

int increment_counter()
{
    counter++;
    return (counter);
}
```

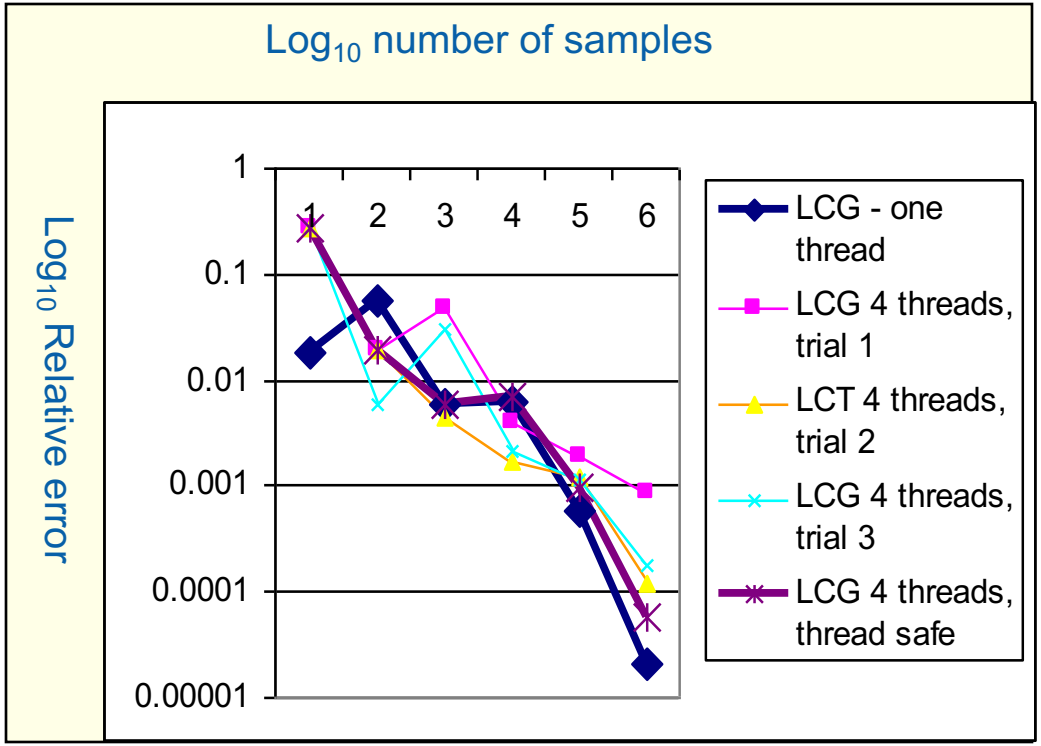
LCG code: threadsafe version

```
static long MULTIPLIER  = 1366;
static long ADDEND      = 150889;
static long PMOD        = 714025;
long random_last = 0;
#pragma omp threadprivate(random_last)
double random ()
{
    long random_next;

    random_next = (MULTIPLIER  * random_last + ADDEND)% PMOD;
    random_last = random_next;

   return  ((double)random_next/(double)PMOD);
}
```

random_last carries state between random number computations,

To make the generator threadsafe, make random_last threadprivate so each thread has its own copy.

Thread Safe Random Number Generators



Thread safe version gives the same answer each time you run the program.

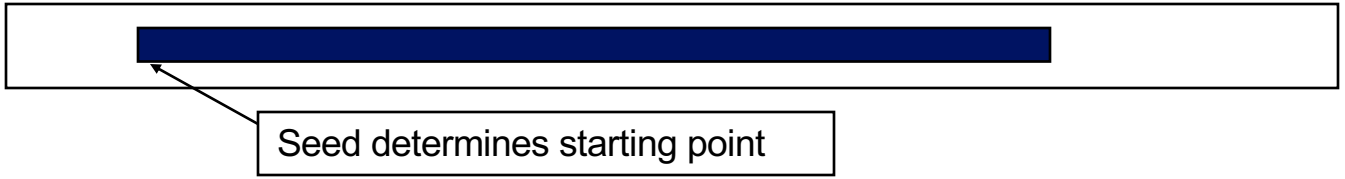
But for large number of samples, its quality is lower than the one thread result!

Why?

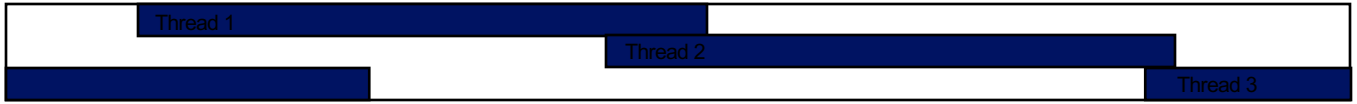
Pseudo Random Sequences

- Random number Generators (RNGs) define a sequence of pseudo-random numbers of length equal to the period of the RNG

- In a typical problem, you grab a subsequence of the RNG range



- Grab arbitrary seeds and you may generate overlapping sequences
  - E.g. three sequences … last one wraps at the end of the RNG period.



- Overlapping sequences = over-sampling and bad statistics … lower quality or even wrong answers!

Now that you understand threadprivate in OpenMP, the concept of thread safe libraries, and the concept of parallel random number generators, let’s move to MPI.

A “Hands-on” Introduction to MPI

Tim Mattson **Human Learning Group.** tgmattso@gmail.com

Download tutorial materials:

git clone https://github.com/infn-esc/esc23.git then go to esc23/hands-on/mpi

* The name “MPI” is the property of the MPI forum (http://www.mpi-forum.org).

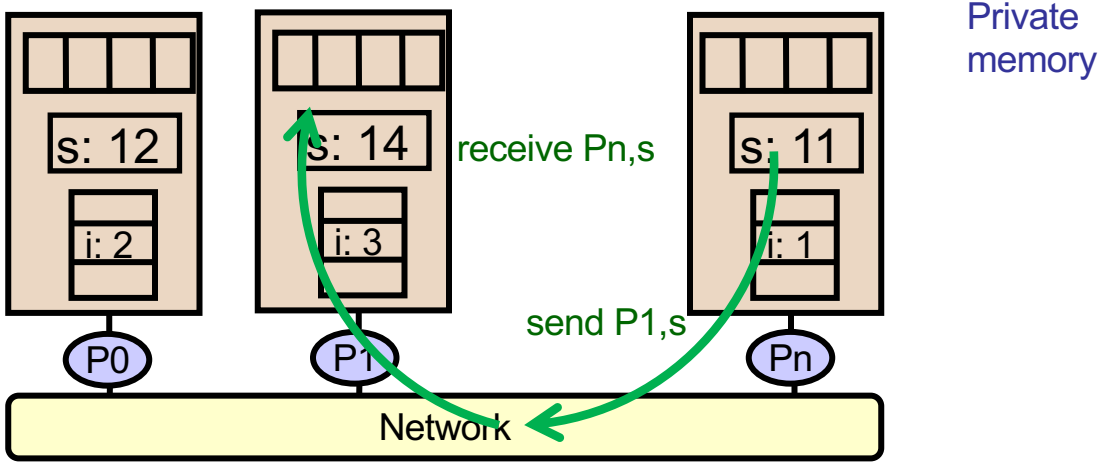
Outline

- MPI and distributed memory systems
- The Bulk Synchronous Pattern and MPI collective operations
- Introduction to message passing
- The diversity of message passing in MPI
- Geometric Decomposition and MPI
- Concluding Comments

Programming Model for distributed memory systems

- Programs execute as a collection of processes.
  - **Number of processes almost always fixed at program startup time**
  - **Local address space per node -- NO physically shared memory.**
  - **Logically shared data is partitioned over local processes.**

- Processes communicate by explicit send/receive pairs
  - **Synchronization is implicit by communication events.**
  - **MPI (Message Passing Interface) is the most commonly used API**



Parallel API's: MPI, the Message Passing Interface

MPI: An API for Writing Applications for Distributed Memory Systems

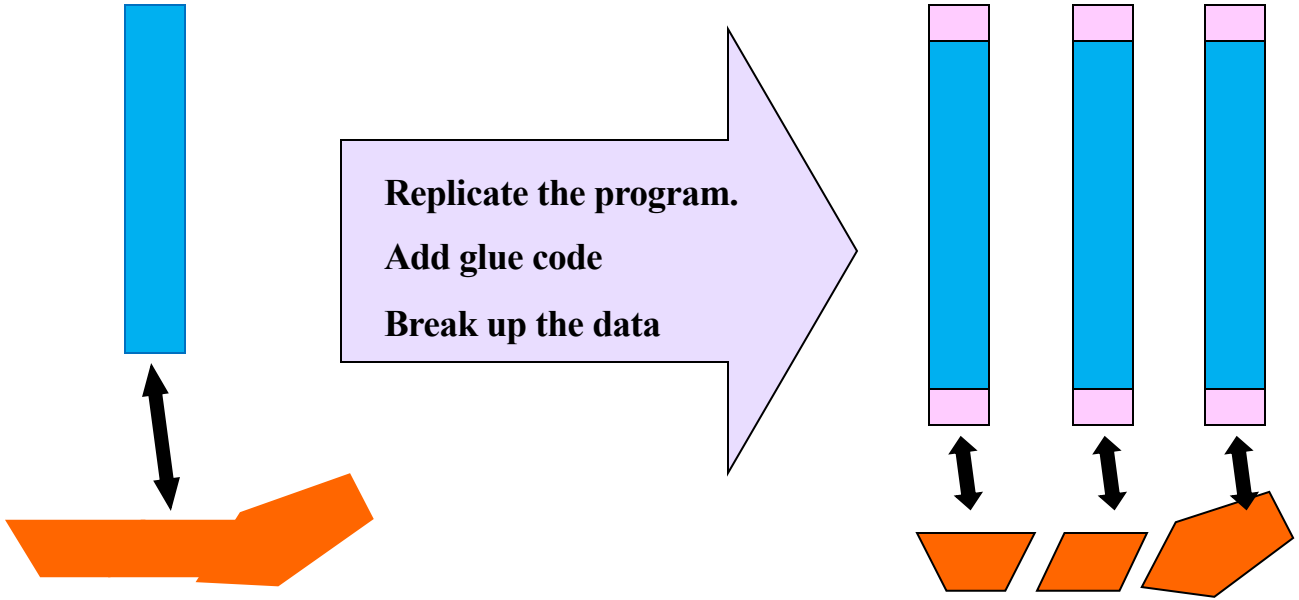
- A library of routines to coordinate the execution of multiple processes.
- Provides point to point and collective communication in Fortran, C and C++
- Unifies last 30 years of cluster computing and MPP* practice

*MPP: Massively Parallel Processing. Clusters use "off the shelf" components. MPP systems include custom system integration.

How do people use MPI?
The SPMD Design Pattern

- A replicated single program working on a decomposed data set.
- Use Node ID (rank) and number of nodes to split up work between processes (ranks)
- Coordination by passing messages.

A sequential program (blue) working on a data set (orange)



Using the ESC cluster with MPI

- Compile your program

```
$ mpicc -fopenmp -O3 -o hi hello.c
```

- Run the program on the local node

```
$ mpirun -np 4 ./hi
```

- Run the program across multiple nodes (with 2 processes … or slots … on each node):

```
$ cat hosts
 hpc-200-06-06 slots=2
 hpc-200-06-17 slots=2
 hpc-200-06-18 slots=2
$ mpirun -hostfile hosts -np 4 ./hi
```

Exercise: Hello world part 1

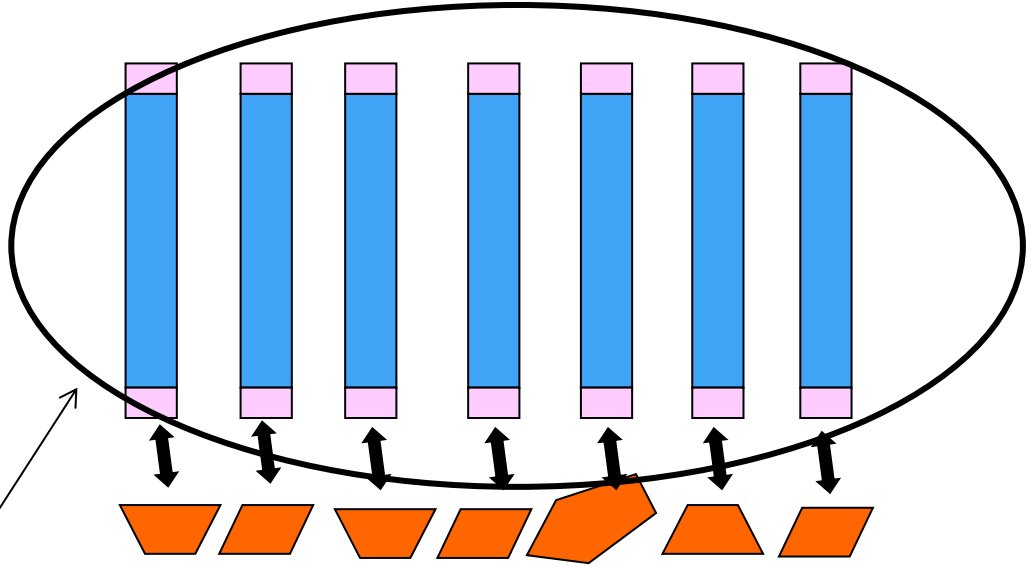
```
$ cat hosts
 hpc-200-06-06 slots=2
 hpc-200-06-17 slots=2
 hpc-200-06-18 slots=2
```

- Goal
  - To confirm that you can run a program in parallel.
- Program
  - Write a program that prints “hello world” to the screen.
  - Execute across the nodes of our cluster using mpirun

- Log in to the ESC cluster making sure to set things up for MPI as instructed.
- Build your MPI program
  ```
  $ mpicc -fopenmp -O3 -o hi hello.c
  ```
- Run the program on the local node
  ```
  $ mpirun -np 4 ./hi
  ```
- Run the program on hosts listed in the hostfile.
  ```
  $ mpirun -hostfile hosts -np 4 ./hi
  ```

An MPI program at runtime

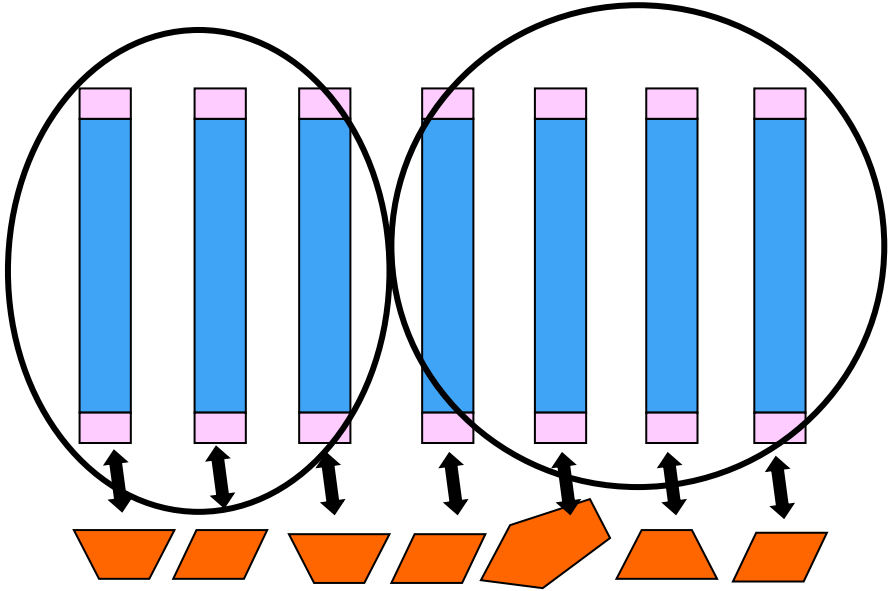
- Typically, when you run an MPI program, multiple processes all running the same program are launched … working on their own block of data.



The collection of processes involved in a computation is called “a **<u>process group</u>**”

An MPI program at runtime

- Typically, when you run an MPI program, multiple processes all running the same program are launched … working on their own block of data.



You can dynamically split a **process group** into multiple subgroups to manage how processes are mapped onto different tasks

MPI Hello World Program

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                              rank, size );
   MPI_Finalize();
   return 0;
}
```

Initializing and finalizing MPI

```
int MPI_Init (int* argc, char* argv[])
```

- Initializes the MPI library … called before any other MPI functions.
- agrc and argv are the command line args passed from main()

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                                rank, size );
   MPI_Finalize();
   return 0;
}
```

```
int MPI_Finalize (void)
```

- Frees memory allocated by the MPI library … close every MPI program with a call to MPI_Finalize

How many processes are involved?

```
int MPI_Comm_size (MPI_Comm comm, int* size)
```

- **MPI_Comm**, an *opaque data type called a communicator.* Default context: MPI_COMM_WORLD (all processes)
- **MPI_Comm_size** returns the number of processes in the process group associated with the communicator

```
#incl
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                                 rank, size );
   MPI_Finalize();
   return 0;
}
```

Communicators consist of two parts, a **context** and a **process group**.

The communicator lets one control how groups of messages interact.

Communicators support modular SW … i.e. I can give a library module its own communicator and know that it's messages can't collide with messages originating from outside the module

Which process “am I” (the rank)

```
int MPI_Comm_rank (MPI_Comm comm, int* rank)
```

- **MPI_Comm**, an *opaque data type,* **a** communicator. Default context: MPI_COMM_WORLD (all processes)
- **MPI_Comm_rank** An integer ranging from 0 to “(num of procs)-1”

```
#incl
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                                rank, size );
   MPI_Finalize();
   return 0;
}
```

Note that other than init() and finalize(), every MPI function has a communicator.

This makes sense .. You need a context and group of processes that the MPI functions impact … and those come from the communicator.

Running the program

- On a 4 node cluster, to run this program (hello):
  > mpirun –np 4 –hostfile hostf hello
- Where “hostf” is a file with the names of the cluster nodes, one to a line.
- Would would this program output?

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                                rank, size );
   MPI_Finalize();
   return 0;
}
```

Running the program

- On a 4 node cluster, to run this program (hello):

  > mpirun –np 4 –hostfile hostf hello

  Hello from process 1 of 4

  Hello from process 2 of 4

  Hello from process 0 of 4

  Hello from process 3 of 4

- Where “hostf” is a file with the names of the cluster nodes, one to a line.

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
    int rank, size;
    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    printf( "Hello from process %d of %d\n",
                                rank, size );
    MPI_Finalize();
    return 0;
}
```

Exercise: Hello world part 2

- Goal
  - To confirm that you can run an MPI program on our cluster
- Program
  - Write a program that prints "hello world" to the screen.
  - Modify it to run as an MPI program … with each printing "hello world" and its rank

- Log in to the ESC cluster making sure to set things up for MPI as instructed.
- Build your MPI program

```
$ mpicc -fopenmp -O3 -o hi hello.c
```

- Run the program on the local node

```
$ mpirun -np 4 ./hi
```

- Run the program on hosts listed in the hostfile.

```
$ mpirun -hostfile hosts -np 4 ./hi
```

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
MPI_Finalize();
```

```
char name[MPI_MAX_PROCESSOR_NAME];
int namLen;

MPI_Get_processor_name(name,&namLen);
printf("%s  %d\n",name,namLen);
```

Running the program

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
   int rank, size;
   MPI_Init (&argc, &argv);
   MPI_Comm_rank (MPI_COMM_WORLD, &rank);
   MPI_Comm_size (MPI_COMM_WORLD, &size);
   printf( "Hello from process %d of %d\n",
                                rank, size );
   MPI_Finalize();
   return 0;
}
```

- run this program (hello) as:

mpirun –hostfile hosts –np 4 hello

Hello from process 1 of 4
Hello from process 2 of 4
Hello from process 0 of 4
Hello from process 3 of 4

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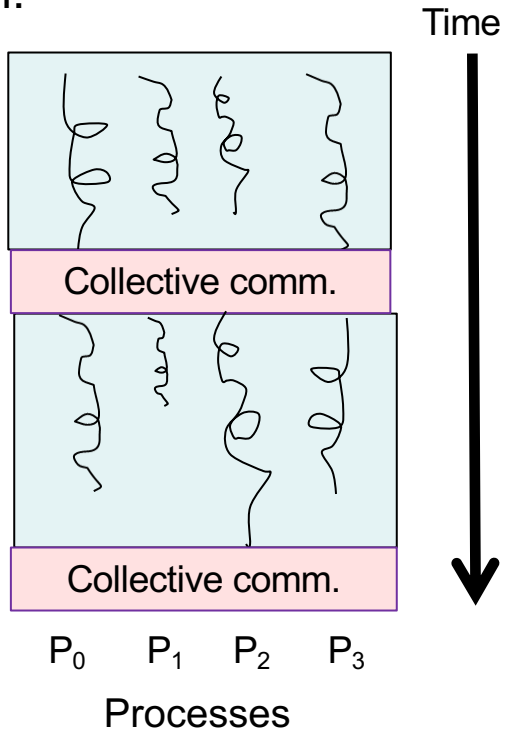
Bulk Synchronous Processing:
BSP, A typical pattern with MPI Programs

- Many MPI applications directly call few (if any) message passing routines. They use the following very common pattern:
  - Use the Single Program Multiple Data pattern
  - Each process maintains a local view of the global data
  - A problem broken down into phases each of which is composed of two subphases:
    - Compute on local view of data
    - Communicate to update global view on all processes (collective communication).
  - Continue phases until complete



This is a subset or the SPMD pattern sometimes referred to as the Bulk Synchronous pattern.

Collective Communication: Reduction

```
int MPI_Reduce (void* sendbuf,
     void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,
     int root, MPI_Comm comm)
```

Returns MPI_SUCCESS if there were no errors

- **`MPI_Reduce`** performs specified reduction operation (**op**) on the **count** values in **sendbuf** from all processes in communicator. Places result in **recvbuf** on the process with rank **root** only.

MPI Data Type*	C Data Type
MPI_CHAR	char
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long
MPI_LONG_DOUBLE	long double
MPI_SHORT	short

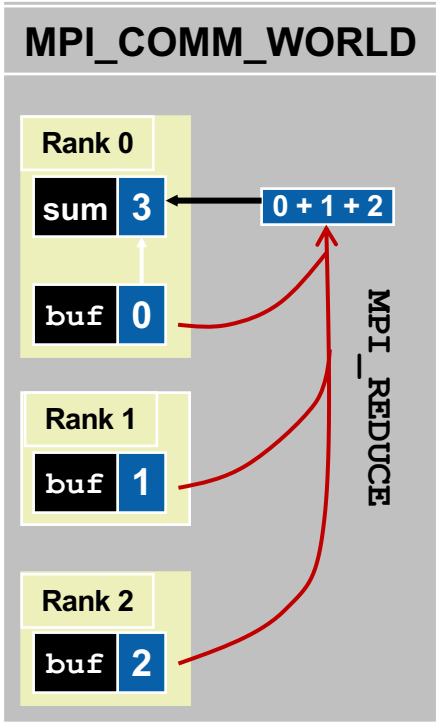
*This is a subset of available MPI types

Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
MPI_LAND	Logical AND

Operation	Function
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
User-defined	It is possible to define new reduction operations

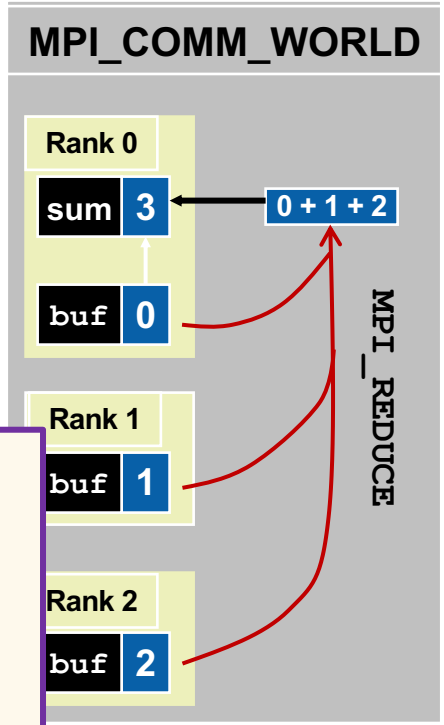
MPI_Reduce() Example

```
#include <mpi.h>

int main(int argc, char* argv[]) {
  int buf, sum, nprocs, myrank;

  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

  sum = 0;
  buf = myrank;

  MPI_Reduce(&buf, &sum, 1, MPI_INT,
          MPI_SUM, 0, MPI_COMM_WORLD);

  MPI_Finalize();
}
```



MPI_Reduce() Example

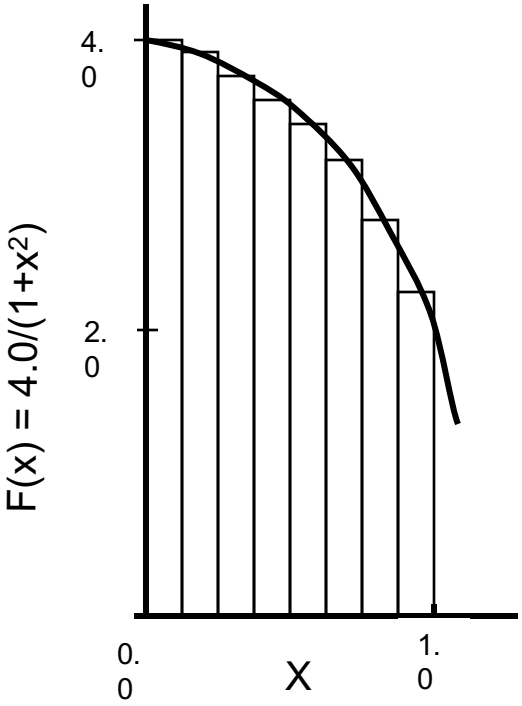
```
#include <mpi.h>

int main(int argc, char* argv[]) {
  int buf, sum, nprocs, myrank;

  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

  sum = 0;
```



C language comments:

- **`char*`** is a pointer to a collection of characters (a string).
- **`char* argv[]`** is the same as **`char **argv`**. They point to a collection of strings
- If you have a variable and you want its address, use the **`&`** character. C is a *call-by-value* language. If you want to pass updated values through a function argument, you need to pass in the address for that argument, for example **`&myrank`**

Example Problem: Numerical Integration



Mathematically, we know that:

$$\int_0^1 \frac{4.0}{(1+x^2)}\,dx = \pi$$

We can approximate the integral as a sum of rectangles:

$$\sum_{i=0}^{N} F(x_i)\Delta x \approx \pi$$

Where each rectangle has width Δx and height $F(x_i)$ at the middle of interval i.

PI Program: an example

```
static long num_steps = 100000;
double step;
void main ()
{       int i;       double x, pi, sum = 0.0;

        step = 1.0/(double) num_steps;
           x = 0.5 * step;
        for (i=0;i<= num_steps; i++){
              x+=step;
              sum += 4.0/(1.0+x*x);
        }
        pi = step * sum;
}
```

Exercise: Pi Program

- Goal
  - To write a simple Bulk Synchronous, SPMD program
- Program
  - Start with the provided “pi program” and using an MPI reduction, write a parallel version of the program.

```
int MPI_Reduce (void* sendbuf, void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,   int root, MPI_Comm comm)
```

MPI_Op	Function
MPI_SUM	Summation

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
MPI_Finalize();
```

MPI Data Type	C Data Type
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long

Pi program in MPI

```
#include <mpi.h>
void main (int argc, char *argv[])
{
        int i, my_id, numprocs;  double x, pi, step, sum = 0.0 ;
        step = 1.0/(double) num_steps ;
        MPI_Init(&argc, &argv) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &my_id) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        my_steps = num_steps/numprocs ;
        for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++)
        {
                x = (i+0.5)*step;
                sum += 4.0/(1.0+x*x);
        }
        sum *= step ;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
;
}
```

Sum values in “sum” from each process and place it in “pi” on process 0

Timing MPI programs

- MPI added a function (which OpenMP copied) to time programs.
- **MPI_Wtime()** returns a double for the time (in seconds) for some arbitrary time in the past.
- As with omp_get_wtime(), call before and after a section of code of interest to get an elapsed time.

Exercise: Pi Program with MPI_Wtime()

- Goal
  - Time your Bulk Synchronous, SPMD program
- Program
  - Start with your parallel “pi program” and use MPI_Wtime() to explore its scalability on your system.

```
int MPI_Reduce (void* sendbuf, void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,   int root, MPI_Comm comm)
```

MPI_Op	Function
MPI_SUM	Summation

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
Double MPI_Wtime();
MPI_Finalize();
```

MPI Data Type	C Data Type
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long

Pi program in MPI

```
#include <mpi.h>
void main (int argc, char *argv[])
{
        int i, my_id, numprocs;  double x, pi, step, sum = 0.0 ;
        step = 1.0/(double) num_steps ;
        MPI_Init(&argc, &argv) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &my_id) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        double init_time = MPI_Wtime();
        my_steps = num_steps/numprocs ;
        for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++)
        {
                x = (i+0.5)*step;
                sum += 4.0/(1.0+x*x);
        }
        sum *= step ;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        if(my_id == 0) printf(" runtime = %lf\n",MPI_Wtime()-init_time);
}
```

MPI Pi program performance (on my laptop)

```
#include <mpi.h>
void main (int argc, char *argv[])
{
        int i, my_id, numprocs;  double x, pi, step, sum = 0.0 ;
        step = 1.0/(double) num_steps ;
        MPI_Init(&argc, &argv) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &my_id) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        double init_time = MPI_Wtime();
        my_steps = num_steps/numprocs ;
        for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++)
        {
                x = (i+0.5)*step;
                sum += 4.0/(1.0+x*x);
        }
        sum *= step ;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        if(my_id == 0) printf(" runtime = %lf\n",MPI_Wtime()-init_time);
}
```

Thread or procs	OpenMP SPMD critical	OpenMP PI Loop	MPI
1	0.85	0.43	0.84
2	0.48	0.23	0.48
3	0.47	0.23	0.46
4	0.46	0.23	0.46

*Intel compiler (icpc) with –O3 on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

MPI Pi program performance (on my laptop)

```
#include <mpi.h>
void main (int argc, char *argv[])
{
        int i, my_id, numprocs;  double x, pi, step, sum = 0.0 ;
        step = 1.0/(double) num_steps ;
        MPI_Init(&argc, &argv) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &my_id) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        double init_time = MPI_Wtime();
        my_steps = num_steps/numprocs ;
        for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++)
        {
                x = (i+0.5)*step;
                sum += 4.0/(1.0+x*x);
        }
        sum *= step ;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        if(my_id == 0) printf(" runtime = %lf\n",MPI_Wtime()-init_time);
}
```

Thread or procs	OpenMP SPMD critical	OpenMP PI Loop	MPI
1	0.85	0.43	0.84
2	0.48	0.23	0.48
3	0.47	0.23	0.46
4	0.46	0.23	0.46

Is this a dependable way to get an elapsed time?

What if instead of a laptop, we are starting processes across a large cluster? Is this time reliable?

*Intel compiler (icpc) with –O3 on Apple OS X 10.7.3 with a dual core (four HW thread) Intel® Core™ i5 processor at 1.7 Ghz and 4 Gbyte DDR3 memory at 1.333 Ghz.

Synchronization in MPI

- Synchronization … establishing ordering constraints among concurrent processes so we can establish happens-before relations.

- As we will see later … the semantics of how messages are passed includes synchronization properties.

- For a stand-alone synchronization construct, we can use a barrier (all processes in the group associated with comm arrive before any proceed):

  - **int MPI_Barrier(MPI_Comm comm)**

Synchronization in MPI

- Synchronization … establishing ordering constraints among concurrent processes so we can establish happens-before relations.

- As we will see later … the semantics of how messages are passed includes synchronization properties.

- For a stand-alone synchronization construct, we can use a barrier (all processes in the group associated with comm arrive before any proceed):

  - int MPI_Barrier(MPI_Comm comm)

What is this int for? All MPI routines other than the timing routines return an int error code. Equals MPI_SUCCESS when everything is OK, other values specific to routines when errors occur

Collective Communication: Reduction

```
int MPI_Reduce (void* sendbuf,
     void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,
     int root, MPI_Comm comm)
```

Returns MPI_SUCCESS if there were no errors

- **`MPI_Reduce`** performs specified reduction operation (**op**) on the **count** values in **sendbuf** from all processes in communicator. Places result in **recvbuf** on the process with rank **root** only.

MPI Data Type*	C Data Type
MPI_CHAR	char
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long
MPI_LONG_DOUBLE	long double
MPI_SHORT	short

*This is a subset of available MPI types

Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
MPI_LAND	Logical AND

Operation	Function
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
User-defined	It is possible to define new reduction operations

Many operations beyond sum

Timing without a barrier

- Another option … forget the barrier. Collect times for all processes and report min, max and average. This is easy to do using the operations available for use in MPI_Reduce.

```
int MPI_Reduce (void* sendbuf,
     void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,
     int root, MPI_Comm comm)
```

Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
MPI_LAND	Logical AND

Exercise: Explore timing MPI programs with the Pi program

- Goal
  - Time your Bulk Synchronous, SPMD program
- Program
  - Use MPI_Wtime(), MPI_Barrier() and other methods explore timing for the pi program.

```
int MPI_Reduce (void* sendbuf, void* recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,   int root, MPI_Comm comm)
```

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
double MPI_Wtime();
int MPI_Barrier();
MPI_Finalize();
```

Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
MPI_LAND	Logical AND

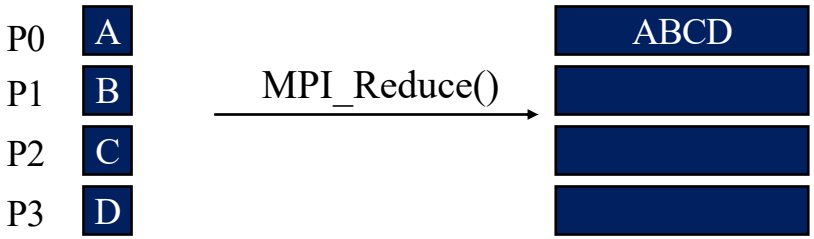
Pi program … return max time

```
#include <mpi.h>
void main (int argc, char *argv[])
{       int i, my_id, numprocs;  double x, pi, step, sum = 0.0, mxtime=0.0;
        step = 1.0/(double) num_steps ;
        MPI_Init(&argc, &argv) ;
        MPI_Comm_rank(MPI_COMM_WORLD, &my_id) ;
        MPI_Comm_size(MPI_COMM_WORLD, &numprocs) ;
        MPI_Barrier(MPI_COMM_WORLD);
        double init_time = MPI_Wtime();
        my_steps = num_steps/numprocs ;
        for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++) {
                x = (i+0.5)*step;
                sum += 4.0/(1.0+x*x);
        }
        sum *= step ;
        MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        double wtime = MPI_Wtime()-init_time
        MPI_Reduce(&wtime, &mxtime, 1, MPI_DOUBLE, MPI_MAX, 0, MPI_COMM_WORLD);
        if(my_id == 0) printf(“ maximum time = %lf”,mxtime);
}
```

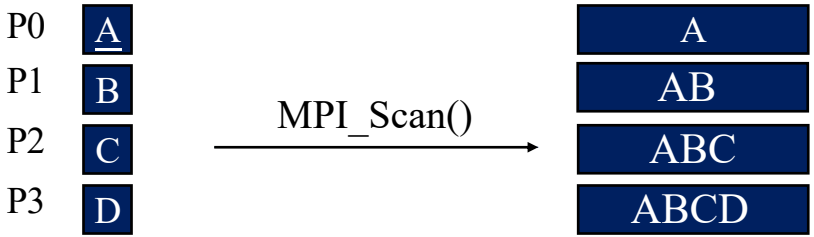
MPI defines a rich set of Collective operations

Collective Computations

Reduction: Take values on each P and combine them with an op (such as add) into a single value on one P.



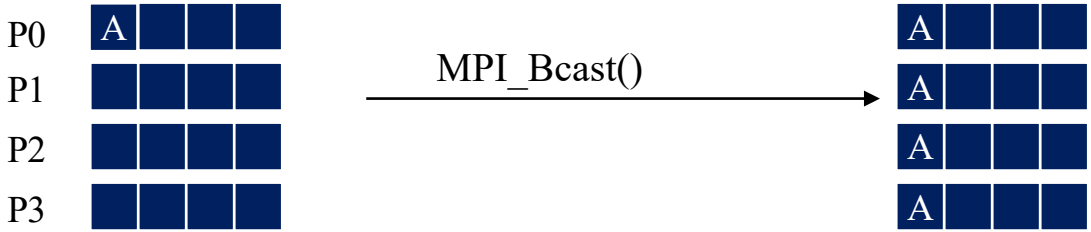
Scan: Take values on each P and combine them with a scan operation and spread the scan array out among all P.




```
int MPI_Reduce(const void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)
int MPI_Scan(const void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)
```

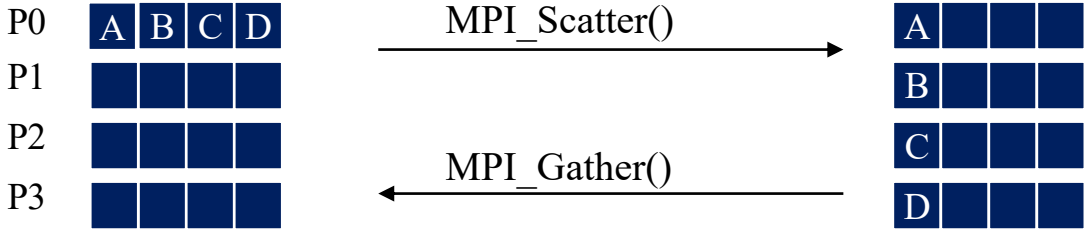
Collective Data Movement

Broadcast a value from P0 (the root) and give a copy to P1, P2 and P3



Scatter an array on P0 (the root) to P1, P2, and P3

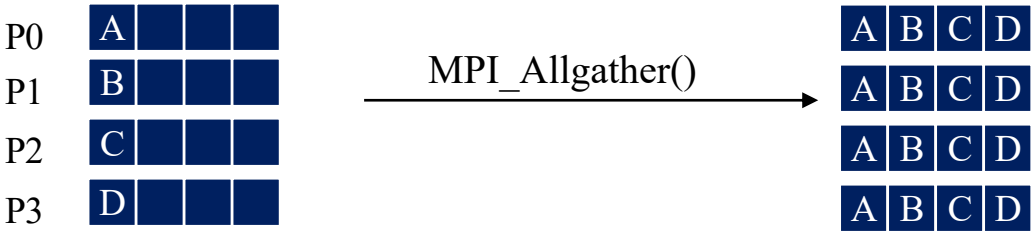
Gather values from P1, P2, and P3 into an array on P0 (the root)



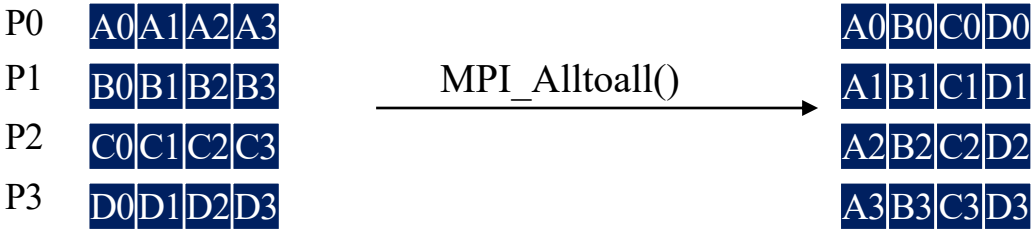

```
int MPI_Bcast( void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm )
int MPI_Gather(const void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
int MPI_Scatter(const void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
```

More Collective Data Movement

Gather a chunk from each P and put it into a single array. Each P gets a copy of the resulting array.



All to All: Take chunks of data on each P and spread them out among the corresponding arrays on each P




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

MPI Collectives: Summary

- Collective communications: called by all processes in the group to create a global result and share with all participating processes.
  - `Allgather, Allgatherv, Allreduce, Alltoall, Alltoallv, Bcast, Gather, Gatherv, Reduce, Reduce_scatter, Scan, Scatter, Scatterv`
- Notes:
  - `Allreduce, Reduce, Reduce_scatter`, and `Scan` use the same set of built-in or user-defined combiner functions.
  - Routines with the "`All`" prefix deliver results to all participating processes
  - Routines with the "`v`" suffix allow chunks to have different sizes
- Global synchronization is available in MPI through a barrier which blocks until all the processes in the process group associated with the communicator call it.
  - `MPI_Barrier( comm )`

Collective operations are powerful … use them when you can

Do not implement them from scratch on your own. Think about how you'd implement, for example, a reduction.

It is MUCH harder than you might think.

Outline

- MPI and distributed memory systems
- The Bulk Synchronous Pattern and MPI collective operations
- Introduction to message passing
- The diversity of message passing in MPI
- Geometric Decomposition and MPI
- Concluding Comments

Message passing: Basic ideas and jargon

- We need to coordinate the execution of processes … which may be spread out over a collection of independent computers
- Coordination:
  1. Process management (e.g., create and destroy)
  2. Synchronization … timing constraints for concurrent processes)
  3. Communication ... Passing a buffer from one machine to another

- A message passing interface builds coordination around messages (either explicitly or implicitly).

- The fundamental (and overly simple) timing model for a message:

$$\text{Time}_{\text{communication}} = \text{latency} + N_{\text{bytes}}/\text{bandwidth}$$

Network fixed costs plus overheads

Network asymptotic bytes per second

Sending and receiving messages

- Pass a buffer which holds “count” values of MPI_TYPE
- The data in a message to send or receive is described by a triple:
  - **(address, count, datatype)**

- The receiving process identifies messages with the double :
  - **(source, tag)**
- Where:
  - Source is the rank of the sending process
  - Tag: a user-defined int to keep track of different messages from a single source

Rank of Destination node

MPI_Send (buff, 100, MPI_DOUBLE, Dest, tag, MPI_COMM_WORLD);

Address of **Local Buffer**

Count

Datatype

tag

Communicator

MPI_Recv (buff, 100, MPI_DOUBLE, Src, tag, MPI_COMM_WORLD, &status);

Rank of Source node

Sending and Receiving messages: More Details

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

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

MPI_Status is a variable that contains information about the message that is received. We can use it to find out information about the received message. The most common usage is to find out how many items were in the message:

```
MPI_Status MyStat;      int count;      float buff[4];
int ierr = MPI_Recv(buf, 4, MPI_FLOAT, 2, 0, MPI_COMM_WORLD, &MyStat);   // receive message from node=2 with message tag = 0
If(ierr == MPI_SUCCESS) MPI_Get_Count(MyStat, MPI_FLOAT, &count);
```

For messages of a known size, we typically ignore the status, in which case use the parameter MPI_STATUS_IGNORE

```
int ierr = MPI_Recv(&buf, 4, MPI_FLOAT, 2, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Sending and Receiving messages: More Details

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

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

C language comments:

- **void*** says the argument can take a pointer to any type. The C compiler won't do any type checking … it just needs a valid address to a block of memory.
- A type with a * means the function expects a pointer to that type. So I would declare a variable as **MPI_Status MyStat** and then put the variable in the function call with an ampersand (**&**) … for example **&MyStat**

MPI_Status is a variable that contains information about the message that is received.
about the received message. The most common usage is to find out how many items v

```
MPI_Status MyStat;      int count;      float buff[4];
int ierr = MPI_Recv(buf, 4, MPI_FLOAT, 2, 0, MPI_COMM_WORLD, &MyStat);   // receive message from node=2 with message tag = 0
If(ierr == MPI_SUCCESS) MPI_Get_Count(MyStat, MPI_FLOAT, &count);
```

For messages of a known size, we typically ignore the status, in which case use the parameter MPI_STATUS_IGNORE

```
int ierr = MPI_Recv(&buf, 4, MPI_FLOAT, 2, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

MPI Data Types for C

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

MPI defines predefined data types that must be specified when passing messages.

Exercise: Ping-Pong Program

- Goal
  - Measure the latency of our communication network.
- Program
  - Create a program to bounce a message (**a single value**) between a pair of processes. Bounce the message back and forth multiple times and report the average one-way communication time. Figure out how to use this so called "ping-pong" program to measure the latency of communication on your system.

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

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

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
double MPI_Wtime();
MPI_Finalize();
```

MPI Data Type	C Data Type
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long

Solution: Ping-Pong Program

```
#include <mpi.h>
#include <stdio.h>
#include <stdlib.h>
#define VAL 42
#define NREPS  10
#define TAG 5

int main(int argc, char **argv)  {
   int rank, size;
   double t0;
   MPI_Init(&argc, &argv);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   MPI_Comm_size(MPI_COMM_WORLD, &size);

   int bsend = VAL;
   int brecv = 0;
   MPI_Status stat;
   MPI_Barrier(MPI_COMM_WORLD);
   if(rank == 0) t0 = MPI_Wtime();
   for(int i=0;i<NREPS; i++){
      if(rank == 0){
         MPI_Send(&bsend, 1, MPI_INT, 1, TAG, MPI_COMM_WORLD);
         MPI_Recv(&brecv, 1, MPI_INT, 1, TAG, MPI_COMM_WORLD, &stat);
         if(brecv != VAL)printf("error: interation %d %d != %d\n",i,brecv,VAL);
         brecv = 0;
      }
      else if(rank == 1){
         MPI_Recv(&brecv, 1, MPI_INT, 0, TAG, MPI_COMM_WORLD, &stat);
         MPI_Send(&bsend, 1, MPI_INT, 0, TAG, MPI_COMM_WORLD);
         if(brecv != VAL)printf("error: interation %d %d != %d\n",i,brecv,VAL);
         brecv = 0;
      }
   }
   if(rank == 0){
      double t = MPI_Wtime() - t0;
      double lat = t/(2*NREPS);
      printf(" lat = %f seconds\n",(float)lat);
   }
   MPI_Finalize();
}
```

Ping Pong for different message sizes … but first a bit of C

- Input parameters from the command line (so you don't need to recompile for each case):

For atoi() you need `#include <stdlib.h>`

```
int main(int argc, char **argv)
{
    if (argc == 3){
        int msg_size = atoi(*++argv);
        int num_pings = atoi(*++argv);
    }
    else{
        int msg_size = 1;
        int num_pings = 10;
    }
```

Argc → number of command line arguments
**argv →Pointer to a set of strings

Argc == 3 → the executable Plus two args

*++argv → increment to point to next string

atoi() →converts a string to an int

Define a default case for when skipped command line are omitted

- Allocate memory and initialize buffer (i.e., a dynamic array of doubles)

```
double *msg = (double*)malloc(msg_size*sizeof(double));
for(int i; i<msg_size; i++) msg[i] = (double) i;
free(msg);
```

Malloc allocates memory as a void*. Cast to the desired type

Msg is a pointer but we treat it like an array

Command Line Arguments

- If I run my program like this:

```
./a.out 1000 10
```

- Then my program ping/pongs a message of size 1000 ten times.

Exercise: Ping-Pong Program with command line args

- Goal
  - Measure the latency of our communication network for different sized messages.
- Program
  - Vary message sizes and number of pings/pongs from the command line.

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

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

```
#include <mpi.h>
int size, rank, argc;   char **argv;
MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);
double MPI_Wtime();
MPI_Finalize();
```

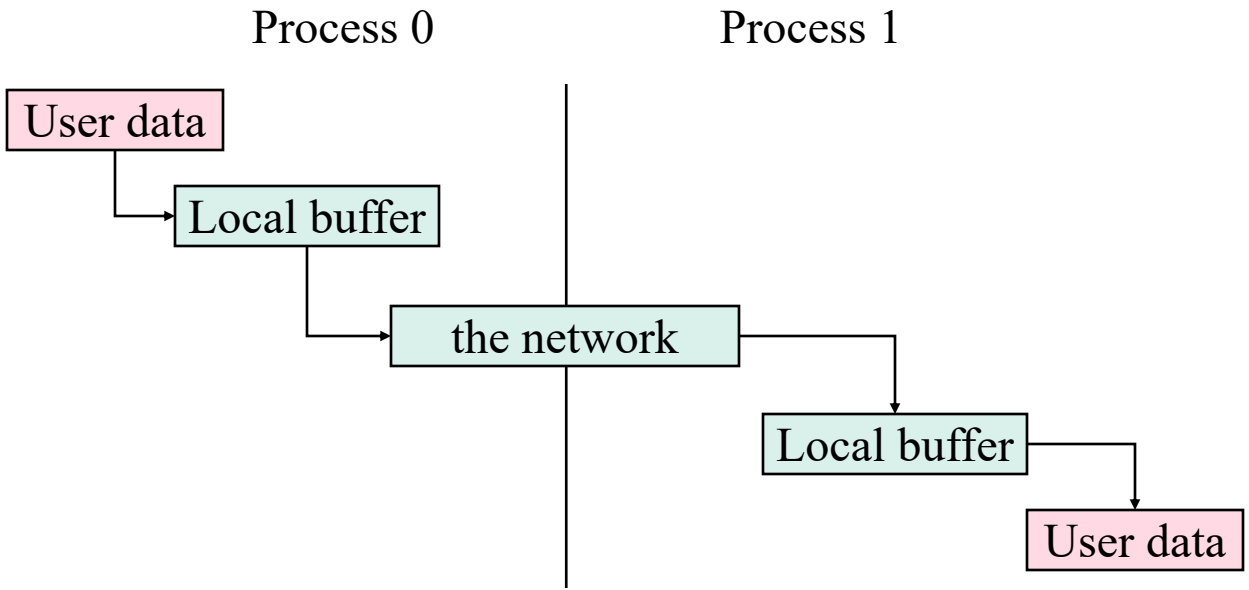
```
int main(int argc, char **argv) {
   if (argc == 3){
     int msg_size = atoi(*++argv);
     int num_pings = atoi(*++argv);
   }
   double *msg = (double*)malloc(msg_size*sizeof(double));
   for(int i; i<msg_size; i++) msg[i] = (double) i;
   free(msg);
```

Outline

- MPI and distributed memory systems
- The Bulk Synchronous Pattern and MPI collective operations
- Introduction to message passing
- The diversity of message passing in MPI
- Geometric Decomposition and MPI
- Concluding Comments

Buffers

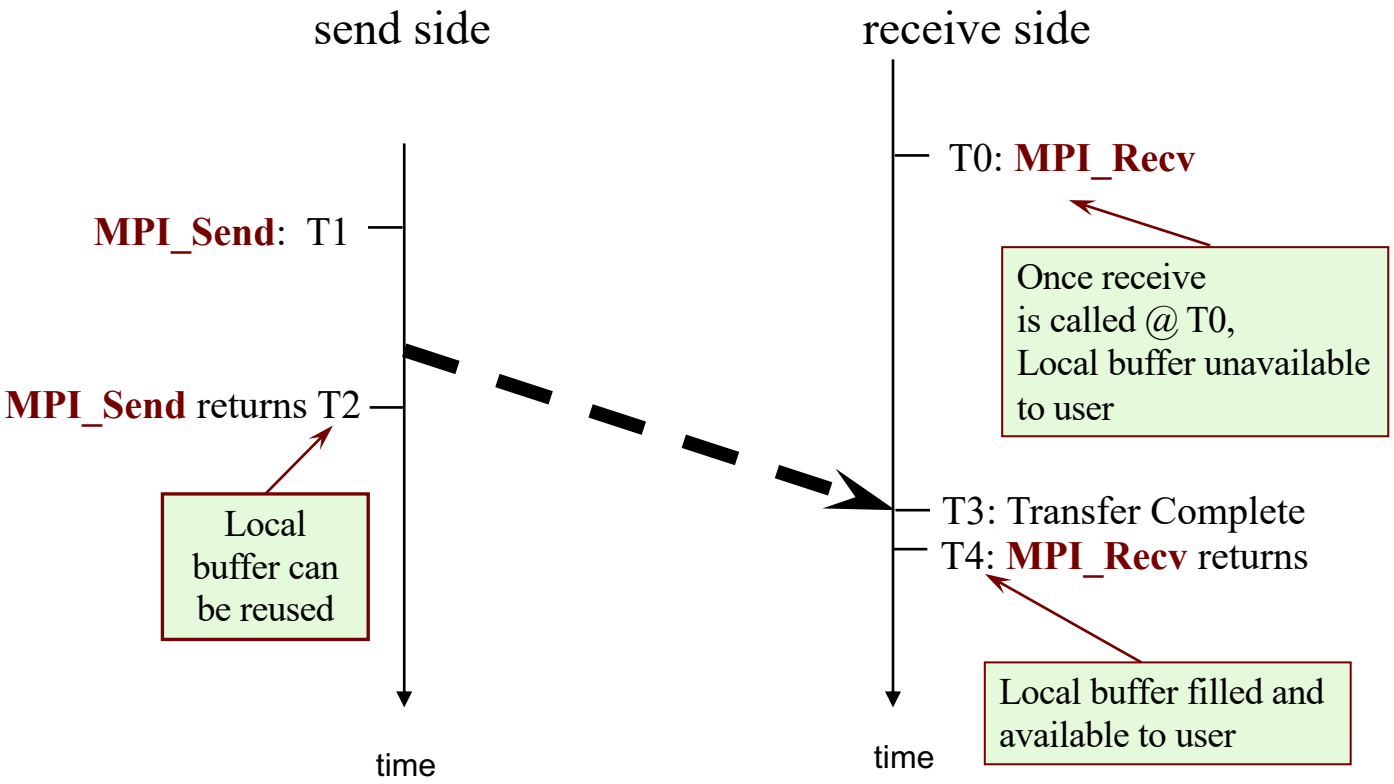
- Message passing is straightforward, but there are subtleties
  - Buffering and deadlock
  - Deterministic execution
  - Performance
- When you send data, where does it go? The following is the typical flow:



Derived from slides provided by Bill Gropp of UIUC

Blocking Send-Receive Timing Diagram

(Receive before Send)



It is important to post the receive before sending, for highest performance.

Exercise: Ring program

- Start with the basic ring program we provide.
- Study the code (ring.c and ring_naive.c) and note how I manage the computation of where the message goes to and where it comes from for each node.
- Run it for a range of message sizes and notes what happens for large messages.

```
double *buff;     int buff_count, to, from, tag=3;   MPI_Status stat;

MPI_Recv (buff, buff_count, MPI_DOUBLE, from, tag, MPI_COMM_WORLD, &stat);
MPI_Send (buff, buff_count, MPI_DOUBLE, to,     tag,  MPI_COMM_WORLD);
```

Sources of Deadlocks

- Send a large message from process 0 to process 1
  - If there is insufficient storage at the destination NIC (Network Interface Unit), the send must wait for the user to provide the memory space (through a receive) to drain buffers inside the NIC
- What happens with this code?

Process 0	Process 1
`Send(to 1)`	`Send(to 0)`
`Recv(from 1)`	`Recv(from 0)`

- This code could deadlock … it depends on the availability of system buffers in which to store the data sent until it can be received

Slide source: based on slides from Bill Gropp, UIUC

Some Solutions to the “deadlock” Problem

- Order the operations more carefully:

Process 0	Process 1
`Send(1)`	**`Recv(0)`**
`Recv(1)`	**`Send(0)`**

- Use a collective “swap” so buffers created when the communication operation is posted:

Process 0	Process 1
`Sendrecv(1)`	**`Sendrecv(0)`**

Slide source: based on slides from Bill Gropp, UIUC

More Solutions to the “unsafe” Problem

- Supply a sufficiently large buffer in the send function

Process 0	Process 1
`Bsend(1)`	`Bsend(0)`
`Recv(1)`	`Recv(0)`

- Use non-blocking operations:

Process 0	Process 1
`Isend(1)`	`Isend(0)`
`Irecv(1)`	`Irecv(0)`
`Waitall`	`Waitall`

Slide source: Bill Gropp, UIUC

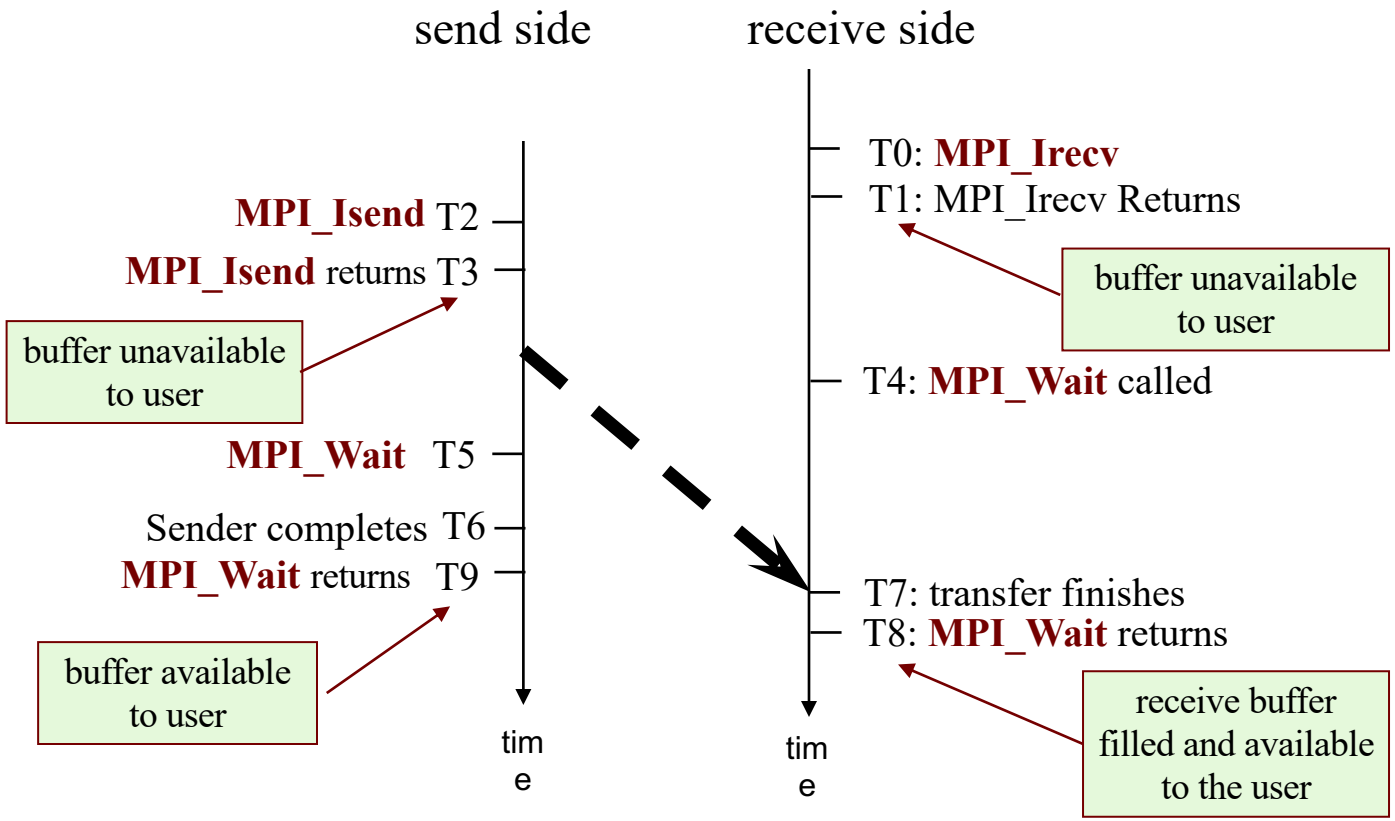
Non-Blocking Communication

- Non-blocking operations return immediately and pass "request handles" that can be waited on and queried
  - **MPI_Isend(start, count, datatype, dest, tag, comm, request)**
  - **MPI_Irecv(start, count, datatype, src, tag, comm, request)**
  - **MPI_Wait(request, status)**
- One can also test without waiting using MPI_TEST
  - **MPI_Test(request, flag, status)**
- Anywhere you use MPI_Send or MPI_Recv, you can use the pair of MPI_Isend/MPI_Wait or MPI_Irecv/MPI_Wait
- Note the MPI types:

```
MPI_Status status;      // type used with the status output from recv
MPI_Request request;    // the type of the handle used with isend/ircv
```

Non-blocking operations are extremely important … they allow you to overlap computation and communication.

Non-Blocking Send-Receive Diagram



Exercise: Ring program

- Start with the basic ring program we provide. Run it for a range of message sizes and notes what happens for large messages.
  - It may deadlock if the network stalls due to there being no place to put a message (i.e. no receives in place so the send blocking on when its buffer can be reused hangs).
- Try to make it more stable for large messages by:
  - Split-phase … have the nodes “send than receive” while the other half “receive then send”.
  - Sendrecv … a collective communication send/receive.
  - Isend/Irecv … nonblocking send receive

```
double *buff;     int buff_count, to, from, tag=3;   MPI_Status stat; MPI_Request request;

MPI_Recv (buff, buff_count, MPI_DOUBLE, from, tag, MPI_COMM_WORLD, &stat);
MPI_Send (buff, buff_count, MPI_DOUBLE, to,     tag,  MPI_COMM_WORLD);
MPI_Isend( Buff, count, datatype, dest, tag, comm, &request )
MPI_Irecv( Buff, count, datatype, src, tag, comm, &request )
MPI_Wait( &request, &status )
MPI_Sendrecv (snd_buff,  buff_count, MPI_DOUBLE, to, tag,
              rcv_buf,     buff_count, MPI_DOUBLE, to, tag, MPI_COMM_WORLD, &stat);
```

Example: shift messages around a ring (part 1 of 2)

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

int main(int argc, char **argv)
{
  int num, rank, size, tag, next, from;
  MPI_Status status1, status2;
  MPI_Request req1, req2;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank( MPI_COMM_WORLD, &rank);
  MPI_Comm_size( MPI_COMM_WORLD, &size);
  tag = 201;
  next = (rank+1) % size;
  from = (rank + size - 1) % size;
  if (rank == 0) {
    printf("Enter the number of times around the ring: ");
    scanf("%d", &num);

    printf("Process %d sending %d to %d\n", rank, num, next);
    MPI_Isend(&num, 1, MPI_INT, next, tag,
                                MPI_COMM_WORLD,&req1);
    MPI_Wait(&req1, &status1);
  }
  do {
    MPI_Irecv(&num, 1, MPI_INT, from, tag,
                                MPI_COMM_WORLD, &req2);
    MPI_Wait(&req2, &status2);

    if (rank == 0) {
      num--;
      printf("Process 0 decremented number\n");
    }

    printf("Process %d sending %d to %d\n", rank, num, next);
    MPI_Isend(&num, 1, MPI_INT, next, tag,
                                MPI_COMM_WORLD, &req1);
    MPI_Wait(&req1, &status1);
  } while (num != 0);

  if (rank == 0) {
    MPI_Irecv(&num, 1, MPI_INT, from, tag,
                                MPI_COMM_WORLD, &req2);
    MPI_Wait(&req2, &status2);
  }
  MPI_Finalize();
  return 0;
}
```

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Example: finite difference methods

- Solve the heat diffusion equation in 1 D:
  - u(x,t) describes the temperature field
  - We set the heat diffusion constant to one
  - Boundary conditions, constant u at endpoints.

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}$$

- map onto a mesh with stepsize h and k

$$x_i = x_0 + ih \qquad t_i = t_0 + ik$$

- Central difference approximation for spatial derivative (at fixed time)

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$$

- Time derivative at $t = t^{n+1}$

$$\frac{du}{dt} = \frac{u^{n+1} - u^n}{k}$$

Example: Explicit finite differences

- Combining time derivative expression using spatial derivative at t = t^n

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

  - Solve for u at time n+1 and step j

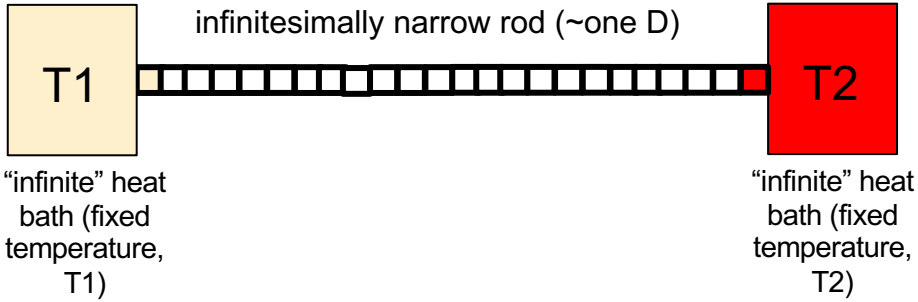
$$u_j^{n+1} = (1-2r)u_j^n + ru_{j-1}^n + ru_{j+1}^n \qquad r = k/h^2$$

  - The solution at t = t_{n+1} is determined explicitly from the solution at t = t_n (assume u[t][0] = u[t][N] = Constant for all t).

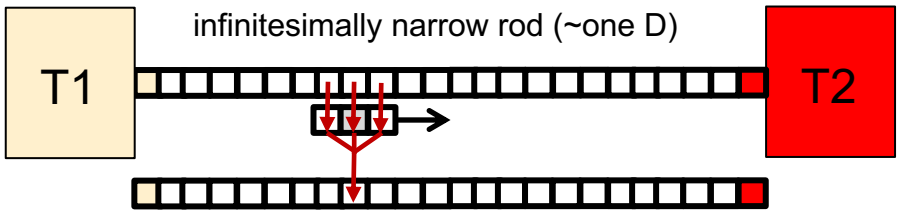
```
for (int t = 0; t < N_STEPS-1; ++t)
   for (int x = 1; x < N-1; ++x)
         u[t+1][x] = u[t][x] + r*(u[t][x+1] - 2*u[t][x] + u[t][x-1]);
```

  - Explicit methods are easy to compute … each point updated based on nearest neighbors. Converges for r<1/2.

Heat Diffusion equation

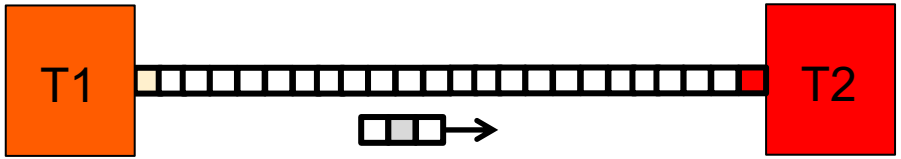


Heat Diffusion equation



Pictorially, you are sliding a three point “stencil” across the domain (u[t]) and computing a new value of the center point (u[t+1]) at each stop.

Heat Diffusion equation

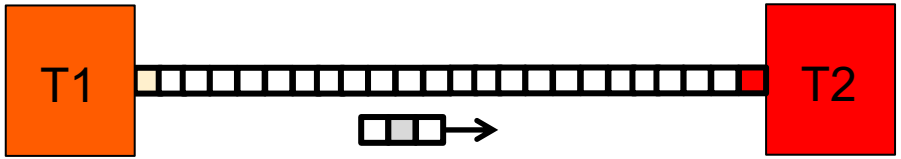



```
int main()
{
   double *u   = malloc (sizeof(double) * (N));
   double *up1 = malloc (sizeof(double) * (N));

   initialize_data(uk, ukp1, N, P); // initialize, set end temperatures
   for (int t = 0; t < N_STEPS; ++t){
      for (int x = 1; x < N-1; ++x)
          up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);

      temp = up1; up1 = u; u = temp;
    }
return 0;
```

Note: I don't need the intermediate "u[t]" values hence "u" is just indexed by x.

A well known trick with 2 arrays so I don't overwrite values from step k-1 as I fill in for step k

Heat Diffusion equation




```
int main()
{
   double *u   = malloc (sizeof(double) * (N));
   double *up1 = malloc (sizeof(double) * (N));

   initialize_data(uk, ukp1, N, P); // initialize, set end temperatures
   for (int t = 0; t < N_STEPS; ++t){
      for (int x = 1; x < N-1; ++x)
          up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);

      temp = up1; up1 = u; u = temp;
    }
return 0;
```

How would you parallelize this program?

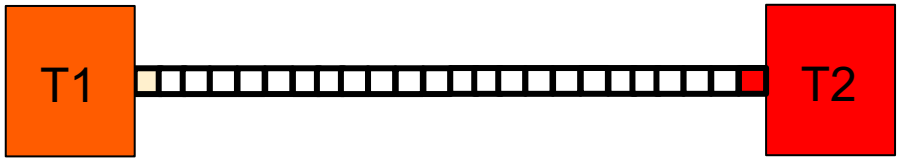
Exercise: Parallel heat diffusion

- Goal
  - Parallelize the heat diffusion code (MPI_Exercises/heat-eqn-seq.c) with OpenMP … should be a quick and easy way to familiarize yourself with the code.
  - As you do this, think about how you might parallelize this with MPI

```
#pragma omp parallel
#pragma omp for
#pragma omp critical
#pragma omp single
#pragma omp barrier
int omp_get_num_threads();
int omp_get_thread_num();
```

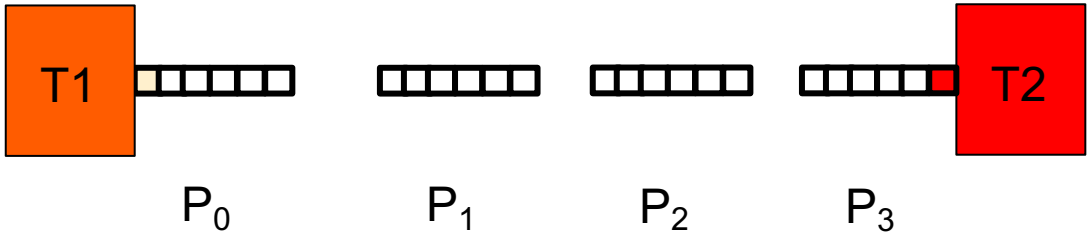
Heat Diffusion equation

- Start with our original picture of the problem … a one dimensional domain with end points set at a fixed temperature.



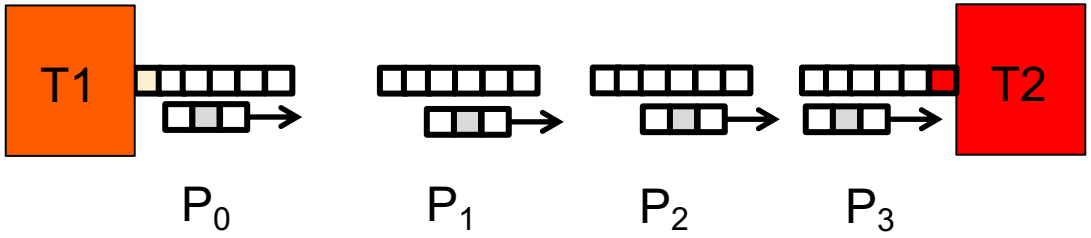
Heat Diffusion equation

- Break it into chunks assigning one chunk to each process.



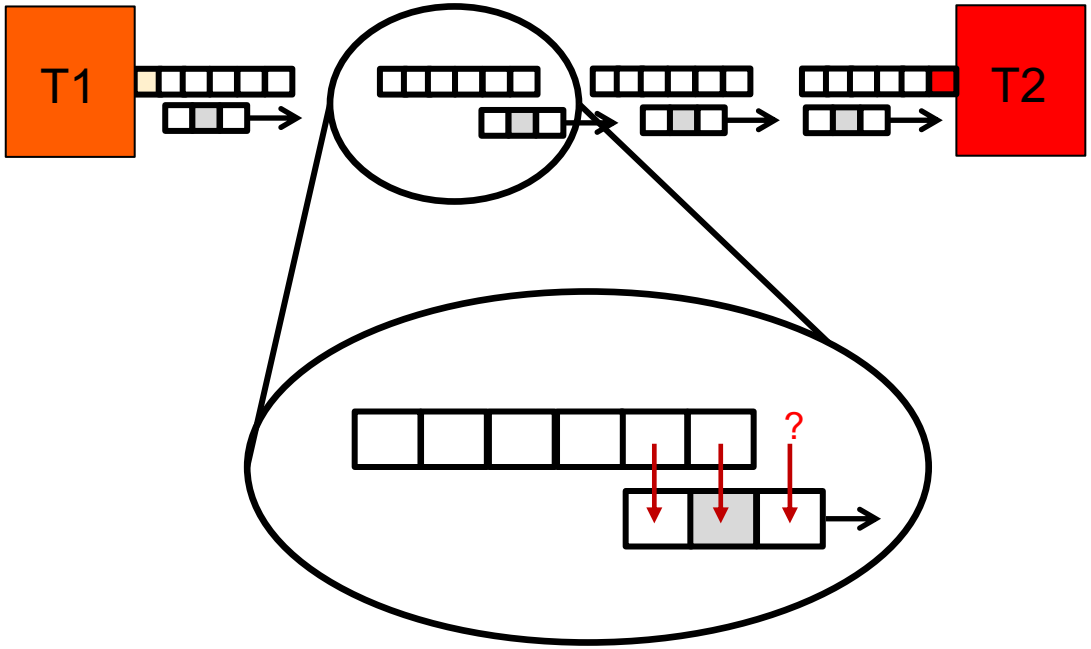
Heat Diffusion equation

- Each process works on it's own chunk … sliding the stencil across the domain to updates its own data.



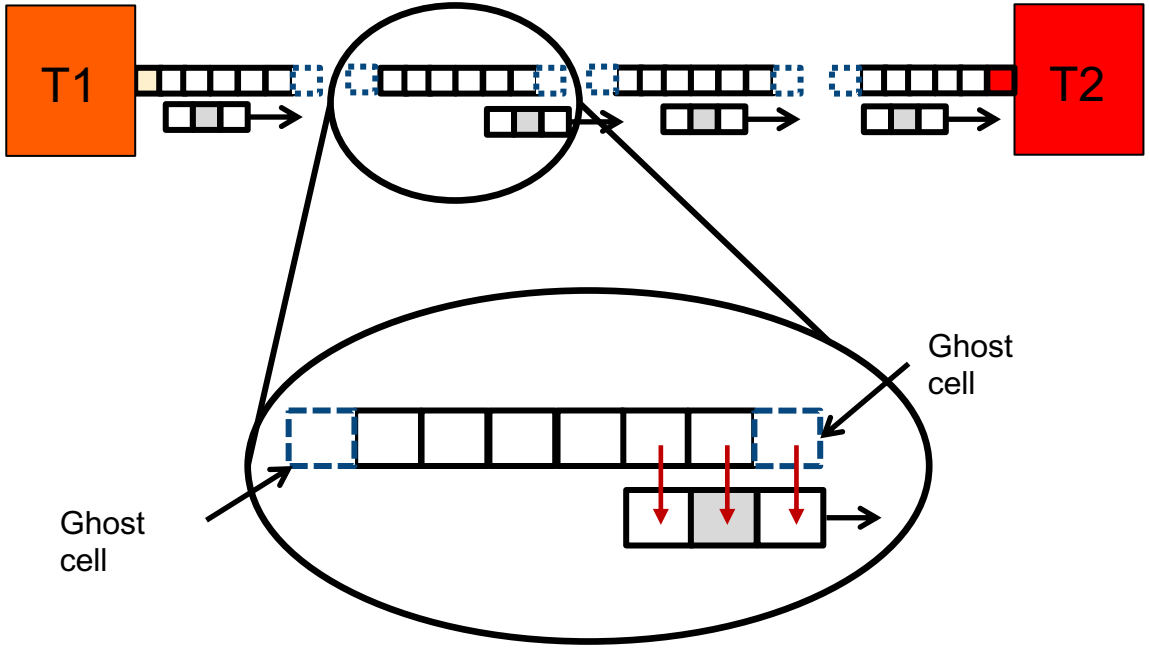
Heat Diffusion equation

- What about the ends of each chunk … where the stencil will run off the end and hence have missing values for the computation?



Heat Diffusion equation

- We add ghost cells to the ends of each chunk, update them with the required values from neighbor chunks at each time step … hence giving the stencil everything it needs on any given chunk to update all of its values.



Heat Diffusion equation

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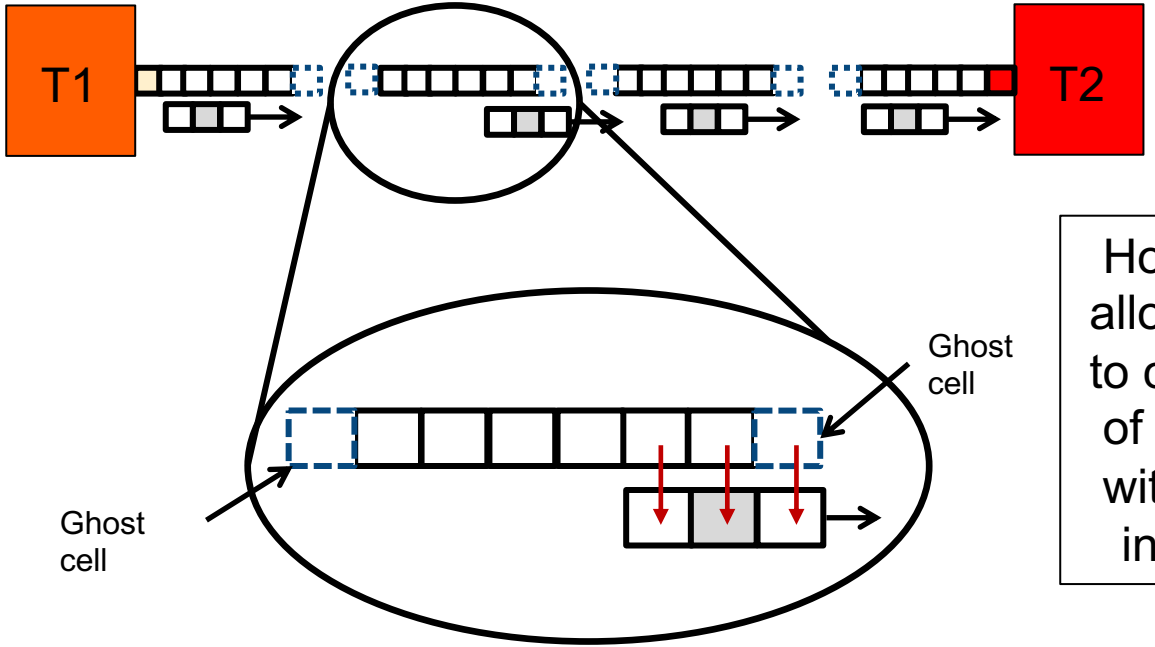
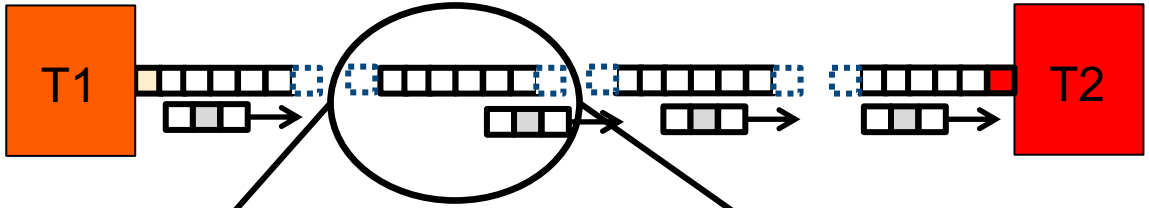


How would you allocate memory to create chunks of the right size with ghost cells in your code?

Heat Diffusion equation

- We add ghost cells to the ends of each chunk, update them with the required values from neighbor chunks at each time step … hence giving the stencil everything it needs on any given chunk to update all of its values.

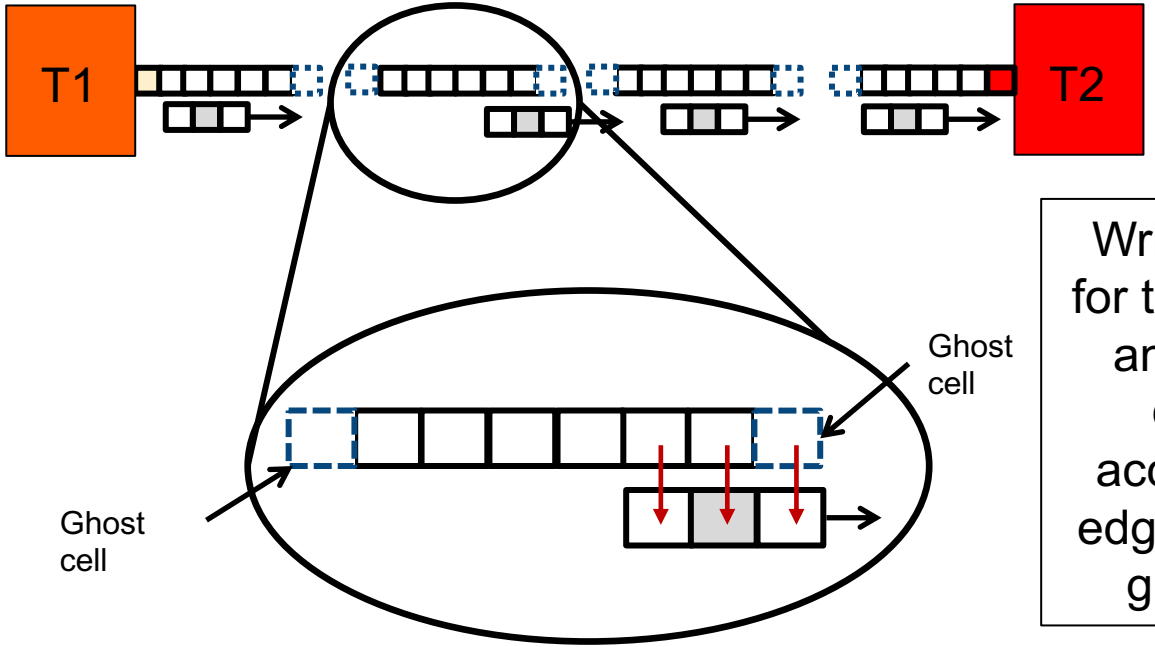


Let's be lazy and assume P is a divisor of N (i.e.; N%P = 0)

```
MPI_Comm_size (MPI_COMM_WORLD, &P);
double *u   = malloc (sizeof(double) * (2 + N/P))
double *up1 = malloc (sizeof(double) * (2 + N/P));
```

Heat Diffusion equation

- We add ghost cells to the ends of each chunk, update them with the required values from neighbor chunks at each time step … hence giving the stencil everything it needs on any given chunk to update all of its values.



Write the code for the update of an individual chunk … accounting for edges using the ghost cells.

Heat Diffusion MPI Example: Updating a chunk

```
// Compute interior of each "chunk"
  for (int x = 2; x < N/P; ++x)
    up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);

// update edges of each chunk keeping the two far ends fixed
// (first element on Process 0 and the last element on process P-1).
  if (myID != 0)
    up1[1] = u[1] + (k / (h*h)) * (u[1+1] - 2*u[1] + u[1-1]);

  if (myID != P-1)
    up1[N/P] = u[N/P] + (k/(h*h)) * (u[N/P+1] - 2*u[N/P] + u[N/P-1]);

// Swap pointers to prepare for next iterations
  temp = up1; up1 = u; u = temp;

} // End of for (int t ...) loop

MPI_Finalize();
return 0;
```

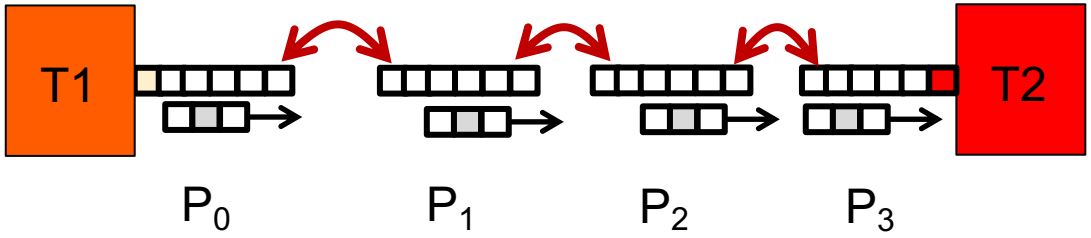
Update array values using local data and values from ghost cells.

u[0] and u[N/P+1] are the ghost cells

Note I was lazy and assumed N was evenly divided by P. Clearly, I'd never do this in a "real" program.

Heat Diffusion MPI Example: Communication

- Each process works on it's own chunk … sliding the stencil across the domain to updates its own data.



Try to write the code for this communication pattern.

Heat Diffusion MPI Example

Note: the edges of domain are held at a fixed temperature.
- Node 0 has no neighbor to the left
- Node P has no neighbor to its right

```
MPI_Init (&argc, &argv);
MPI_Comm_size (MPI_COMM_WORLD, &P);
MPI_Comm_rank (MPI_COMM_WORLD, &myID);
double *u   = malloc (sizeof(double) * (2 + N/P))  // include "Ghost Cells” to hold
double *up1 = malloc (sizeof(double) * (2 + N/P)); // values from my neighbors

initialize_data(uk, ukp1, N, P);
for (int t = 0; t < N_STEPS; ++t){
```

Send my “left” boundary value to the neighbor on my “left’

```
  if (myID != 0) MPI_Send (&u[1], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD);
```

Receive my “right” ghost cell from the neighbor to my “right’

```
  if (myID != P-1) MPI_Recv (&u[N/P+1], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD, &status);
```

Send my “right” boundary value to the neighbor to my “right’

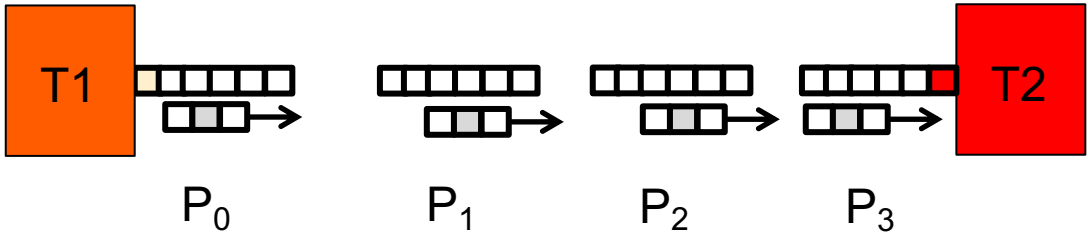
```
  if (myID != P-1) MPI_Send (&u[N/P], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD);
```

Receive my “left” ghost cell from the neighbor to my “left”

```
  if (myID != 0) MPI_Recv (&u[0], 1, MPI_DOUBLE, myID-1, 0,MPI_COMM_WORLD, &status);
```

Heat Diffusion equation

- Each process works on it's own chunk … sliding the stencil across the domain to updates its own data.



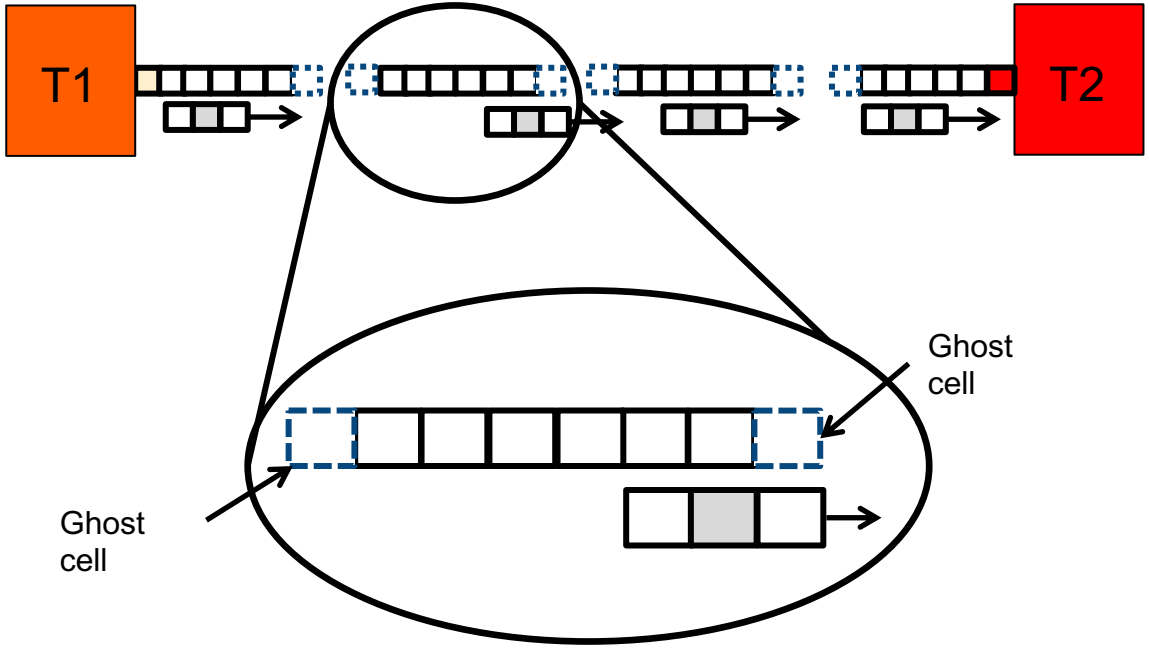
We now put all the pieces together for the full program

Heat Diffusion MPI Example

```
MPI_Init (&argc, &argv);
MPI_Comm_size (MPI_COMM_WORLD, &P);
MPI_Comm_rank (MPI_COMM_WORLD, &myID);
double *u   = malloc (sizeof(double) * (2 + N/P))  // include "Ghost Cells” to hold
double *up1 = malloc (sizeof(double) * (2 + N/P)); // values from my neighbors

initialize_data(uk, ukp1, N, P);
for (int t = 0; t < N_STEPS; ++t){
  if (myID != 0)  MPI_Send (&u[1], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD);
  if (myID != P-1) MPI_Recv (&u[N/P+1], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD, &status);
  if (myID != P-1) MPI_Send (&u[N/P], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD);
  if (myID != 0)   MPI_Recv (&u[0], 1, MPI_DOUBLE, myID-1, 0,MPI_COMM_WORLD, &status);

  for (int x = 2; x < N/P; ++x)
    up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
  if (myID != 0)
    up1[1] = u[1] + (k / (h*h)) * (u[1+1] - 2*u[1] + u[1-1]);
  if (myID != P-1)
    up1[N/P] = u[N/P] + (k/(h*h)) * (u[N/P+1] - 2*u[N/P] + u[N/P-1]);
  temp = up1; up1 = u; u = temp;

} // End of for (int t ...) loop

MPI_Finalize();
return 0;
```

The Geometric Decomposition Pattern

- This is an instance of a very important design pattern … the Geometric decomposition pattern.



Partitioned Arrays

- Realistic problems are 2D or 3D; require more complex data distributions.
- We need to parallelize the computation by partitioning this index space
- Example: Consider a 2D domain over which we wish to solve a PDE using an explicit finite difference solver . The figure shows a five point stencil … update a value based on its value and its 4 neighbors.
- Start with an array and stencil →

$a_{0,0}$	$a_{0,1}$	$a_{0,2}$	$a_{0,3}$	$a_{0,4}$	$a_{0,5}$	$a_{0,6}$	$a_{0,7}$
$a_{1,0}$	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$	$a_{1,4}$	$a_{1,5}$	$a_{1,6}$	$a_{1,7}$
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$a_{3,0}$	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$	$a_{3,4}$	$a_{3,5}$	$a_{3,6}$	$a_{3,7}$
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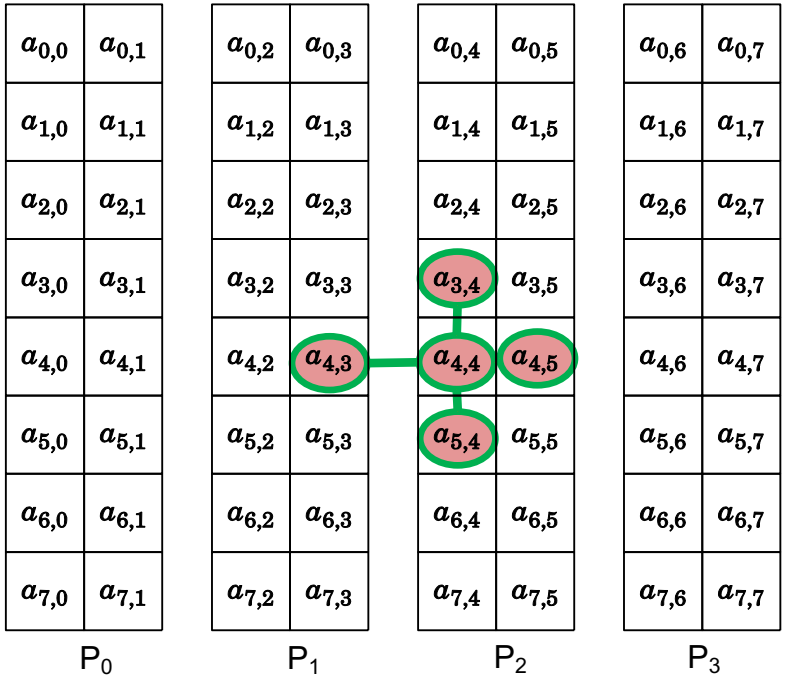
$a_{5,0}$	$a_{5,1}$	$a_{5,2}$	$a_{5,3}$	$a_{5,4}$	$a_{5,5}$	$a_{5,6}$	$a_{5,7}$
$a_{6,0}$	$a_{6,1}$	$a_{6,2}$	$a_{6,3}$	$a_{6,4}$	$a_{6,5}$	$a_{6,6}$	$a_{6,7}$
$a_{7,0}$	$a_{7,1}$	$a_{7,2}$	$a_{7,3}$	$a_{7,4}$	$a_{7,5}$	$a_{7,6}$	$a_{7,7}$

Partitioned Arrays: Column block distribution

- Split the non-unit-stride dimension (P-1) times to produce P chunks, assign the ith chunk to P_i. …. To keep things simple, assume N%P = 0
- In a 2D finite-differencing program (exchange edges), how much do we have to communicate? **O(N) values** per processor

P is the # of processors

N is the order of our square matrix



Partitioned Arrays: Block distribution

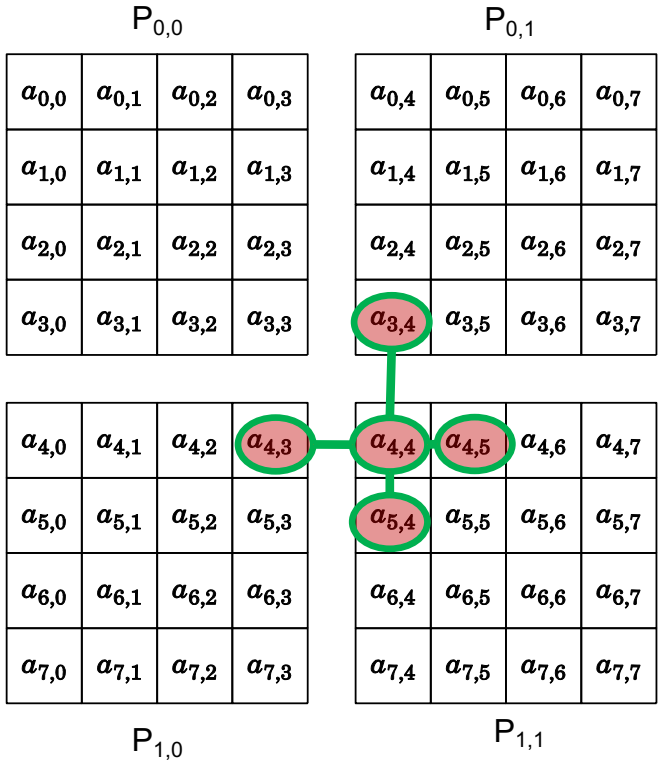
- If we parallelize in both dimensions, then we have $(N/P^{1/2})^2$ elements per processor, and we need to send **$O(N/P^{1/2})$ values** from each processor. Asymptotically better than O(N).

P is the # of processors

Assume a p by p square mesh … $p=P^{1/2}$

N is the order of our square matrix

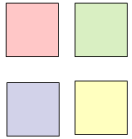
Dimension of each block is $N/P^{1/2}$



Partitioned Arrays: block cyclic distribution

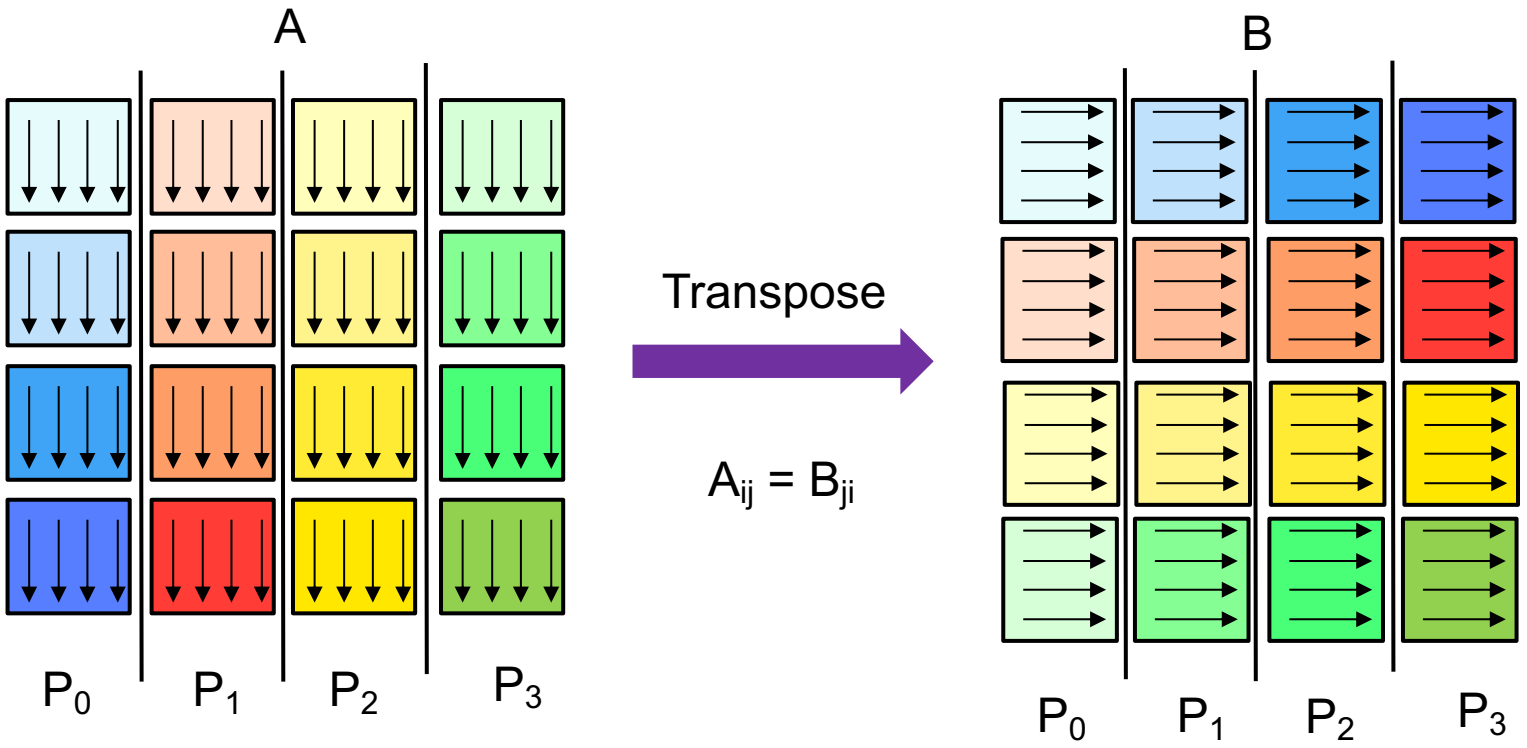
- LU decomposition (A= LU) .. Move down the diagonal transform rows to “zero the column” below the diagonal.

  - Zeros fill in the right lower triangle of the matrix … less work to do.
  - Balance load with cyclic distribution of blocks of A mapped onto a grid of nodes (2x2 in this case … colors show the mapping to nodes).



Matrix Transpose: Column block decomposition

You can only learn this stuff by doing it so we're going to design an algorithm to transpose a matrix using a partitioned array model based on column blocks.



Let's keep things simple. The order of A and B is N. N = blk*P where blk is the order of the square subblocks

Matrix Transposition

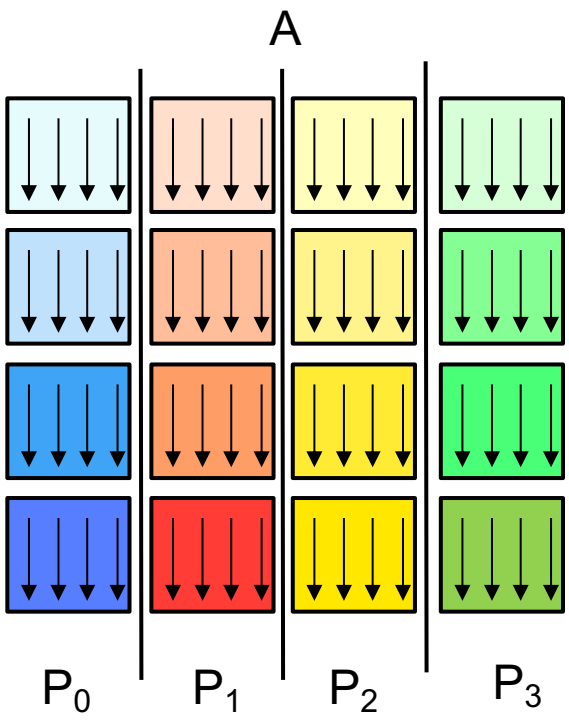
We are going to create a transpose program that uses the SPMD pattern.

That's Single Program Multiple Data.

We'll run the same program on each node.

What is the high level structure of this algorithm?

That is … how will each Processor march through its set of blocks?



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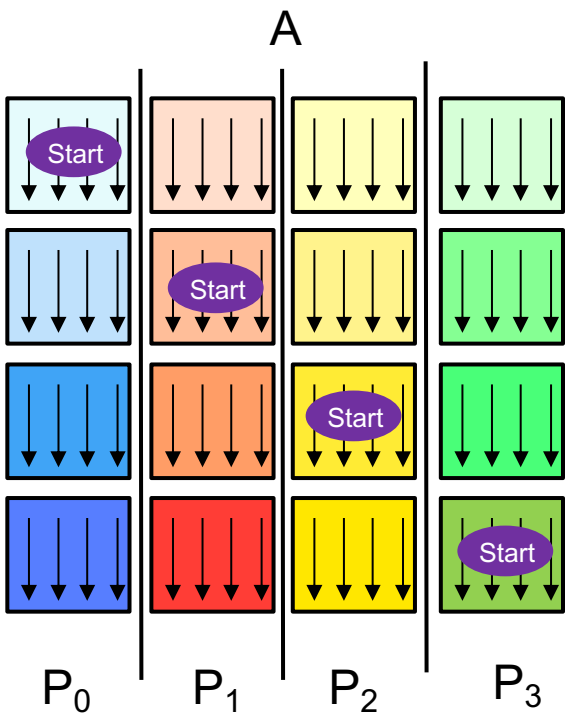

There is no one way to do this.

Since its an SPMD program, you want a symmetric path through the blocks on each processor.

A great approach is for everyone to start from their diagonal and shift down until they hit the bottom of their column.

Phase 0 … transpose your diagonal

Let's keep things simple. N = blk*P where blk is the order of the square subblocks

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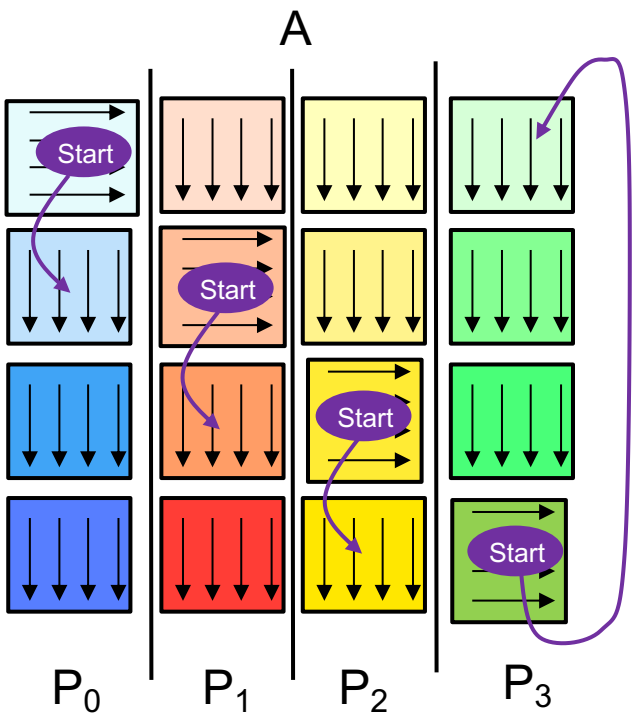

Shift down (with a circular shift pattern … i.e. when you run off an edge, wrap around to the opposite edge.

Phase 0 … transpose your diagonal
Phase 1 … deal with next block "down"

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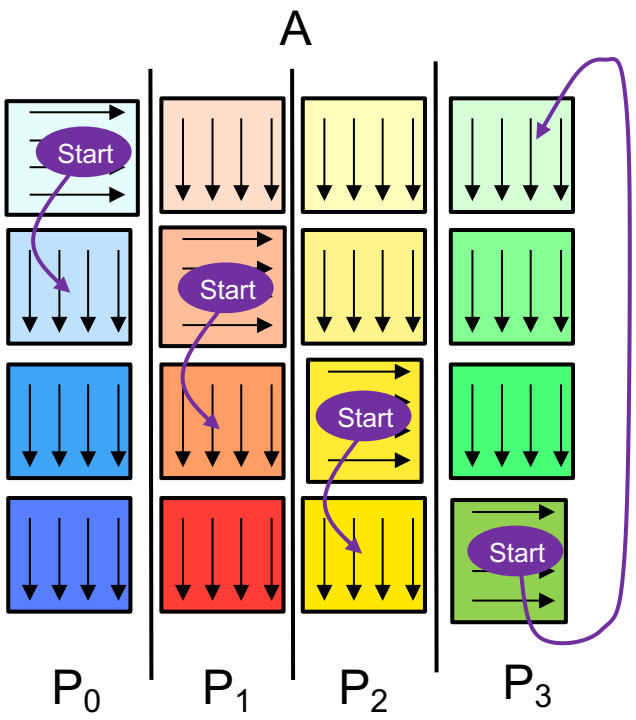

Shift down (with a circular shift pattern … i.e. when you run off an edge, wrap around to the opposite edge.

Phase 0 … transpose your diagonal
Phase 1 … deal with next block "down"

We know the sender … who receives the block?

Let's keep things simple. N = blk*P where blk is the order of the square subblocks

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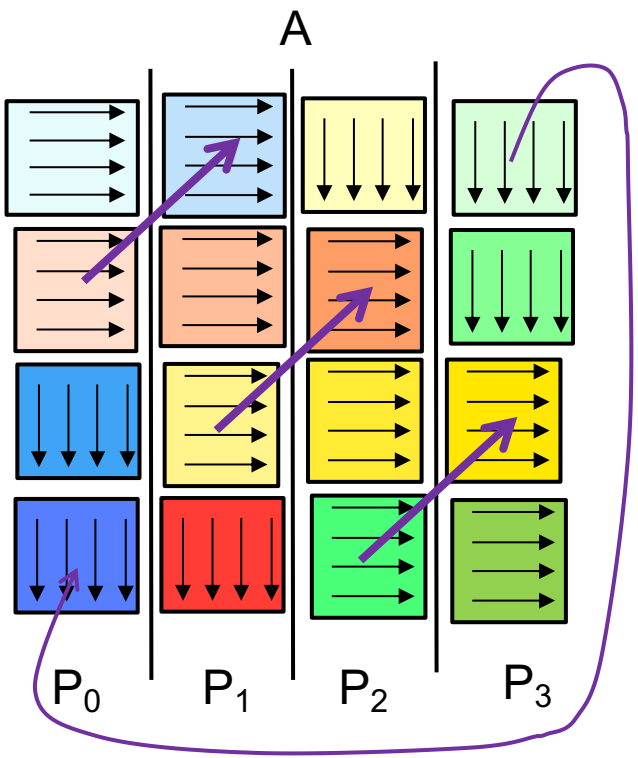

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Phase 0 … transpose your diagonal
Phase 1 … deal with next block "down"

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Exercise: Matrix Transpose Program

- Start with the basic transpose program we provide (transpose.c and several trans_*.c functions).
- Your task … deduce a general expression for the sender and receiver (FROM and TO) for each phase.
- Go to trans_sendrcv.c and enter your definitions for the TO and FROM macros (what is there now is wrong … I just wanted something to show how macros work).
- Test and verify correctness
- Try different message passing approaches.
- Can you overlap the local transpose and the communication between nodes?

```
double *buff;     int buff_count, to, from, tag=3;   MPI_Status stat, MPI_Request request;

MPI_Recv (buff, buff_count, MPI_DOUBLE, from, tag, MPI_COMM_WORLD, &stat);
MPI_Send (buff, buff_count, MPI_DOUBLE, to,     tag,  MPI_COMM_WORLD);
MPI_Isend( Buff, count, datatype, dest, tag, comm, &request )
MPI_Irecv( Buff, count, datatype, src, tag, comm, &request )
MPI_Wait( &request, &status )
MPI_Sendrecv (snd_buff,  buff_count, MPI_DOUBLE, to, tag,
              rcv_buf,     buff_count, MPI_DOUBLE, to, tag, MPI_COMM_WORLD, &stat);
```

Outline

- MPI and distributed memory systems
- The Bulk Synchronous Pattern and MPI collective operations
- Introduction to message passing
- The diversity of message passing in MPI
- Geometric Decomposition and MPI
- Concluding Comments

The 12 core functions in MPI

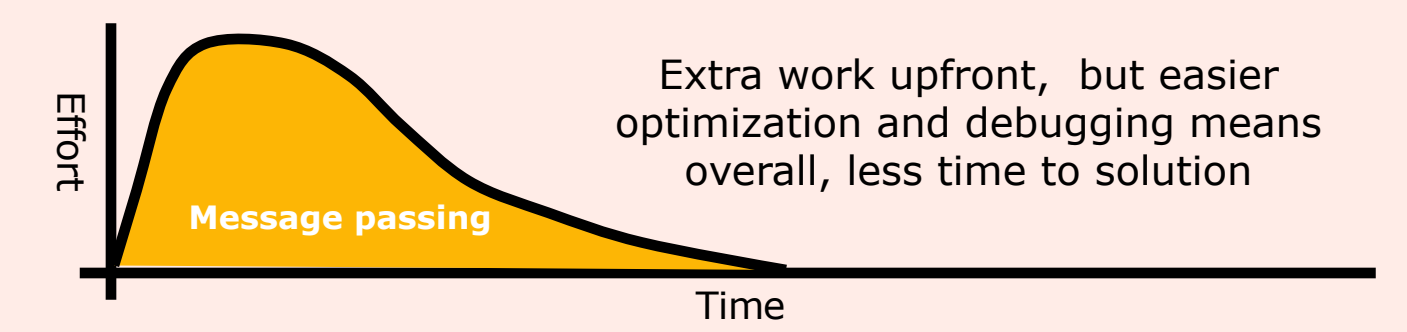
- MPI_Init
- MPI_Finish
- MPI_Comm_size
- MPI_Comm_rank
- MPI_Send
- MPI_Recv
- MPI_Reduce
- MPI_Isend
- MPI_Irecv
- MPI_Wait
- MPI_Wtime
- MPI_Bcast

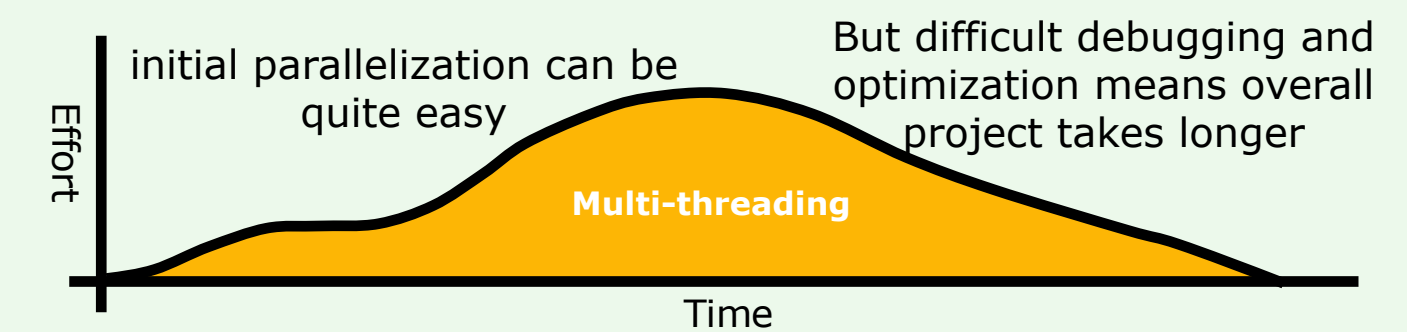
The ~~12~~ 10 core functions in MPI

- MPI_Init
- MPI_Finish
- MPI_Comm_size
- MPI_Comm_rank
- ~~MPI_Send~~
- ~~MPI_Recv~~
- MPI_Reduce
- MPI_Isend
- MPI_Irecv
- MPI_Wait
- MPI_Wtime
- MPI_Bcast

Real Programmers always try to overlap communication and computation .. Post your receives using MPI_Irecv() then where appropriate, MPI_Isend().

Does a shared address space make programming easier?



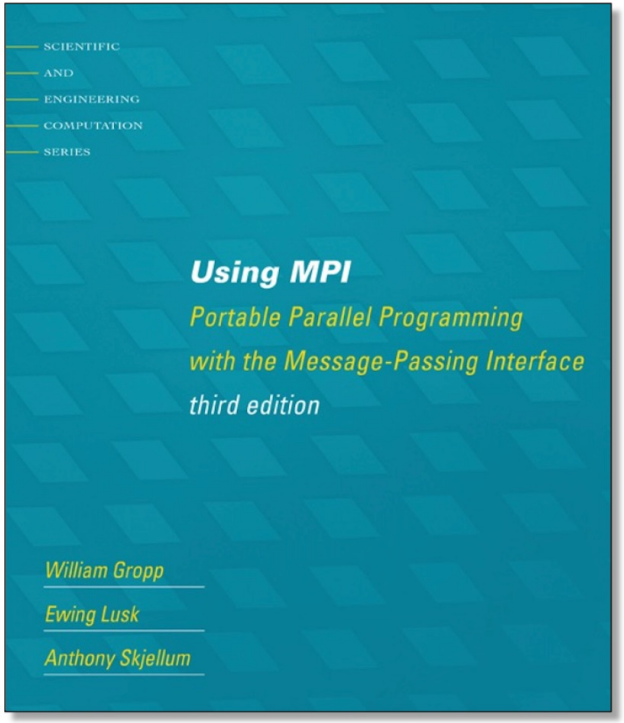


Proving that a shared address space program using semaphores is race free is an NP-complete problem*

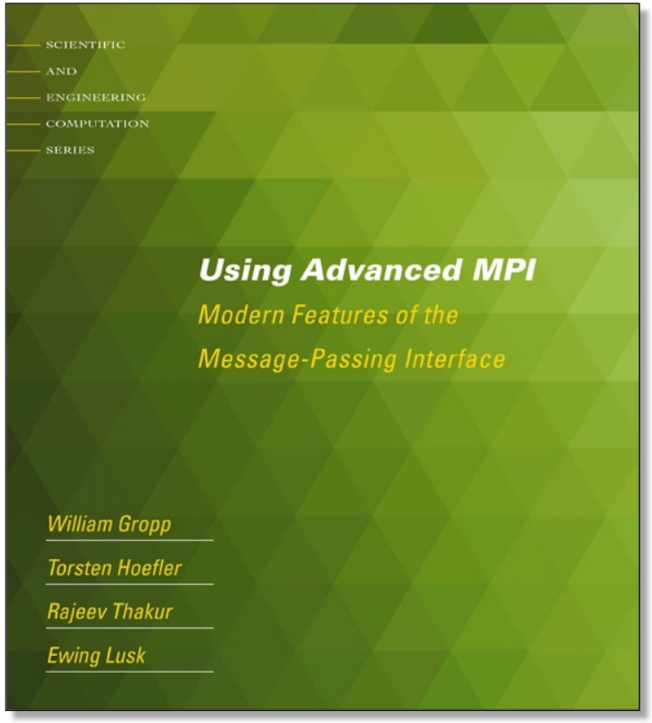
*P. N. Klein, H. Lu, and R. H. B. Netzer, Detecting Race Conditions in Parallel Programs that Use Semaphores, Algorithmica, vol. 35 pp. 321–345,

MPI References

- The Standard itself at http://www.mpi-forum.org
- Additional tutorial information at http://www.mcs.anl.gov/mpi
- The core reference books:



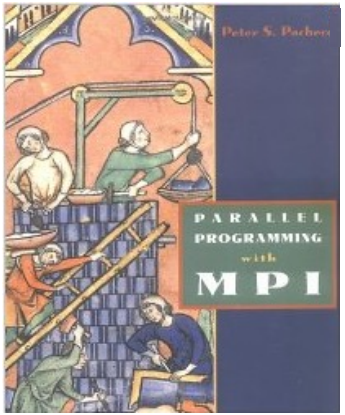
Basic MPI



Advanced MPI, including MPI-3

Additional books to help you master MPI

- *Parallel Programming with MPI*, by Peter Pacheco, Morgan-Kaufmann, 1997.
  - Only covers MPI 1.0 so it's out of date, but it is a very friendly and gentle introduction.
  - Peter Pacheco is a teacher first and foremost and that shows in the way he organizes the material in this book.



- *Patterns for Parallel Programing*, by Tim Mattson, Beverly Sanders, and Berna Massingill.
  - Only covers MPI 1.0 so it's out of date.
  - Focusses on how to use MPI, not the structure of the standard itself.
  - Shows how patterns are expressed across MPI, OpenMP, and concurrent Java