The Parallel Programming world beyond OpenMP

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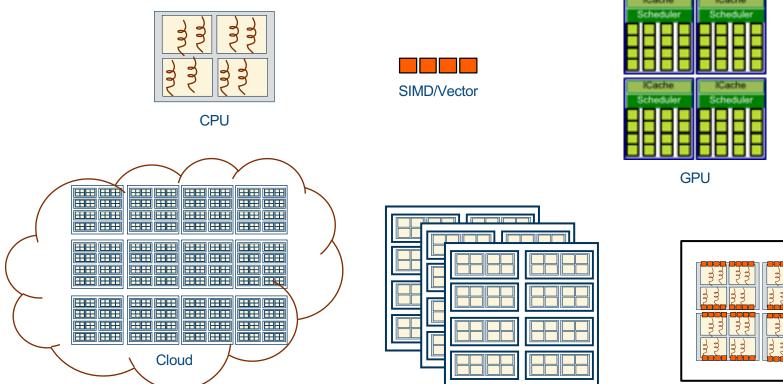
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- The views expressed in this talk are those of the speaker and not his employer.
- If I say something "smart" or worthwhile:
 - Credit goes to the many smart people I work with.
- If I say something stupid...
 - It's my own fault

I work in Intel's research labs. I don't build products. Instead, I get to poke into dark corners and think silly thoughts... just to make sure we don't miss any great ideas.

Hence, my views are by design far "off the roadmap".

Hardware is diverse ... and its only getting worse!!!



Cluster



Heterogeneous node

The Big Three

- 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.

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

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.

The Big Three

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

- 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.

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• 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.



A "Hands-on" Introduction to MPI

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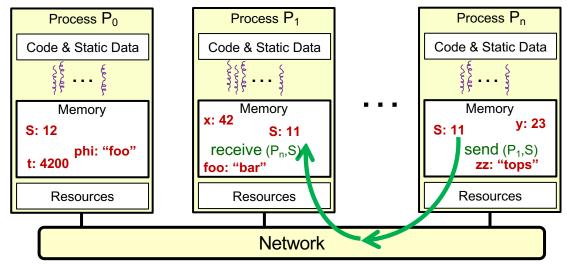


Outline

- 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

Execution Model: Distributed memory, CSP*

- Program consists of a collection of named processes.
 - Number of processes almost always fixed at program startup time
 - Local address space per node -- NO physically shared memory.
- Processes communicate by explicit send/receive pairs
 - Coordination is implicit in every communication event.
 - 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

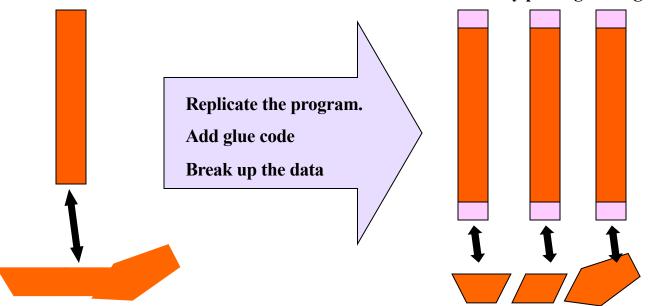
MPI_Alltoallv

MPI_Send

How do people use MPI? The SPMD Design Pattern

A sequential program working on a data set

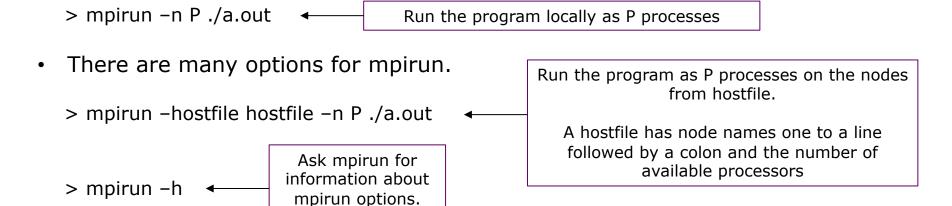
- •A single program working on a decomposed data set.
- •Use Node ID and numb of nodes to split up work between processes
- Coordination by passing messages.



Running MPI programs

The programs **mpirun** or **mpiexec** are largely equivalent and are used to launch a job on the processes across a cluster. On our cluster, we'll use **mpirun**

- MPI implementations include a way to start "P processes" on the system.
- For MPIch (the most common MPI implementation), this is done with the mpirun command:



Exercise: Hello world part 1

- Goal
 - To confirm that you can run a program in parallel.
- Program
 - Write a program that prints "hello world" to the screen.
 - Use mpirun to launch multiple copies of the program.
 - Run them on your shared memory node
 - mpirun -n 4 ./a.out
 - Run them across the nodes of a cluster (hint: you'll need a hostfile)
 - To run 3 processes on one node and 4 on another, my hostfile would be (assuming my two nodes are named node0 and node1):

node0:3 node1:4

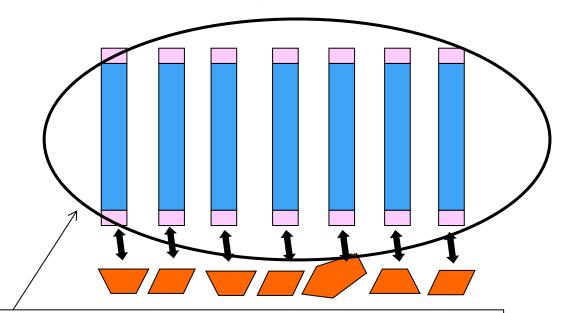
To run the executable hello on 2 processes on my local machine type: > mpiexec -n 4 ./a.out

To run the executable hello on 4 processes on my two node cluster:

> mpiexec -hostfile hostfile -n 4 ./a.out

An MPI program at runtime

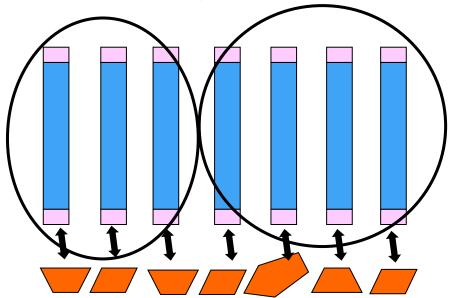
• Typically, when you run an MPI program, multiple processes all running the same program are launched ... working on their own block of data.



The collection of processes involved in a computation is called "a process group"

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 **<u>process group</u>** into multiple subgroups to manage how processes are mapped onto different tasks

MPI Hello World

```
#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

```
other MPI functions.

    agrc and argv are the command line args passed

#include <stdio.h>
                                         from main()
#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
```

int MPI Init (int* argc, char* argv[])

Initializes the MPI library ... called before any

every MPI program with a call to MPI Finalize

How many processes are involved?

```
int MPI Comm size (MPI Comm comm, int* size)
#include <stdio.h>
                             returns the number of processes in the process group
#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;
```

How many processes are involved?

```
#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_Comm_size (MPI_Comm comm, int* size)

returns the number of processes in the process group

What is MPI_COMM_WORLD?

It's a communicator (of type MPI Comm)

MPI_COMM_WORLD defines a name space for the communication events inside MPI. This includes the process group and any other meta-data about the set of cooperating processes.

How many processes are involved?

```
int MPI Comm size (MPI Comm comm, int* size)
#include <stdio.h>
                              returns the number of processes in the process group
#include <mpi.h>
                                                       Other than init() and finalize(),
int main (int argc, char **argv){
                                                       every MPI function has a
   int rank, size;
                                                       communicator.
   MPI_Init (&argc, &argv);
   MPI Comm rank (MPI COMM WORLD) &rank);
                                                       You can build your own
   MPI Comm size (MPI COMM WORLD, &size);
                                                       communicators to support
                                                       libraries or segregate
   printf( "Hello from process %d of %d\n",
                                                       operations into different
                                 rank, size );
                                                       process groups.
   MPI Finalize();
   return 0;
                                                       But most of us just use the one
                                                       global communicator,
                                                       MPI COMM WORLD
```

Which process "am I" (the rank)

```
int MPI Comm rank (MPI Comm comm, int* rank)
                         ■ MPI Comm rank An integer ranging from 0 to "(num of procs)-1"
#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, I'd run this program (hello) as:> mpiexec -n 4 hello
- What would this program would 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;
```

Exercise: Hello world part 2

- Goal
 - To confirm that you can run an MPI program on our cluster
- Program

Get the name of the

node you're running on

- 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
- Compile with mpicc ... a wrapper around the C compiler that understands most C compiler options
 % mpicc hello.c –o hello

```
#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 MPI_Get_processor_name( char *name, int *resultLen )
```

To run the executable hello on 4 processes on my local node: > mpirun –n 4 hello

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;
```

On a 4 node cluster, I'd run this program (hello) as:
 > mpirun -n 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

Outline

MPI and distributed memory systems

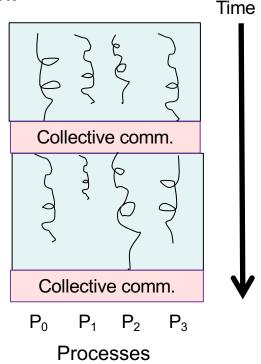


- The Bulk Synchronous Pattern and MPI collective operations
 - Introduction to message passing
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A typical pattern with MPI Programs

- 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

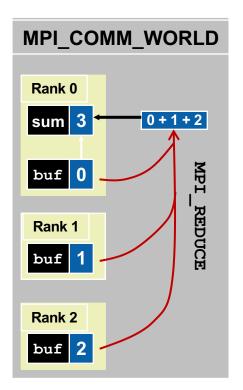
*This is a subset of available MPI types	*This	is a	subset	of	available	MPI	types
--	-------	------	--------	----	-----------	-----	-------

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

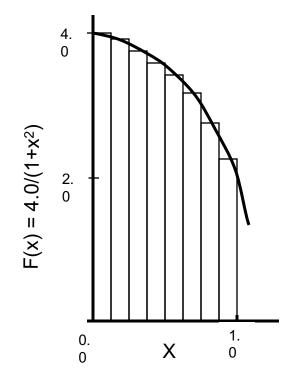
Operation	Function
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
User-defined	It is possible to define new reduction operations

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;
 msg = myrank;
 MPI Reduce (&buf, &sum, 1, MPI INT,
          MPI SUM, 0, MPI COMM WORLD);
 MPI Finalize();
```



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\leq 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. Explore its scalability on your system.

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 values in "sum" from
           sum += 4.0/(1.0+x*x);
                                              each process and place it
                                                 in "pi" on process 0
     sum *= step ;
     MPI Reduce(&sum, &pi, 1, MPI DOUBLE, MPI SUM, 0,
     MPI COMM WORLD);
```

MPI Pi program performance

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 values in "sum" from
           sum += 4.0/(1.0+x*x);
                                              each process and place it
                                                in "pi" on process 0
     sum *= step;
     MPI Reduce(&sum, &pi, 1, MPI DOUBLE, MPI SUM, 0,
     MPI COMM WORLD):
```

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

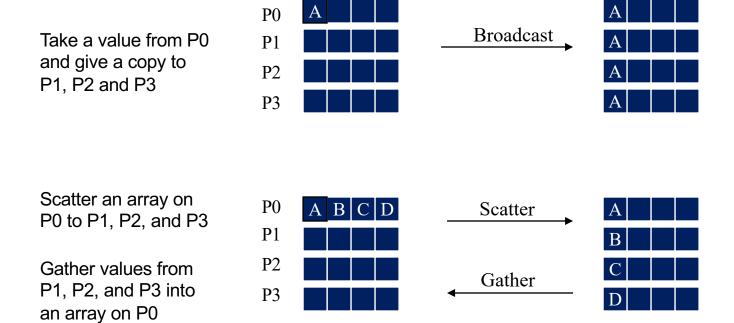
Note: OMP loop used a Blocked loop distribution. The others used a cyclic distribution. Serial .. 0.43

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

MPI Collective Routines

- 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, 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
 - MPI Barrier (comm)
- Blocks until all processes in the group of the communicator comm call it.

Collective Data Movement

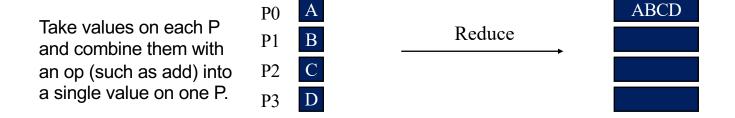


More Collective Data Movement

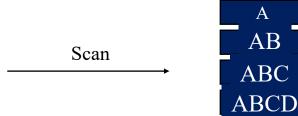




Collective Computation



P0 Take values on each P P1 and combine them with a scan operation and spread the scan array P3 out among all P.



AB

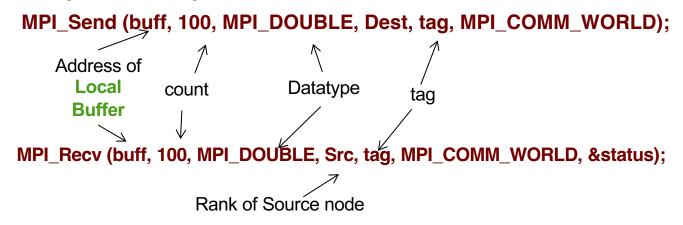
ABC

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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 is a user-defined integer to help the receiver keep track of different messages from a single source



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);
```

Exercise: Ping-Pong Program

Goal

- Measure the latency of our communication network.

Program

 Create a program to bounce a message 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.

```
#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;
 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();
```

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		

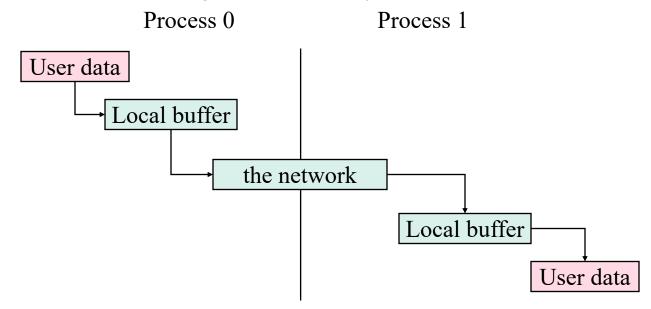
MPI provides predefined data types that must be specified when passing messages.

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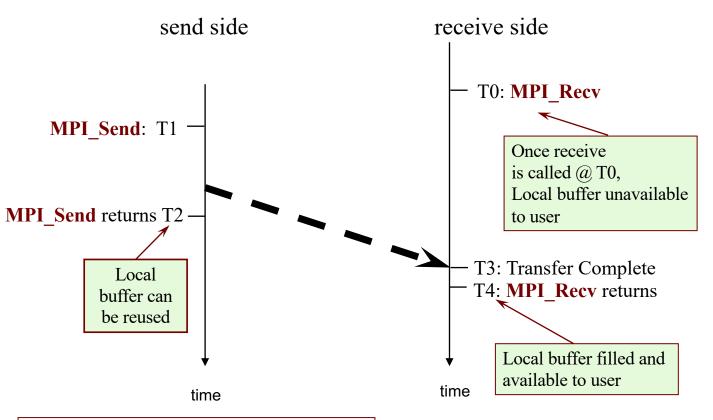
Buffers

- Message passing is straightforward, but there are subtleties
 - Buffering and deadlock
 - Deterministic execution
 - Performance
- When you send data, where does it go? One possibility is:



Blocking Send-Receive Timing Diagram

(Receive before Send)



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

Sources of Deadlocks

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

Process 0	Process 1		
Send(1)	Send(0)		
Recv(1)	Recv(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

Some Solutions to the "deadlock" Problem

• Order the operations more carefully:

Process 0	Process 1		
Send(1)	Recv(0)		
Recv(1)	Send(0)		

• Supply receive buffer at same time as send:

Process 0	Process 1		
Sendrecv(1)	Sendrecv(0)		

More Solutions to the "unsafe" Problem

• Supply a sufficiently large buffer in the send function

Process 1		
Bsend(0) Recv(0)		

• Use non-blocking operations:

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

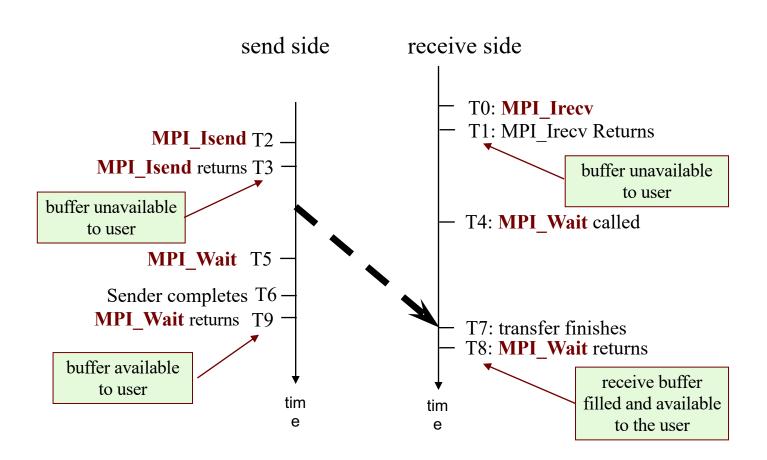
Non-Blocking Communication

- 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

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(&reg1, &status1);
```

```
do {
 MPI Irecv(&num, 1, MPI INT, from, tag,
                           MPI COMM WORLD, &req2);
 MPI Wait(&reg2, &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, &reg2);
 MPI Wait(&req2, &status2);
MPI Finalize();
return 0;
```

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
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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.
 - map onto a mesh with stepsize h and k

 Central difference approximation for spatial derivative (at fixed time)

■ Time derivative at t = tⁿ⁺¹

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

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

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

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

Example: Explicit finite differences

Combining time derivative expression using spatial derivative at t = tⁿ

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

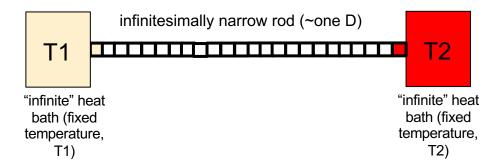
Solve for u at time n+1 and step j

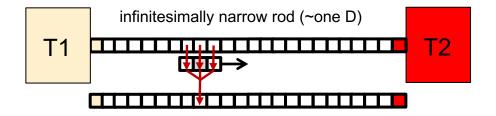
$$u_{j}^{n+1} = (1-2r)u_{j}^{n} + ru_{j-1}^{n} + ru_{j+1}^{n}$$

$$r = k/h^{2}$$

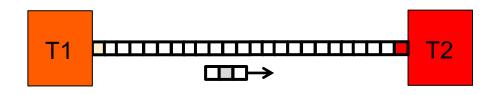
■ The solution at $t = t_{n+1}$ is determined explicitly from the solution at $t = t_n$ (assume u[t][0] = u[t][N] = Constant for all t).

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

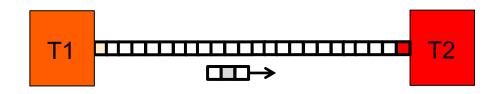




Pictorially, you are sliding a three point "stencil" across the domain (u[t]) and computing a new value of the center point (u[t+1]) at each stop.

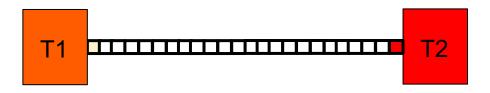


```
int main()
                                                             Note: I don't need the
                                                           intermediate "u[t]" values
   double *u = malloc (sizeof(double) * (N));
                                                         hence "u" is just indexed by x.
   double *up1 = malloc (sizeof(double) * (N));
   initialize data(uk, ukp1, N, P); // init to zero, 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]);
                                                   A well known trick with 2 arrays so I
      femp = up1; up1 = u; u = temp;
                                                   don't overwrite values from step k-1
                                                   as I fill in for step k
return 0;
```

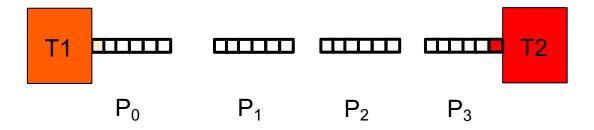


```
int main()
                                                      How would you
  double *u = malloc (sizeof(double) * (N));
                                                      parallelize this program?
  double *up1 = malloc (sizeof(double) * (N));
  initialize data(uk, ukp1, N, P); // init to zero, 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;
```

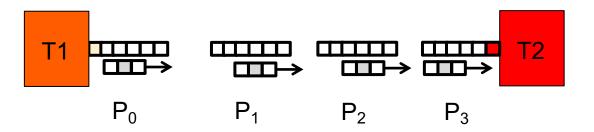
 Start with our original picture of the problem ... a one dimensional domain with end points set at a fixed temperature.



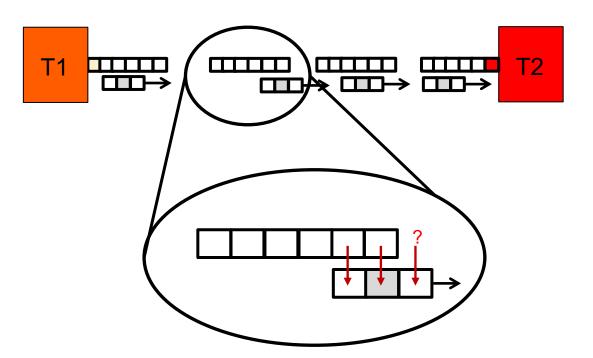
• Break it into chunks assigning one chunk to each process.



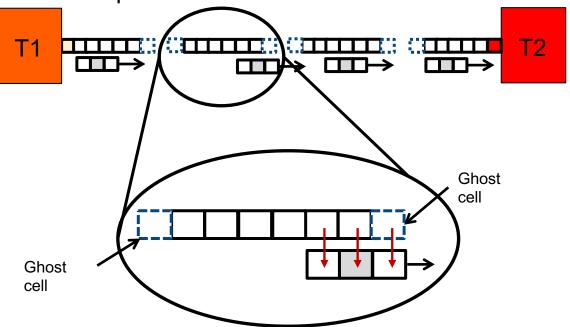
• Each process works on it's own chunk ... sliding the stencil across the domain to updates its own data.



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



 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 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"
double *up1 = malloc (sizeof(double) * (2 + N/P)); // to hold 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;
```

We write/explain this part first and then address the communication and data structures

Heat Diffusion MPI Example

return 0;

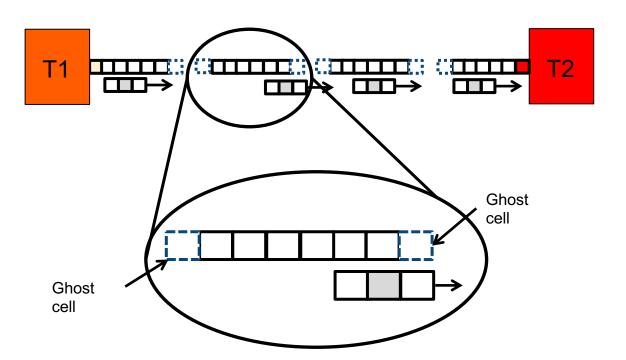
```
// Compute interior of each "chunk"
                                               Update array values using local data
                                               and values from ghost cells.
  for (int x = 2; x < N/P; ++x)
    up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
// update edges of each chunk keeping the two far ends fixed
// (first element on Process 0 and the last element on process P-1).
  if (mvID != 0)
    up1[1] = u[1] + (k / (h*h)) * (u[1+1] - 2*u[1] + u[1-1]);
                                                                       u[0] and
                                                                    u[N/P+1] are the
                                                                      ahost cells
  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
                                        Note I was lazy and assumed N was evenly
                                        divided by P. Clearly, I'd never do this in a
                                        "real" program.
MPI_Finalize();
```

Heat Diffusion MPI Example

```
MPI Init (&argc, &argv);
                                         1D PDE solver ... the simplest "real" message
MPI Comm size (MPI_COMM_WORLD, &P);
                                        passing code I can think of. Note: edges of
MPI_Comm_rank (MPI_COMM_WORLD, &myID); domain held at a fixed temperature
double *u = malloc (sizeof(double) * (2 + N/P)) // include "Ghost Cells"
double *up1 = malloc (sizeof(double) * (2 + N/P)); // to hold values
                                                     // from my neighbors
initialize data(uk, ukp1, N, P);
for (int t = 0; t < N STEPS; ++t){
  if (myID != 0) Send my "left" boundary value to the neighbor on my "left"
    MPI Send (&u[1], 1, MPI DOUBLE, myID-1, 0, MPI COMM WORLD);
  if (myID != P-1) Receive my "right" ghost cell from the neighbor to my "right"
    MPI Recv (&u[N/P+1], 1, MPI DOUBLE, myID+1, 0, MPI COMM WORLD, &status);
  if (myID != P-1) Send my "right" boundary value to the neighbor to my "right"
    MPI Send (&u[N/P], 1, MPI DOUBLE, myID+1, 0, MPI COMM WORLD);
  if (myID != 0) Receive my "left" ghost cell from the neighbor to my "left"
    MPI Recv (&u[0], 1, MPI DOUBLE, myID-1, 0, MPI COMM WORLD, &status);
/* continued on previous slide */
```

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 →

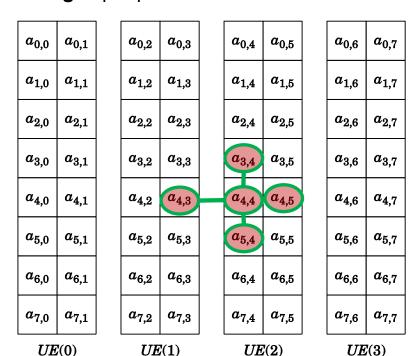
$a_{0,0}$	$a_{0,1}$	$a_{0,2}$	$a_{0,3}$	$a_{0,4}$	$a_{0,5}$	$a_{0,6}$	$a_{0,7}$
$a_{1,0}$	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$	$a_{1,4}$	$a_{1,5}$	$a_{1,6}$	$a_{1,7}$
$a_{2,0}$	$a_{2,1}$	$a_{2,2}$	$a_{2,3}$	$a_{2,4}$	$a_{2,5}$	$a_{2,6}$	$a_{2,7}$
$a_{3,0}$	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$	a _{3,4}	$a_{3,5}$	$a_{3,6}$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

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/P) messages** per processor

P is the # of processors

N is the order of our square matrix



UE = unit of execution ... think of it as a generic term for "process or thread"

Partitioned Arrays: Block distribution

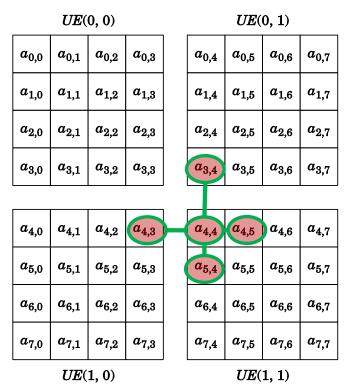
 If we parallelize in both dimensions, then we have (N/p)² elements per processor, and we need to send ~4*(n/p) messages from each processor. Asymptotically better than 2*sqrt(N).

P is the # of processors

Assume a p by p square mesh ... p=sqrt(P)

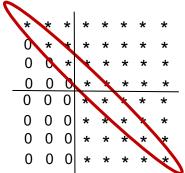
N is the order of our square matrix

Dimension of each block is N/P

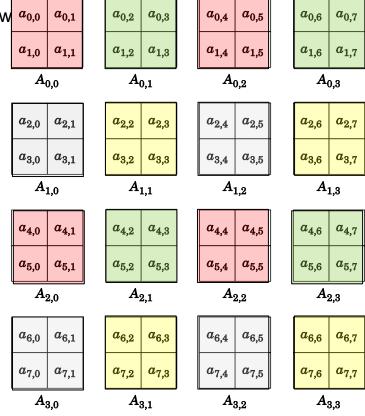


Partitioned Arrays: block cyclic distribution

• LU decomposition (A= LU) .. Move down the diagonal transform rows to "zero the column" below the diagonal.

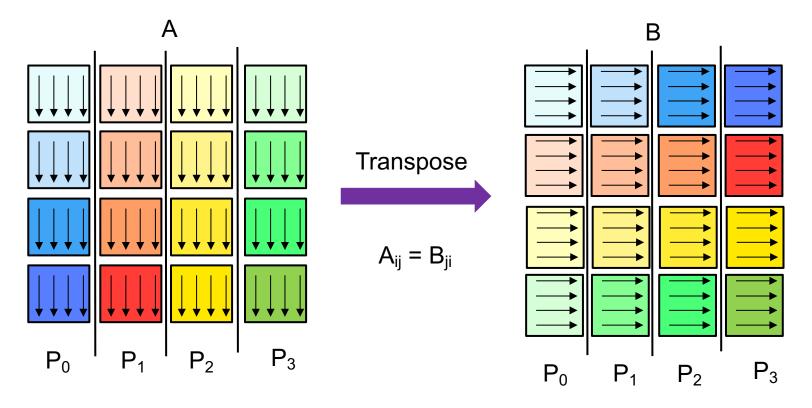


- Zeros fill in the right lower triangle of the matrix ... less work to do.
- Balance load with cyclic distribution of blocks of A mapped onto a grid of nodes (2x2 in this case ... colors show the mapping to nodes).



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.



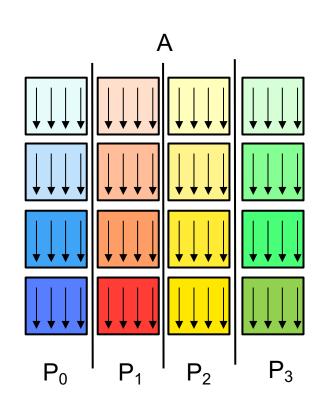
We are going to create a transpose program that uses the SPMD pattern.

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 ... who will each Processor march through its set of blocks?



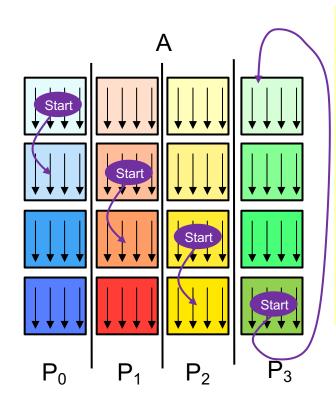
We are going to create a transpose program that uses the SPMD pattern.

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?



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

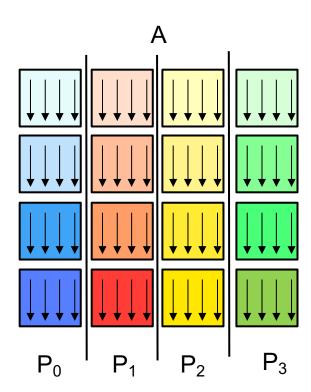
Phase 0 ... transpose your diagonal Phase 1 ... deal with next block "down"

How many phases for our case? 3

What is the communication pattern for each phase?

Which block is sent?
Who receives that block?
Where do they put it?

Remember, this is SPMD. You have a single program so how will you structure it so each processor does the right thing for each block.

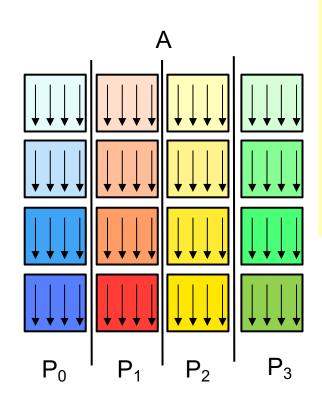


The three phases shown for P₁

What is the communication pattern for each phase?

Which block is sent?
Who receives that block?
Where do they put it?

Remember, this is SPMD. You have a single program so how will you structure it so each processor does the right thing for each block.



Communication pattern

Phase 0 ... no communication ... just a local transpose on block ID (the diagonal)

Phase k ... Send block (ID+k) to your kth neighbor

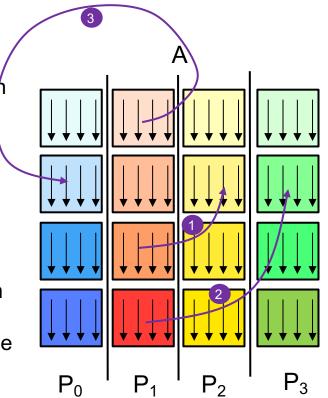
On the receiving end, the block **from** neighbor ID goes to your row-block number ID. Why?

The three phases shown for P₁

What is the communication pattern for each phase?

Which block is sent?
Who receives that block?
Where do they put it?

Remember, this is SPMD. You have a single program so how will you structure it so each processor does the right thing for each block.



Communication pattern

Phase 0 ... no communication ... just a local transpose on block ID (the diagonal)

Phase k ... Send block (ID+k) to your kth neighbor

On the receiving end, the block **from** neighbor ID goes to your row-block number ID. Why?

We have a column block decomposition so column block indices are the rank (ID). Plus in a transpose you map column blocks to row blocks

Remember to transpose the block ... either before you send it or after it arrives.

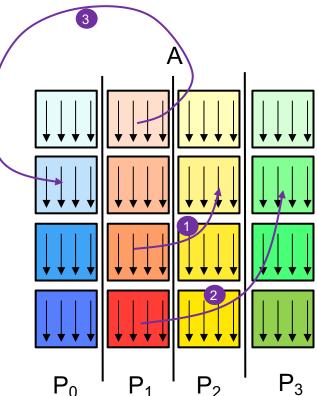
Exercise/discussion The three phases shown for P₁ Now for the tricky part. This is an SPMD pattern. Every node will run the same program. So using just the rank (ID), the phase, and the number of processes (P) ... write expressions for the communication patterns for each phase and each processor. Hint: you have to account for wrap-around (e.g. phase three P_3 in the figure)

The three phases shown for P₁

Now for the tricky part. This is an SPMD pattern. Every node will run the same program.

So using just the rank (ID), the phase, and the number of processes (P) ... write expressions for the communication patterns for each phase and each processor.

Hint: you have to account for wrap-around (e.g. phase three in the figure)



In a given phase, each process will need to send a block TO another process and receive a block FROM another process.

You need expressions for TO and FROM.

We will put this in a C macro.

A macro in S replaces code in the program text BEFORE coompiltion.

Example: (note: this is NOT the right answer ... I don't want to make this too easy)

#define TO(ID, Phase) (ID/PHASE)%N

Exercise: transpose program

- Start with the basic transpose program we provide.
- Go to trans_sendrcv.c and enter your definitions for the TO and FROM macros.
- Test and verify correctness
- Try different message passing approaches.
- Can you overlap the local transpose and the communication between nodes?

Outline

- MPI and distributed memory systems
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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

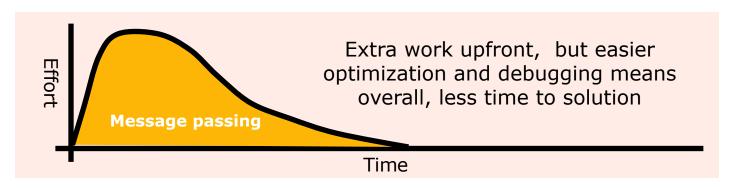
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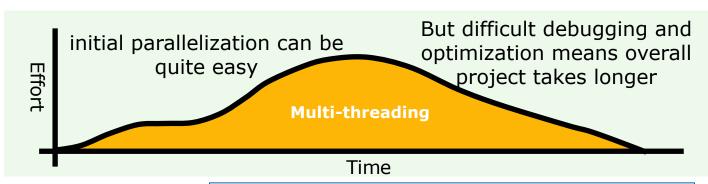
The 12 core functions in MPI

- MPI Init
- MPI Finish
- MPI_Comm_size
- MPI_Comm_rank
- MPI_Send
- MPI_Rocv
- 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*

MPI References

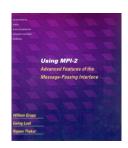
- The Standard itself:
 - at http://www.mpi-forum.org
 - All MPI official releases, in both postscript and HTML
- Other information on Web:
 - at http://www.mcs.anl.gov/mpi
 - pointers to lots of stuff, including other talks and tutorials, a FAQ, other MPI pages

Books for learning MPI

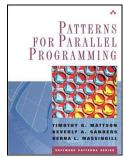
• Using MPI-2: Portable Parallel Programming with the Message-Passing Interface, by Gropp, Lusk, and Thakur, MIT Press, 1999..



Patterns for Parallel Programing, by Tim Mattson, Beverly Sanders, and Berna Massingill.





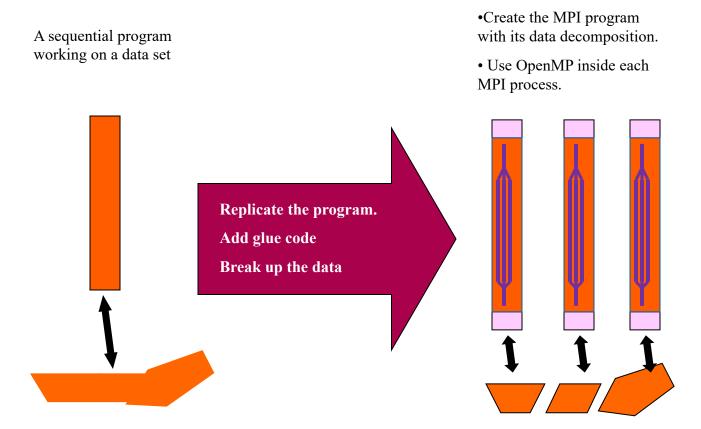


Backup



Loading MPI on your system

How do people mix MPI and OpenMP?



Pi program with MPI and OpenMP

Get the MPI part done first, then add OpenMP pragma where it makes sense to do so

```
#include <mpi.h>
#include "omp.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;
#pragma omp parallel for reduction(+:sum) private(x)
     for (i=my id*my steps; i<(m 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);
```

Key issues when mixing OpenMP and MPI

- 1. Messages are sent to a process not to a particular thread.
 - Not all MPIs are threadsafe. MPI 2.0 defines threading modes:
 - MPI_Thread_Single: no support for multiple threads
 - MPI_Thread_Funneled: Mult threads, only master calls MPI
 - MPI_Thread_Serialized: Mult threads each calling MPI, but they do it one at a time.
 - MPI_Thread_Multiple: Multiple threads without any restrictions
 - Request and test thread modes with the function:
 MPI_init_thread(desired_mode, delivered_mode, ierr)
- 2. Environment variables are not propagated by mpirun. You'll need to broadcast OpenMP parameters and set them with the library routines.

Dangerous Mixing of MPI and OpenMP

• The following will work only if MPI_Thread_Multiple is supported ... a level of support I wouldn't depend on.

```
MPI Comm Rank(MPI COMM WORLD, &mpi id);
#pragma omp parallel
   int tag, swap neigh, stat, omp id = omp thread num();
   long buffer [BUFF SIZE], incoming [BUFF SIZE];
   big ugly calc1(omp id, mpi id, buffer);
                                               // Finds MPI id and tag so
   neighbor(omp id, mpi id, &swap neigh, &tag); // messages don't conflict
   MPI Send (buffer, BUFF SIZE, MPI LONG, swap neigh,
           tag, MPI COMM WORLD);
   MPI Recv (incoming, buffer count, MPI LONG, swap neigh,
           tag, MPI COMM WORLD, &stat);
   big ugly calc2(omp id, mpi id, incoming, buffer);
#pragma critical
  consume(buffer, omp id, mpi id);
```

Messages and threads

- Keep message passing and threaded sections of your program separate:
 - Setup message passing outside OpenMP parallel regions (MPI_Thread_funneled)
 - Surround with appropriate directives (e.g. critical section or master) (MPI_Thread_Serialized)
 - For certain applications depending on how it is designed it may not matter which thread handles a message. (MPI_Thread_Multiple)
 - -Beware of race conditions though if two threads are probing on the same message and then racing to receive it.

Safe Mixing of MPI and OpenMP Put MPI in sequential regions

```
MPI Init(&arge, &argv); MPI Comm Rank(MPI COMM WORLD, &mpi id);
// a whole bunch of initializations
#pragma omp parallel for
for (I=0;I<N;I++) {
   U[I] = big calc(I);
   MPI Send (U, BUFF SIZE, MPI DOUBLE, swap neigh,
           tag, MPI COMM WORLD);
   MPI Recv (incoming, buffer count, MPI DOUBLE, swap neigh,
           tag, MPI COMM WORLD, &stat);
#pragma omp parallel for
for (I=0;I<N;I++) {
   U[I] = other big calc(I, incoming);
consume(U, mpi id);
```

Technically Requires
MPI_Thread_funneled, but I
have never had a problem with
this approach ... even with
pre-MPI-2.0 libraries.

Safe Mixing of MPI and OpenMP Protect MPI calls inside a parallel region

```
MPI Init(&argc, &argv); MPI Comm Rank(MPI COMM WORLD, &mpi id);
// a whole bunch of initializations
                                                     Technically Requires
                                                     MPI_Thread_funneled, but I
#pragma omp parallel
                                                     have never had a problem with
#pragma omp for
                                                     this approach ... even with
  for (I=0;I<N;I++) U[I] = big calc(I);
                                                     pre-MPI-2.0 libraries.
#pragma master
  MPI Send (U, BUFF SIZE, MPI DOUBLE, neigh, tag, MPI COMM WORLD);
  MPI Recv (incoming, count, MPI DOUBLE, neigh, tag, MPI COMM WORLD, &stat);
#pragma omp barrier
#pragma omp for
  for (I=0;I<N;I++) U[I] = other big calc(I, incoming);
#pragma omp master
  consume(U, mpi id);
```

Hybrid OpenMP/MPI works, but is it worth it?

- Literature* is mixed on the hybrid model: sometimes its better, sometimes MPI alone is best.
- There is potential for benefit to the hybrid model
 - MPI algorithms often require replicated data making them less memory efficient.
 - Fewer total MPI communicating agents means fewer messages and less overhead from message conflicts.
 - Algorithms with good cache efficiency should benefit from shared caches of multi-threaded programs.
 - The model maps perfectly with clusters of SMP nodes.
- But really, it's a case by case basis and to large extent depends on the particular application.

Backup

Mixing OpenMP and MPI



MPIch library on Apple Laptops: MacPorts

- To use MPI on your Apple laptop:
 - Download Xcode. Be sure to choose the command line tools that match your OS.
 - Install MacPorts (if you haven't already ... use the installer for your OS from macports.org).

sudo port selfupdate

sudo port install mpich-qcc9

mpicc hello.c
mpiexec -n 4 ./a.out

Update to latest version of MacPorts

Graph the library that matches the version of your gcc compiler.

Test the installation with a simple program