CS 267 Lecture 9: Distributed Memory Machines and Programming

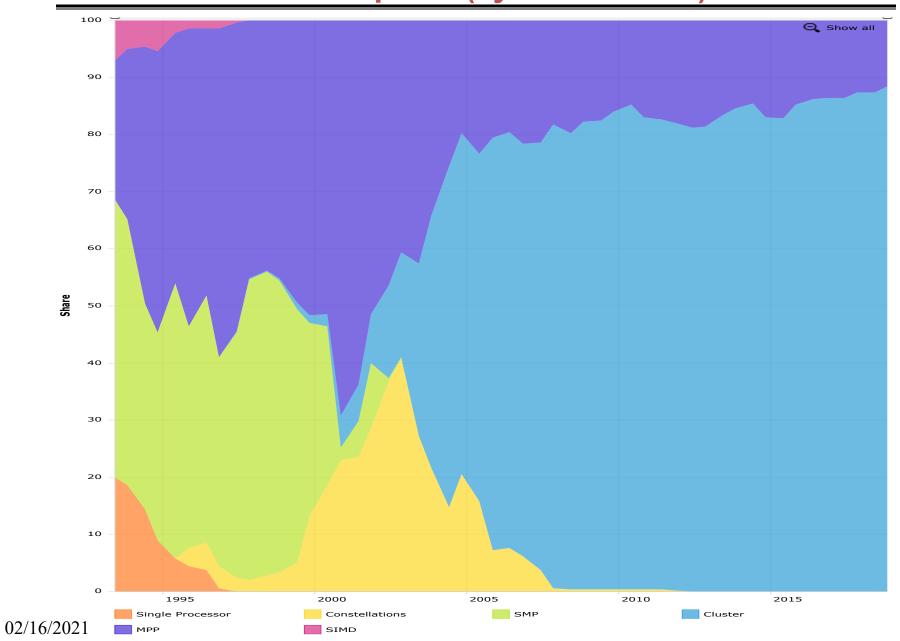
Aydin Buluc

https://sites.google.com/lbl.gov/cs267-spr2021/

Outline

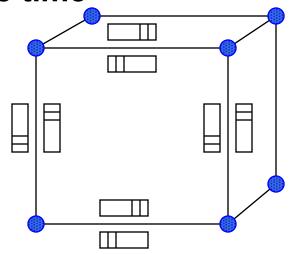
- Distributed Memory Architectures
 - Properties of communication networks
 - Topologies
 - Performance models
- ° Programming Distributed Memory Machines using Message Passing
 - Overview of MPI
 - Basic send/receive use
 - Non-blocking communication
 - Collectives

Architectures in Top 500 (systems share)



Historical Perspective

- ° Early distributed memory machines were:
 - Collection of microprocessors.
 - Communication was performed using bi-directional queues between nearest neighbors.
- Messages were forwarded by processors on path.
 - "Store and forward" networking
- There was a strong emphasis on topology in algorithms, in order to minimize the number of hops = minimize time



Network Analogy

To have a large number of different transfers occurring at once, you need a large number of distinct wires

Not just a bus, as in shared memory

Networks are like streets:

- Link = street.
- Switch = intersection.
- Distances (hops) = number of blocks traveled.
- Routing algorithm = travel plan.

Properties:

Latency: how long to get between nodes in the network.

Street: time for one car = dist (miles) / speed (miles/hr)

Bandwidth: how much data can be moved per unit time.

- Street: cars/hour = density (cars/mile) * speed (miles/hr) * #lanes
- Network bandwidth is limited by the bit rate per wire and #wires

Design Characteristics of a Network

- * Topology (how things are connected)
 - Crossbar; ring; 2-D, 3-D, higher-D mesh or torus; hypercube; tree; butterfly; perfect shuffle, dragon fly, ...
- ° Routing algorithm:
 - Example in 2D torus: all east-west then all north-south (avoids deadlock).
- ° Switching strategy:
 - Circuit switching: full path reserved for entire message, like the telephone.
 - Packet switching: message broken into separately-routed packets, like the post office, or internet
- Flow control (what if there is congestion):
 - Stall, store data temporarily in buffers, re-route data to other nodes, tell source node to temporarily halt, discard, etc.

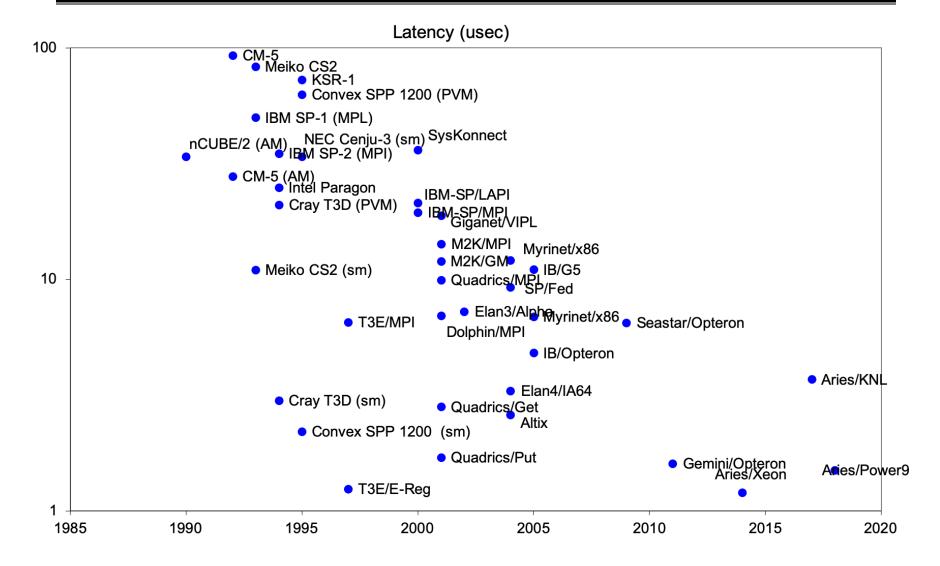
Performance Properties of a Network: Latency

- Diameter: the maximum (over all pairs of nodes) of the shortest path between a given pair of nodes.
- Latency: delay between send and receive times
 - Latency tends to vary widely across architectures
 - Vendors often report hardware latencies (wire time)
 - Application programmers care about software latencies (user program to user program)

° Observations:

- Latencies differ by 1-2 orders across network designs
- Software/hardware overhead at source/destination dominate cost (1s-10s usecs)
- Hardware latency varies with distance (10s-100s nsec per hop)
 but is small compared to overheads
- ° Latency is key for programs with many small messages

End to End Latency (1/2 roundtrip) Over Time



· Latency has not improved significantly, unlike Moore's Law

Performance Properties of a Network: Bandwidth

- ° The bandwidth of a link = # wires / time-per-bit
- Bandwidth typically in Gigabytes/sec (GB/s), i.e., 8* 2²⁰ bits per second
- Effective bandwidth is usually lower than physical link bandwidth due to packet overhead.

Bandwidth is important for applications with mostly large messages

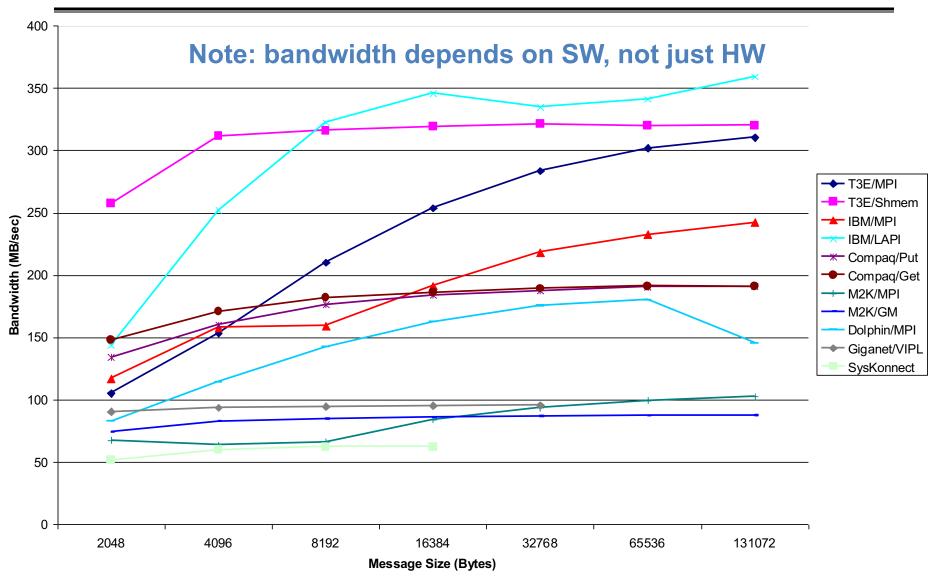
Routing and control header

Data payload

Error code

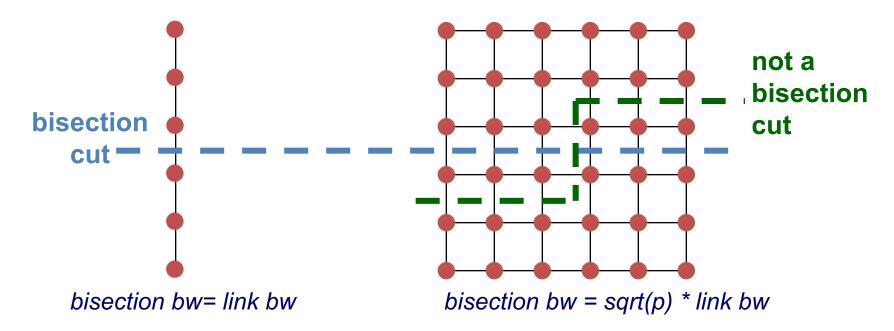
Trailer

Bandwidth Chart



Performance Properties of a Network: Bisection Bandwidth

- Bisection bandwidth: bandwidth across smallest cut that divides network into two equal halves
- ° Bandwidth across "narrowest" part of the network



 Bisection bandwidth is important for algorithms in which all processors need to communicate with all others

Linear and Ring Topologies

° Linear array



- Diameter = n-1; average distance ~n/3.
- Bisection bandwidth = 1 (in units of link bandwidth).
- ° Torus or Ring

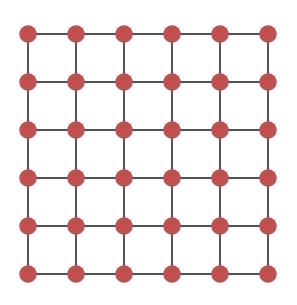


- Diameter = n/2; average distance ~ n/4.
- Bisection bandwidth = 2.
- Natural for algorithms that work with 1D arrays.

Meshes and Tori – used in Hopper

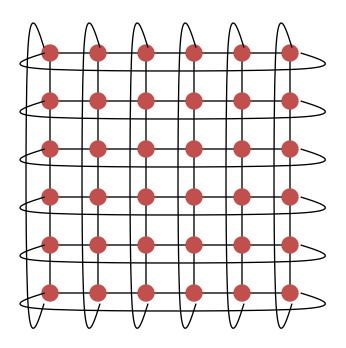
Two dimensional mesh

- Diameter = 2 * (sqrt(n) 1)
- Bisection bandwidth = sqrt(n)



Two dimensional torus

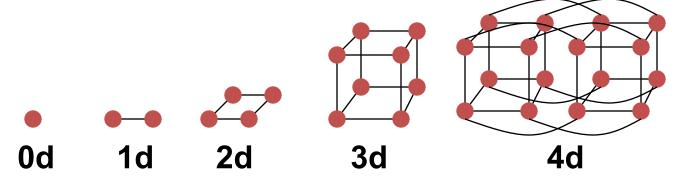
- Diameter = sqrt(n)
- Bisection bandwidth = 2* sqrt(n)



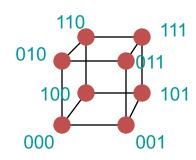
- Generalizes to higher dimensions
 - Cray XT (eg Hopper@NERSC) uses 3D Torus
- Natural for algorithms that work with 2D and/or 3D arrays (matmul)

Hypercubes

- Number of nodes n = 2^d for dimension d.
 - Diameter = d.
 - Bisection bandwidth = n/2.

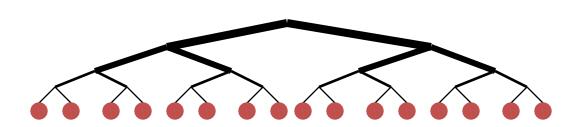


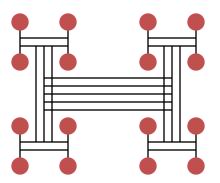
- ° Popular in early machines (Intel iPSC, NCUBE).
 - Lots of clever algorithms.
 - See 1996 online CS267 notes.
- ° Greycode addressing:
 - Each node connected to d others with 1 bit different.



Trees

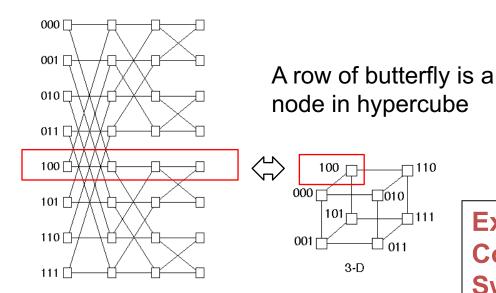
- ° Diameter = log n.
- Bisection bandwidth = 1.
- ° Easy layout as planar graph.
- ° Many tree algorithms (e.g., summation).
- ° Fat trees avoid bisection bandwidth problem:
 - More (or wider) links near top.
 - Example: Thinking Machines CM-5.

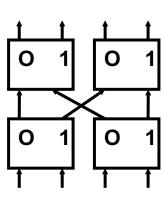




Butterflies

- Really an unfolded version of hypercube.
- A d-dimensional butterfly has (d+1) 2^d "switching nodes" (not to be confused with processors, which is n = 2^d)
- Butterfly was invented because hypercube required increasing radix of switches as the network got larger; prohibitive at the time
- Diameter = log n. Bisection bandwidth = n
- No path diversity: bad with adversarial traffic



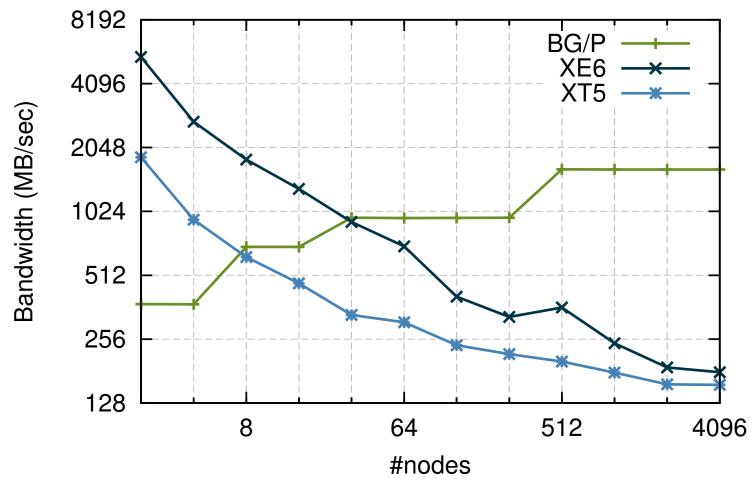


butterfly switch

Ex: to get from proc 101 to 110, Compare bit-by-bit and Switch if they disagree, else not

Does Topology Matter?





See EECS Tech Report UCB/EECS-2011-92, August 2011

Why so many topologies?

Different systems have different needs

Size of the system (data center vs. NIC)

Complexity vs. optimality

Physical constraints

Innovations in HW enable previously infeasible technologies

° Two recent technological changes:

- Higher radix (number of ports supported) switches economical, which is really a consequence of Moore's law
- Fiber optic is feasible → distance doesn't matter

Dragonflies – used in Edison and Cori

- Motivation: Exploit gap in cost and performance between optical interconnects (which go between cabinets in a machine room) and electrical networks (inside cabinet)
 - Optical (fiber) more expensive but higher bandwidth when long
 - Electrical (copper) networks cheaper, faster when short

° Combine in hierarchy:

- Several groups are connected together using all to all links, i.e. each group has at least one link directly to each other group.
- The topology inside each group can be any topology.

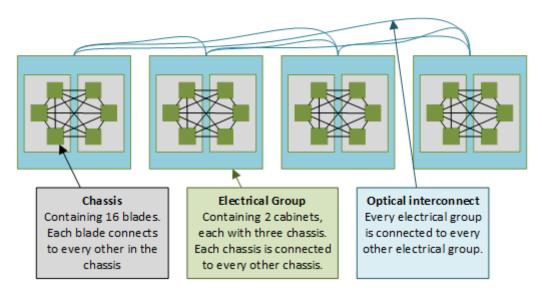
Uses a randomized routing algorithm

- ° Outcome: programmer can (usually) ignore topology, get good performance
 - Important in virtualized, dynamic environment
 - Drawback: variable performance

"Technology-Drive, Highly-Scalable Dragonfly Topology," ISCA 2008

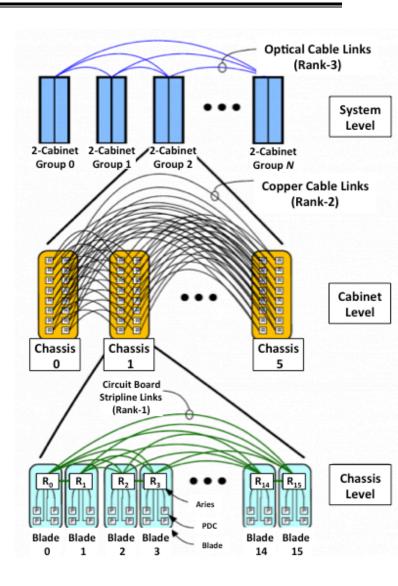
Dragonfly in practice

Aries interconnect for an 8 cabinet Cray XC40

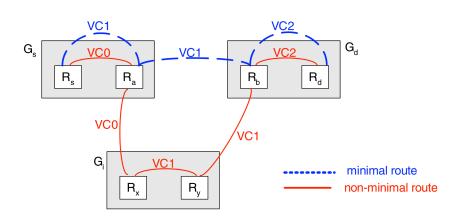


Source: European Centre for Medium-Range Weather Forecasts

Source of image on the right (and more info): http://www.nersc.gov/users/computational-systems/edison/configuration/interconnect/



Why randomized routing?



Minimal routing:

- If Gs ≠ Gd and Rs has no connection to Gd, route within Gs from Rs to Ra, which has a global channel to Gd.
- 2. If Gs ≠ Gd, traverse the global channel from Ra to router Rb in Gd.
- 3. If $Rb \neq Rd$, route from Rb to Rd.

Minimal routing works well when things are load balanced, potentially catastrophic in adversarial traffic patterns.

Randomization idea: For each packet sourced at router $Rs \in Gs$ and addressed to a router in another group $Rd \in Gd$, first route it to an intermediate group Gi.

- This requires at most two group-level link traversals
- And at most 5 total link traversals

Valiant, Leslie G. "A scheme for fast parallel communication." SIAM journal on computing 11.2 (1982): 350-361.

Performance Models

Shared Memory Performance Models

- Parallel Random Access Memory (PRAM)
- All memory access operations complete in one clock period -- no concept of memory hierarchy ("too good to be true").
 - OK for understanding whether an algorithm has enough parallelism at all (see CS273).
 - Parallel algorithm design strategy: first do a PRAM algorithm, then worry about memory/communication time (sometimes works)
- ° Slightly more realistic versions exist
 - E.g., Concurrent Read Exclusive Write (CREW) PRAM.
 - Still missing the memory hierarchy

Latency and Bandwidth Model

° Time to send message of length n is roughly

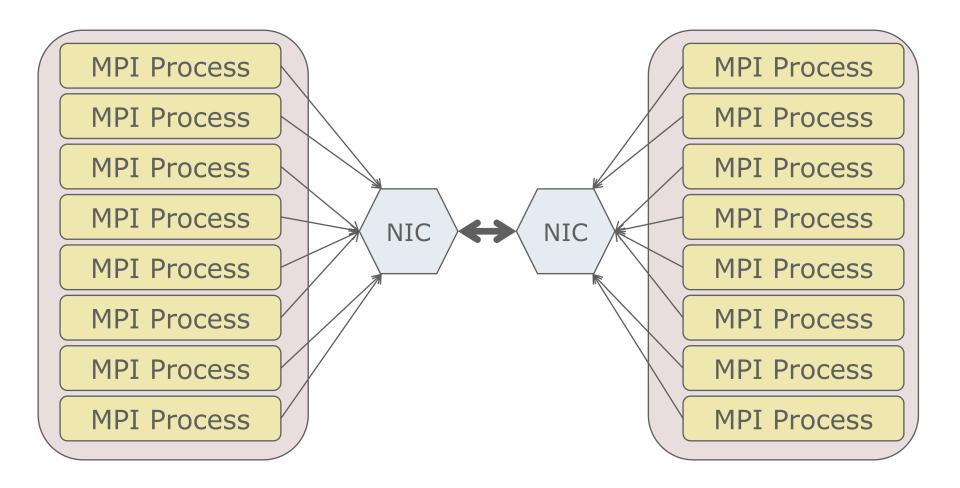
- * Topology is assumed irrelevant.
- ° Often called " α - β model" and written Time = α + n* β
- ° Usually $\alpha >> \beta >>$ time per flop.
 - One long message is cheaper than many short ones.
 - Can do hundreds or thousands of flops for cost of one message.

$$\alpha + n*\beta << n*(\alpha + 1*\beta)$$

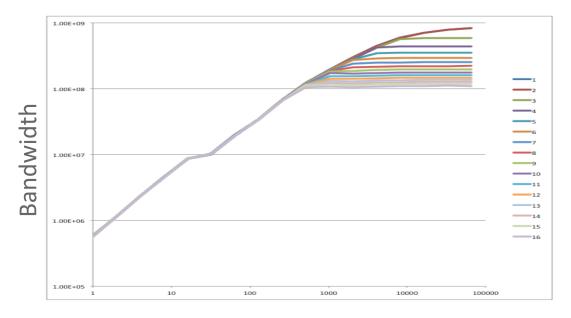
- ° Lesson: Need large computation-to-communication ratio to be efficient.
- ° LogP more detailed model (Latency/overhead/gap/Proc.)

Latency and Bandwidth Model in 2010 and beyond+

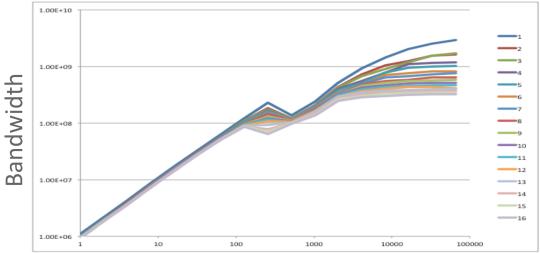
Processors are multi-core and many nodes are multi-chip



NIC bandwidth bottleneck



- Ping-pong between 2 nodes using 1-16 cores on each node
- Top: BG/Q,
- Bottom Cray XE6
- X-axis is message size



Alpha-beta model
 predicts a single curve –
 rates independent of
 the number of
 communicating
 processes

Programming Distributed Memory Machines with Message Passing

Slides by
Aydin Buluc, Jonathan Carter, Jim Demmel,
Bill Gropp, Kathy Yelick

Message Passing Libraries (1)

Many "message passing libraries" were once available

- Chameleon, from ANL.
- CMMD, from Thinking Machines.
- Express, commercial.
- MPL, native library on IBM SP-2.
- NX, native library on Intel Paragon.
- Zipcode, from LLL.
- PVM, Parallel Virtual Machine, public, from ORNL/UTK.
- Others...
- MPI, Message Passing Interface, now the industry standard.
- Need standards to write portable code.

Message Passing Libraries (2)

- All communication, synchronization require subroutine calls
 - No shared variables
 - Program run on a single processor just like any uniprocessor program, except for calls to message passing library
- $^{\circ}\,$ Subroutines for
 - Communication
 - Pairwise or point-to-point: Send and Receive
 - Collectives all processor get together to
 - Move data: Broadcast, Scatter/gather
 - Compute and move: sum, product, max, prefix sum, ... of data on many processors
 - Synchronization
 - Barrier
 - No locks because there are no shared variables to protect
 - Enquiries
 - How many processes? Which one am I? Any messages waiting?

Novel Features of MPI

- Communicators encapsulate communication spaces for library safety
- Datatypes reduce copying costs and permit heterogeneity
- Multiple communication <u>modes</u> allow precise buffer management
- Extensive <u>collective operations</u> for scalable global communication
- Process topologies permit efficient process placement, user views of process layout
- Profiling interface encourages portable tools

MPI References

The Standard itself:

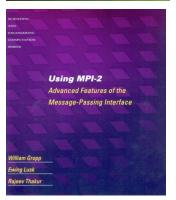
- at http://www.mpi-forum.org
- All MPI official releases, in both postscript and HTML
- Latest version MPI 3.1, released June 2015
- ° Other information on Web:
 - at <u>http://www.mcs.anl.gov/research/projects/mpi/index.ht</u> m
 - pointers to lots of stuff, including other talks and tutorials, a FAQ, other MPI pages

Books on MPI

- * Using MPI: Portable Parallel Programming with the Message-Passing Interface (third edition), by Gropp, Lusk, and Skjellum, MIT Press, 2014.
- [°] Using Advanced MPI: Modern Features of the Message-Passing Interface, by Gropp, Hoefler, Thakur, and Lusk, MIT Press, 2014
- * Using MPI-2: Portable Parallel Programming with the Message-Passing Interface, by Gropp, Lusk, and Thakur, MIT Press, 1999.
- Otto, Huss-Lederman, Walker, and Dongarra, MIT Press, 1998.
- * MPI: The Complete Reference Vol 2 The MPI Extensions, by Gropp, Huss-Lederman, Lumsdaine, Lusk, Nitzberg, Saphir, and Snir, MIT Press, 1998.
- ° **Designing and Building Parallel Programs**, by Ian Foster, Addison-Wesley, 1995.
- ° Parallel Programming with MPI, by Peter Pacheco, Morgan-Kaufmann, 1997.







Finding Out About the Environment

- ° Two important questions that arise early in a parallel program are:
 - How many processes are participating in this computation?
 - Which one am I?
- ° MPI provides functions to answer these questions:
 - •MPI_Comm_size reports the number of processes.
 - •MPI_Comm_rank reports the rank, a number between 0 and size-1, identifying the calling process

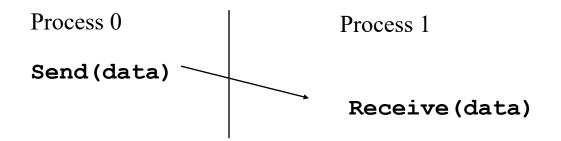
Hello (C)

```
#include "mpi.h"
#include <stdio.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( "I am %d of %d\n", rank, size );
    MPI Finalize();
    return 0;
```

Notes on Hello World

- ° All MPI programs begin with MPI_Init and end with MPI_Finalize
- ° MPI_COMM_WORLD is defined by mpi.h (in C) or mpif.h (in Fortran) and designates all processes in the MPI "job"
- Each statement executes independently in each process
 - including the printf/print statements
- The MPI-1 Standard does not specify how to run an MPI program, but many implementations provide
 mpirun −np 4 a.out

$^{\circ}\,$ We need to fill in the details in



Things that need specifying:

- How will "data" be described?
- How will processes be identified?
- How will the receiver recognize/screen messages?
- What will it mean for these operations to complete?

Some Basic Concepts

- Processes can be collected into groups
- Each message is sent in a <u>context</u>, and must be received in the same context
 - Provides necessary support for libraries
- A group and context together form a <u>communicator</u>
- A process is identified by its <u>rank</u> in the group associated with a communicator
- There is a default communicator whose group contains all initial processes, called MPI COMM WORLD

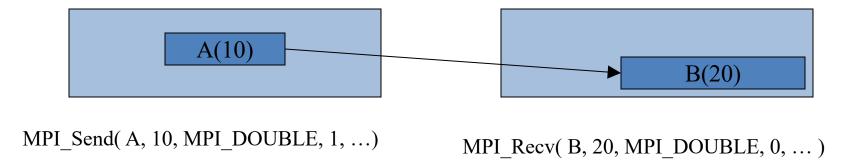
MPI Datatypes

- The data in a message to send or receive is described by a triple (address, count, datatype), where
- An MPI datatype is recursively defined as:
 - predefined, corresponding to a data type from the language (e.g., MPI_INT, MPI_DOUBLE)
 - a contiguous array of MPI datatypes
 - a strided block of datatypes
 - an indexed array of blocks of datatypes
 - an arbitrary structure of datatypes
- There are MPI functions to construct custom datatypes, in particular ones for subarrays
- May hurt performance if datatypes are complex

MPI Tags

- Messages are sent with an accompanying userdefined integer tag, to assist the receiving process in identifying the message
- Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying MPI_ANY_TAG as the tag in a receive
- Some non-MPI message-passing systems have called tags "message types". MPI calls them tags to avoid confusion with datatypes

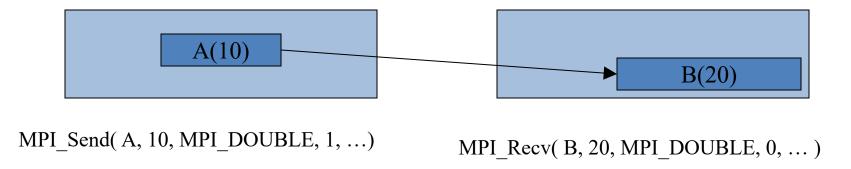
MPI Basic (Blocking) Send



MPI_SEND(start, count, datatype, dest, tag, comm)

- The message buffer is described by (start, count, datatype).
- The target process is specified by dest, which is the rank of the target process in the communicator specified by comm.
- When this function returns, the data has been delivered to the system and the buffer can be reused. The message may not have been received by the target process.

MPI Basic (Blocking) Receive



MPI_RECV(start, count, datatype, source, tag,
 comm, status)

- Waits until a matching (both source and tag) message is received from the system, and the buffer can be used
- source is rank in communicator specified by comm, or MPI_ANY_SOURCE
- tag is a tag to be matched or MPI_ANY_TAG
- receiving fewer than count occurrences of datatype is OK, but receiving more is an error
- status contains further information (e.g. size of message) 41

A Simple MPI Program

```
#include "mpi.h"
#include <stdio.h>
int main( int argc, char *argv[])
  int rank, buf;
 MPI Status status;
 MPI Init(&argv, &argc);
 MPI Comm rank( MPI COMM WORLD, &rank );
  /* Process 0 sends and Process 1 receives */
  if (rank == 0) {
   buf = 123456;
   MPI Send( &buf, 1, MPI INT, 1, 0, MPI COMM WORLD);
  else if (rank == 1) {
    MPI Recv( &buf, 1, MPI INT, 0, 0, MPI COMM WORLD,
              &status );
    printf( "Received %d\n", buf );
 MPI Finalize();
  return 0;
```

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Retrieving Further Information

- ° Status is a data structure allocated in the user's program.
- ° In C:

```
int recvd_tag, recvd_from, recvd_count;
MPI_Status status;
MPI_Recv(..., MPI_ANY_SOURCE, MPI_ANY_TAG, ..., &status)
recvd_tag = status.MPI_TAG;
recvd_from = status.MPI_SOURCE;
MPI_Get_count( &status, datatype, &recvd_count);
```

MPI can be simple

- ° Claim: most MPI applications can be written with only 6 functions (although which 6 may differ)
- Using point-to-point:
 - MPI INIT
 - MPI FINALIZE
 - MPI COMM SIZE
 - MPI COMM RANK
 - MPI SEND
 - MPI RECEIVE

- Using collectives:
 - MPI INIT
 - MPI FINALIZE
 - MPI COMM SIZE
 - MPI COMM RANK
 - MPI BCAST
 - MPI_REDUCE

You may use more for convenience or performance

But is that small subset the practical usage?

- What aspects of the MPI standard do you use in your application in its current form?

 * (multiple)
- 36 What aspects of the MPI standard appear in performance-critical sections of your current application? * (multiple)
- 37 What aspects of the MPI standard do you anticipate using in the "exascale" version of your application? * (multiple)

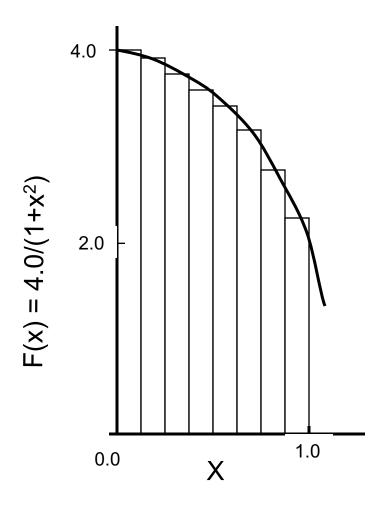
	Q35:	Curre	nt Usage	Q37:	Exasca	ale Usage	Q36:	Perform	nance Critical
Responses	AD	\mathbf{ST}	Overall	\mathbf{AD}	\mathbf{ST}	Overall	AD	\mathbf{ST}	Overall
Point-to-point com- munications	96%	79%	88%	89%	71%	80%	93%	75%	84%
MPI derived datatypes	25%	21%	23%	21%	21%	21%	14%	7%	11%
Collective communications	86%	75%	80%	96%	68%	82%	64%	64%	64%
Neighbor collective communications	14%	14%	14%	32%	25%	29%	7%	11%	9%
Communicators and group manage- ment	68%	54%	61%	61%	50%	55%	29%	7%	18%
Process topologies	14%	7%	11%	32%	11%	21%	4%	4%	4%
RMA (one-sided communications)	36%	7%	21%	50%	36%	43%	21%	7%	14%
RMA shared win- dows	18%	7%	12%	21%	18%	20%	7%	7%	7%
MPI I/O (called directly)	25%	18%	21%	21%	18%	20%	4%	7%	5%
MPI I/O (called through a third- party library)	32%	21%	27%	36%	25%	30%	7%	11%	9%
MPI profiling interface /16/2021	11%	0%	14%	11%	21%	16%	0%	4%	2%

But is that small subset the practical usage?

No.	Question and Responses	AD	\mathbf{ST}	Overall		
38	What is the dominant communication in your application? Check	all that	apply,	recognizing		
	that many applications have different communication patterns in different	phases	s. (mult	tiple)		
	Each process talks to (almost) every other process	25%	21%	23%		
	Processes communicate in fixed "neighborhoods" of limited size	46%	46%	46%		
	Processes communicate in "neighborhoods" of limited size that may	42%	36%	39%		
	change in different phases of the application or evolve over the course					
	of a run					
	Communication is largely irregular	18%	21%	20%		
39	39 Can your application take advantage of non-blocking point-to-point operations (mul-					
	tiple)					
	To overlap communication with computation?	89%	71%	80%		
	To allow asynchronous progress?	64%	64%	64%		
	To allow event-based programming?	43%	29%	36%		
40	Can your application take advantage of non-blocking collective of	perati	ons	(multiple)		
	To overlap communication with computation?	71%	46%	59%		
	To allow asynchronous progress?	46%	29%	38%		
	To allow event-based programming?	25%	14%	20%		

https://info.ornl.gov/sites/publications/Files/Pub108588.pdf

PI redux: 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:

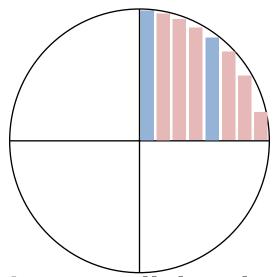
$$\sum_{i=0}^{N} F(x_i) \Delta x \approx \pi$$

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

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Example: Calculating Pi

E.g., in a 4-process run, each process gets every 4th interval. Process 0 slices are in red.



- Simple program written in a data parallel style in MPI
 - E.g., for a reduction (recall "data parallelism" lecture), each process will first reduce (sum) its own values, then call a collective to combine them
- ° Estimates pi by approximating the area of the quadrant of a unit circle
- Each process gets 1/p of the intervals (mapped round robin, i.e., a cyclic mapping)

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Example: PI in C - 1/2

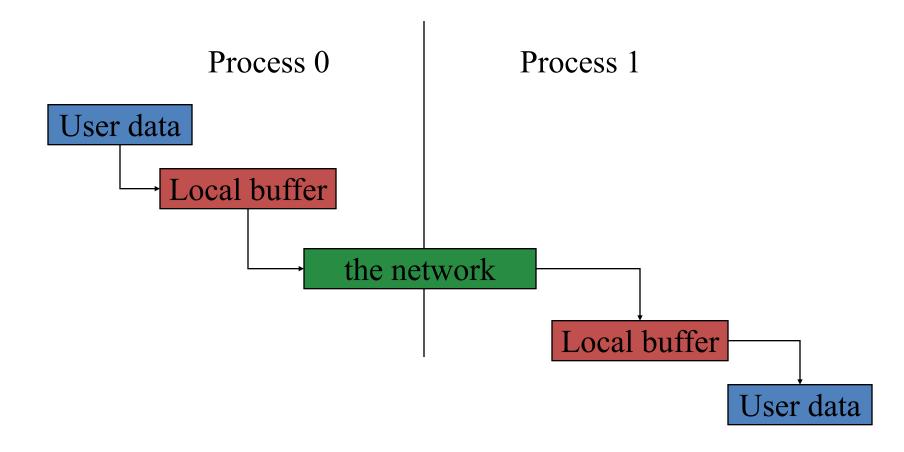
```
#include "mpi.h"
#include <math.h>
#include <stdio.h>
int main(int argc, char *argv[])
  int done = 0, n, myid, numprocs, i, rc;
  double PI25DT = 3.141592653589793238462643;
  double mypi, pi, h, sum, x, a;
  MPI Init(&argc,&argv);
  MPI Comm size(MPI COMM WORLD, &numprocs);
  MPI Comm rank (MPI COMM WORLD, &myid);
  while (!done) {
    if (myid == 0) {
      printf("Enter the number of intervals: (0 quits) ");
      scanf("%d",&n);
    MPI_Bcast(&n, 1, MPI INT, 0, MPI COMM WORLD);
    if (n == 0) break;
```

Example: PI in C - 2/2

```
h = 1.0 / (double) n;
  sum = 0.0;
  for (i = myid + 1; i \le n; i += numprocs) {
    x = h * ((double)i - 0.5);
    sum += 4.0 * sqrt(1.0 - x*x);
  mypi = h * sum;
  MPI Reduce (&mypi, &pi, 1, MPI DOUBLE, MPI SUM, 0,
             MPI COMM WORLD);
  if (myid == 0)
    printf("pi is approximately %.16f, Error is .16f\n",
            pi, fabs(pi - PI25DT));
MPI Finalize();
return 0;
```

Buffers

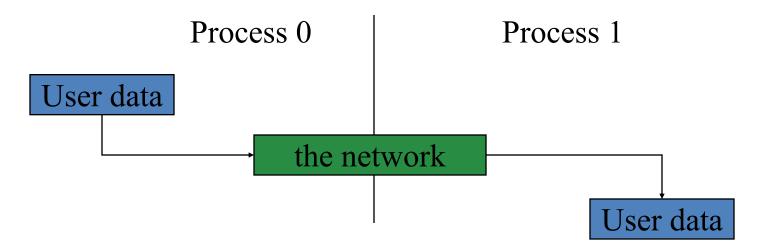
 $^\circ$ When you send data, where does it go? One possibility is:



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Avoiding Buffering

- Avoiding copies uses less memory
- ° May use more or less time



This requires that MPI_Send wait on delivery, or that MPI_Send return before transfer is complete, and we wait later.

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Blocking and Non-blocking Communication

- So far we have been using blocking communication:
 - MPI_Recv does not complete until the buffer is full (available for use).
 - MPI_Send does not complete until the buffer is empty (available for use).
- ° Completion depends on size of message and amount of system buffering.

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 is called "unsafe" because it depends on the availability of system buffers in which to store the data sent until it can be received

Some Solutions to the "unsafe" 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:

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

More Solutions to the "unsafe" Problem

Supply own space as buffer for send

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

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MPI's Non-blocking Operations

Non-blocking operations return (immediately) "request handles" that can be tested and waited on:

One can also test without waiting:

```
MPI Test(&request, &flag, &status);
```

Accessing the data buffer without waiting is undefined

Multiple Completions

It is sometimes desirable to wait on multiple requests:

```
MPI_Waitall(count, array_of_requests,
    array_of_statuses)

MPI_Waitany(count, array_of_requests,
    &index, &status)

MPI_Waitsome(count, array_of_requests,
    array of indices, array of statuses)
```

There are corresponding versions of test for each of these.

Communication Modes

- MPI provides multiple modes for sending messages:
 - Synchronous mode (MPI_Ssend): the send does not complete until a matching receive has begun. (Unsafe programs deadlock.)
 - Buffered mode (MPI_Bsend): the user supplies a buffer to the system for its use. (User allocates enough memory to make an unsafe program safe.
 - Ready mode (MPI_Rsend): user guarantees that a matching receive has been posted.
 - Allows access to fast protocols
 - undefined behavior if matching receive not posted
- Non-blocking versions (MPI_Issend, etc.)
- MPI_Recv receives messages sent in any mode.
- See <u>www.mpi-forum.org</u> for summary of all flavors of send/receive