CS 267
Lecture 9: Distributed Memory Machines and Programming

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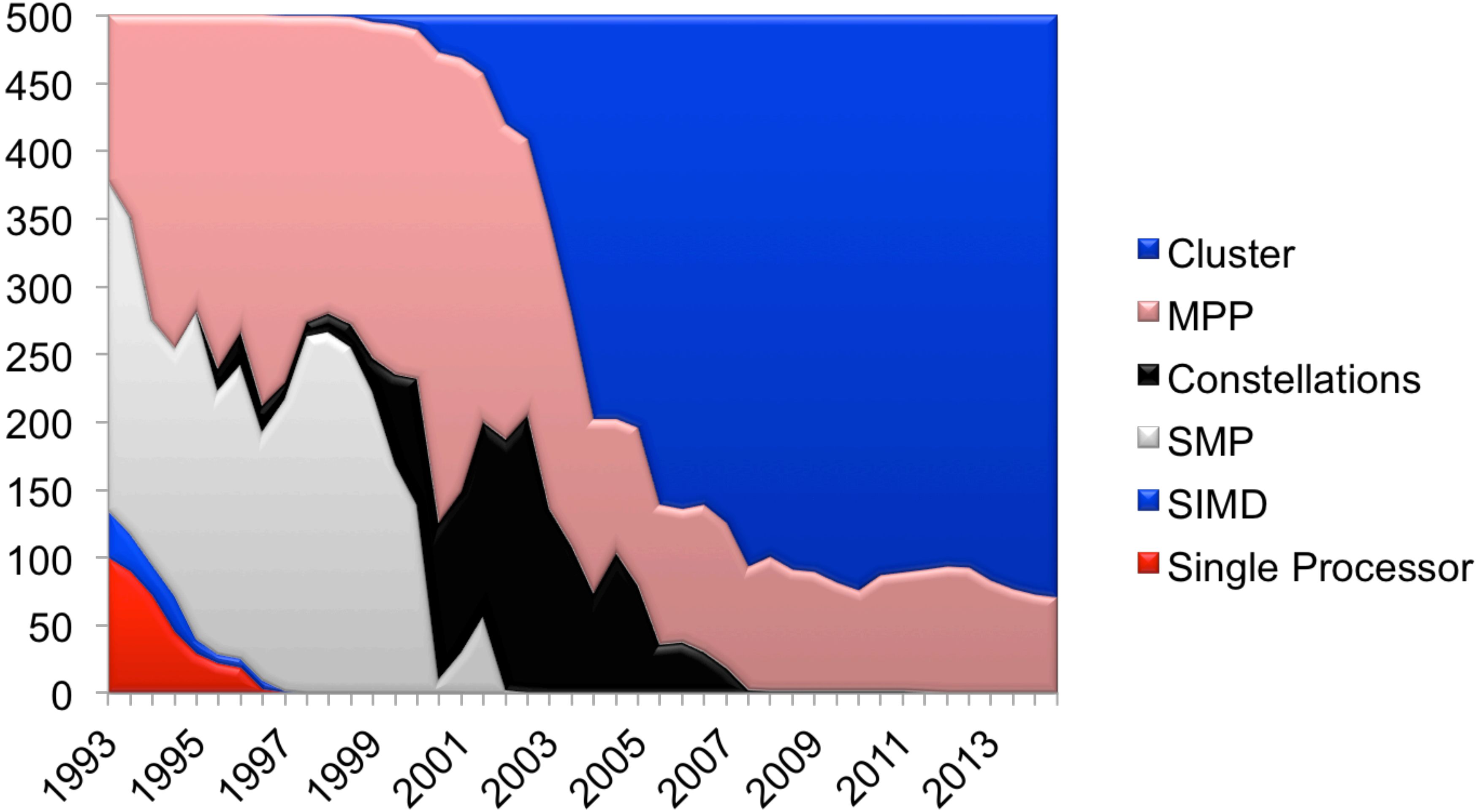
https://sites.google.com/lbl.gov/cs267-spr2018/

Outline

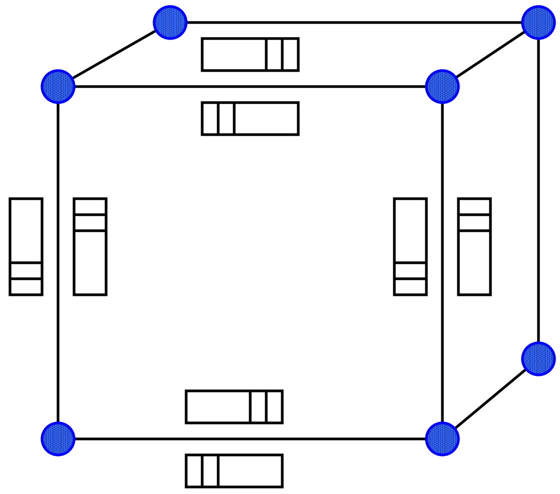
- Distributed Memory Architectures
  - Properties of communication networks
  - Topologies
  - Performance models
- Programming Distributed Memory Machines using Message Passing
  - Overview of MPI
  - Basic send/receive use
  - Non-blocking communication
  - Collectives

Architectures in Top 500, Nov 2014



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

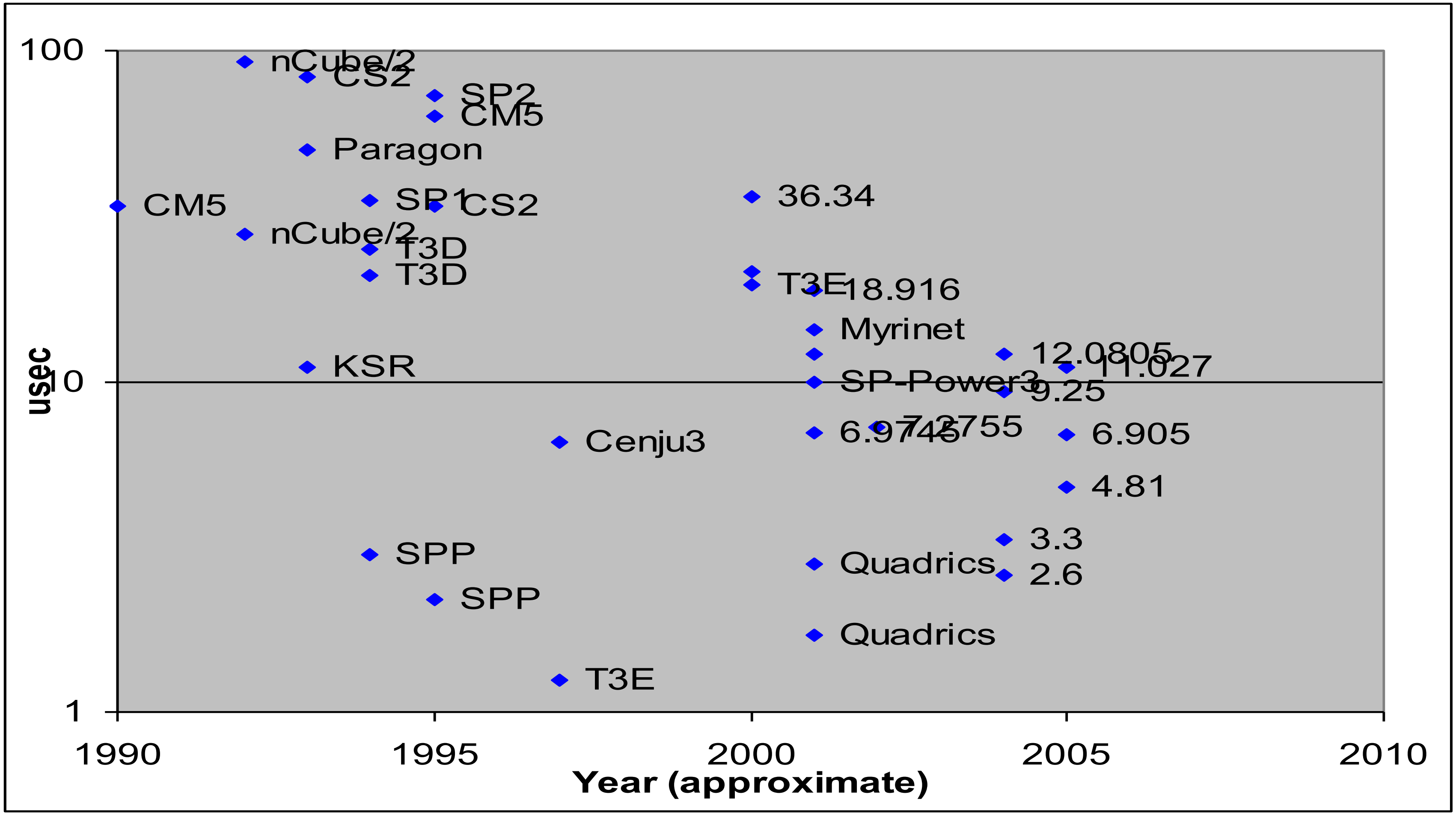
Design Characteristics of a Network

- **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

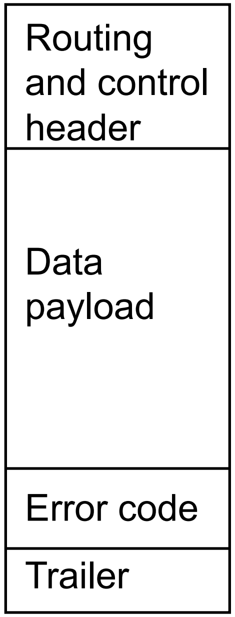


- Latency has not improved significantly, unlike Moore's Law
    - T3E (shmem) was lowest point – in 1997

Data from Kathy Yelick

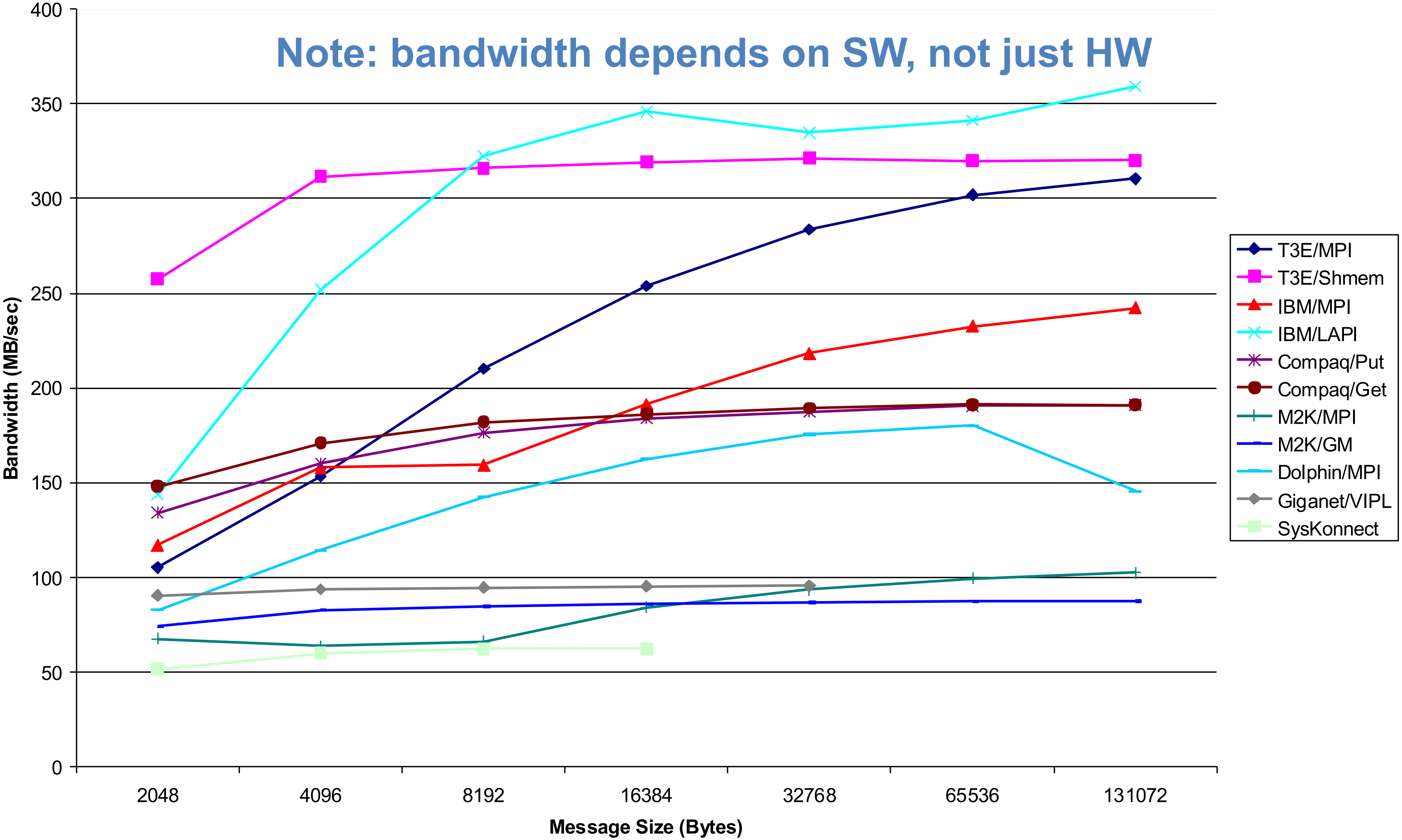
Performance Properties of a Network: Bandwidth

- The bandwidth of a link = # wires / time-per-bit
- Bandwidth typically in Gigabytes/sec (GB/s), i.e., $8 * 2^{20}$ 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

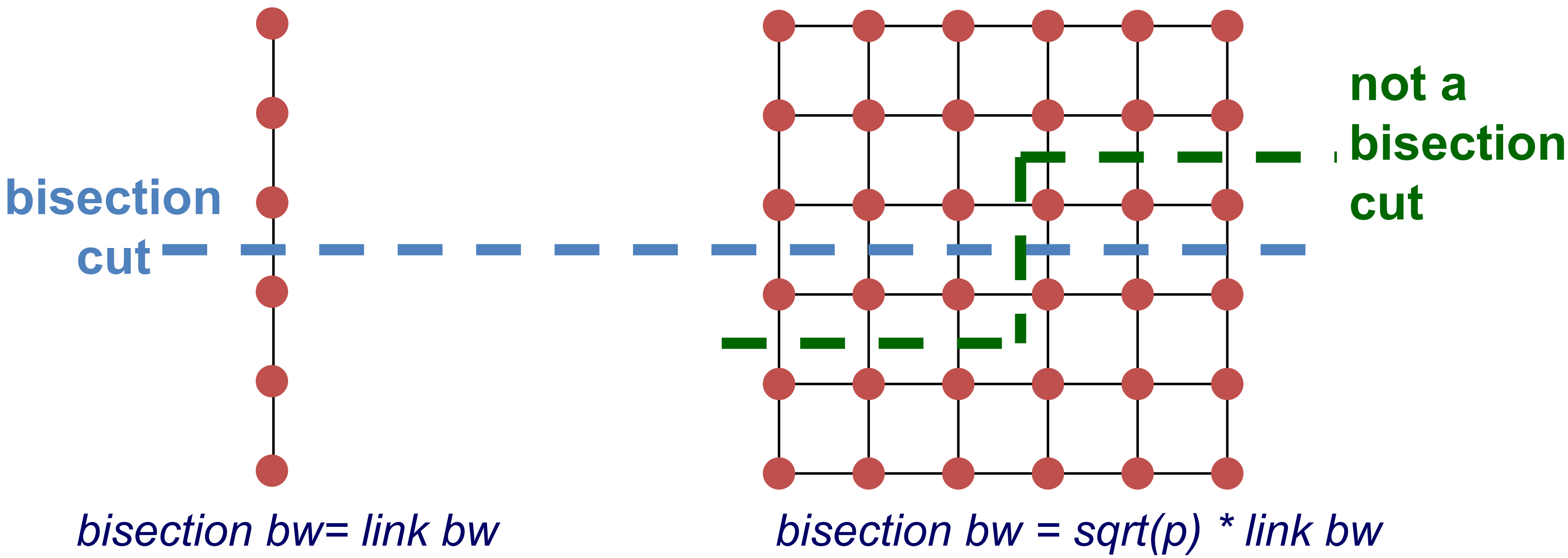
Bandwidth Chart



Data from Mike Welcome, NERSC

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

Network Topology

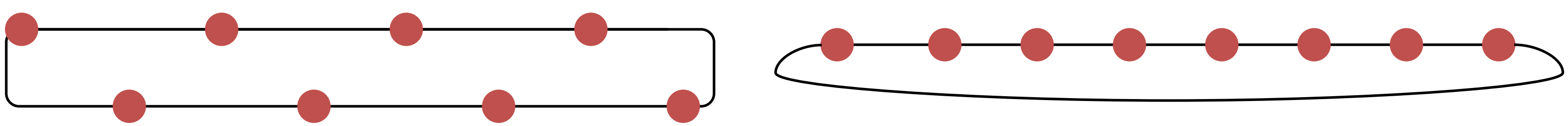
- In the past, there was considerable research in network topology and in mapping algorithms to topology.
  - Key cost to be minimized: number of "hops" between nodes (e.g. "store and forward")
  - Modern networks hide hop cost (i.e., "wormhole routing"), so topology less of a factor in performance of many algorithms
- Example: On IBM SP system, hardware latency varies from 0.5 usec to 1.5 usec, but user-level message passing latency is roughly 36 usec.
- Need some background in network topology
  - Algorithms may have a communication topology
  - Example later of big performance impact

Linear and Ring Topologies

- Linear array

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

- Torus or Ring

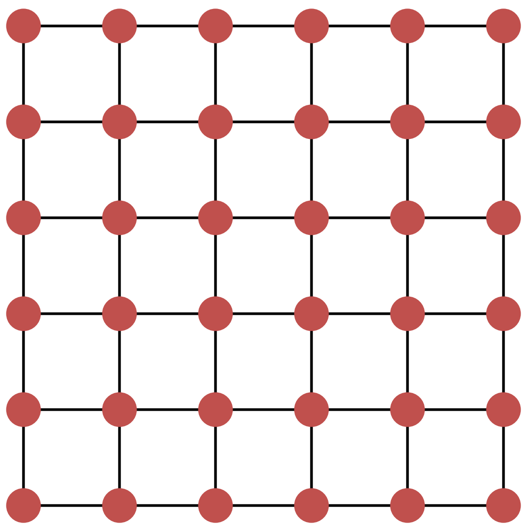


  - Diameter = n/2; average distance ~ n/4.
  - Bisection bandwidth = 2.
  - Natural for algorithms that work with 1D arrays.

Meshes and Tori – used in Hopper

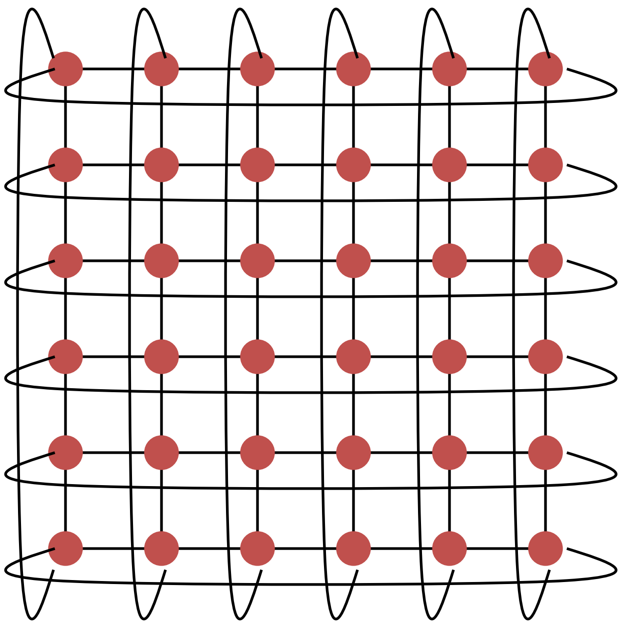
Two dimensional mesh

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



Two dimensional torus

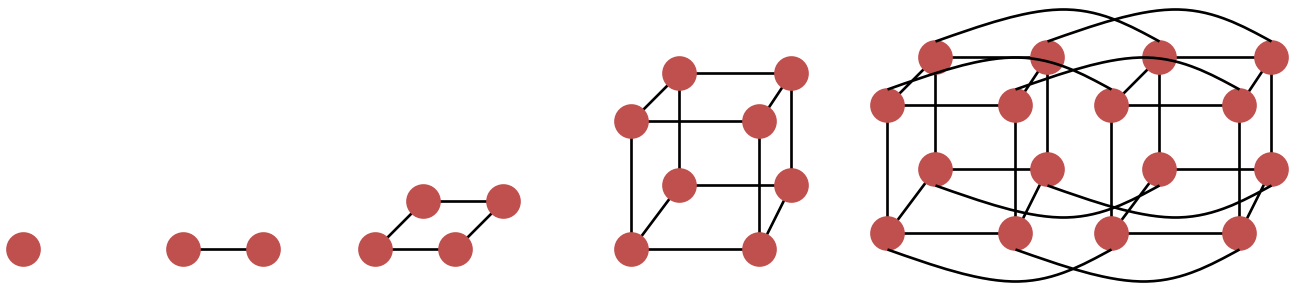
- Diameter = sqrt(n)
- Bisection bandwidth = 2* sqrt(n)



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

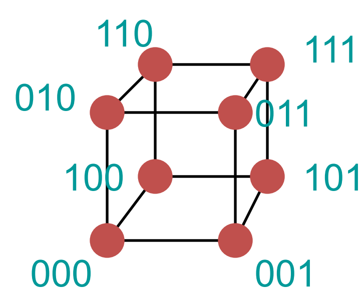
Hypercubes

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



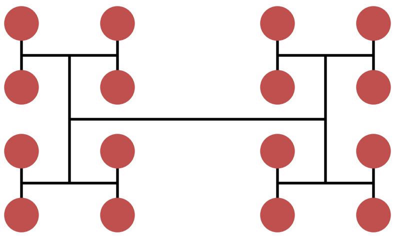
0d 1d 2d 3d 4d

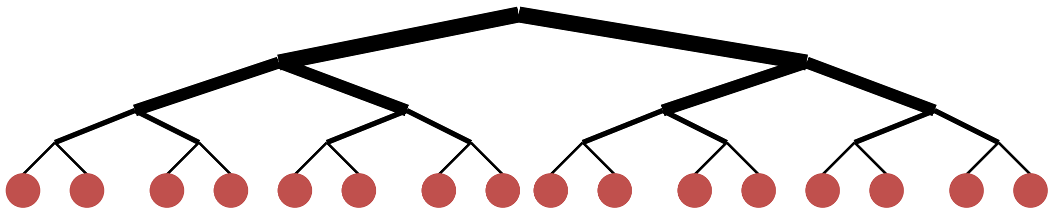
- Popular in early machines (Intel iPSC, NCUBE).
  - Lots of clever algorithms.
  - See 1996 online CS267 notes.
- Greycode addressing:
  - Each node connected to d others with 1 bit different.

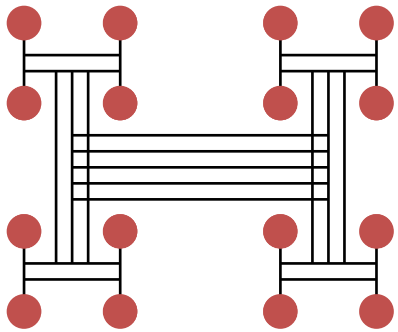


Trees

- 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.



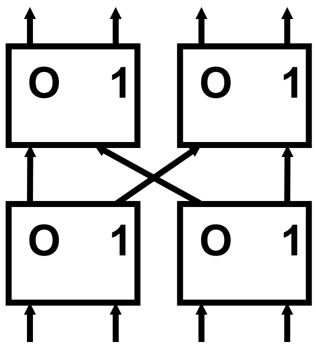




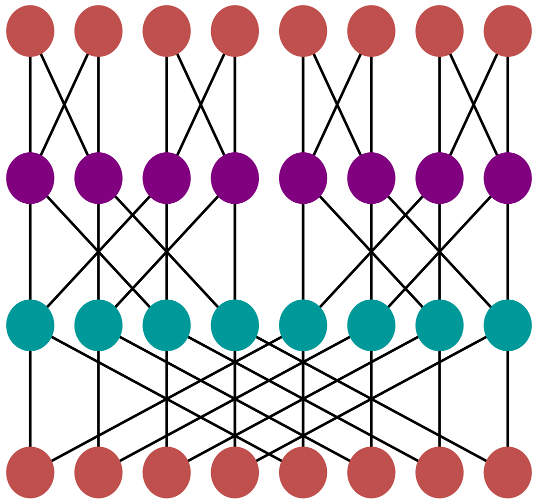
Butterflies

- Diameter = log n.
- Bisection bandwidth = n.
- Cost: lots of wires.
- Used in BBN Butterfly.
- Natural for FFT.

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

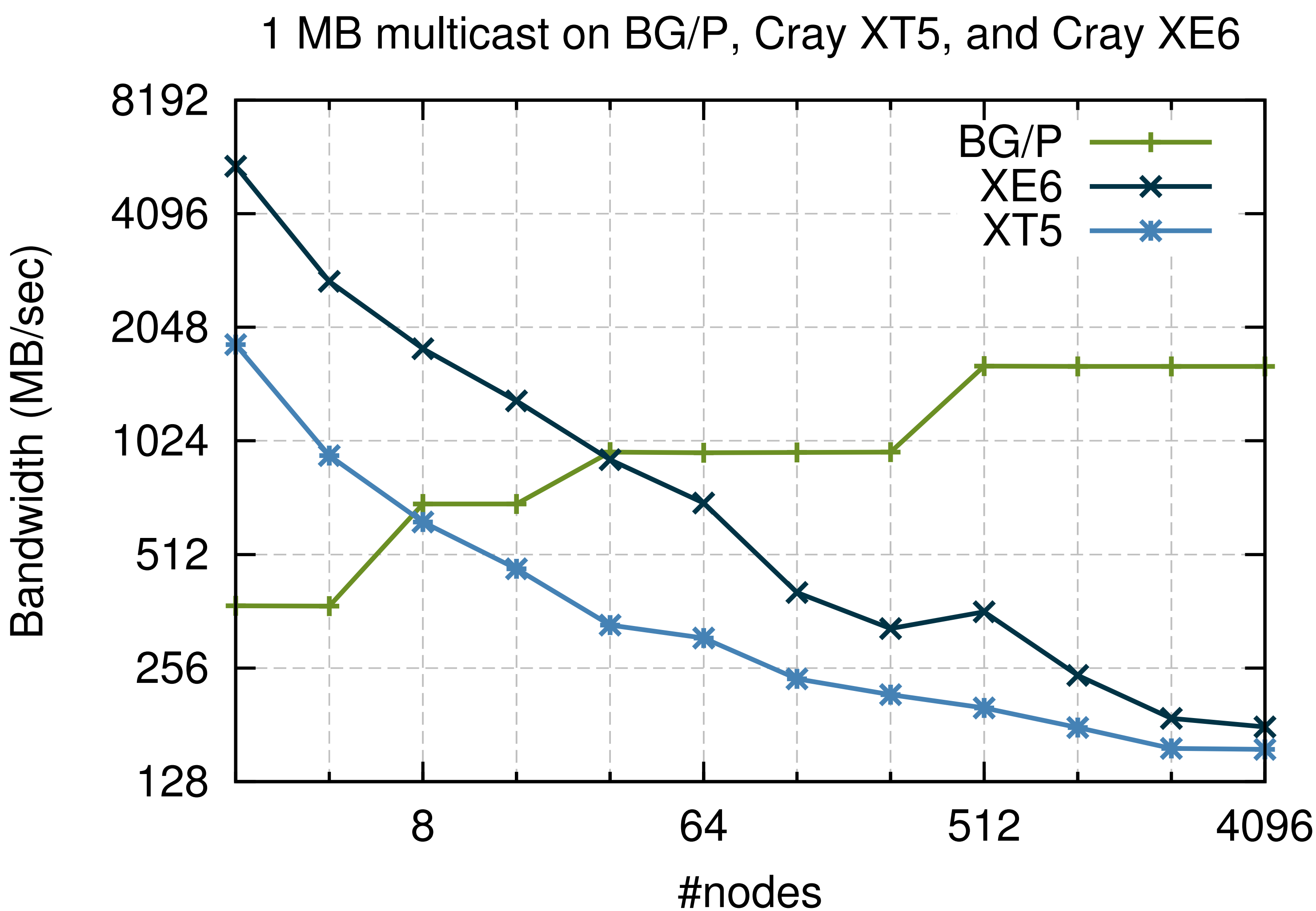


butterfly switch



multistage butterfly network

Does Topology Matter?



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

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 more expensive but higher bandwidth when long
- Electrical 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.

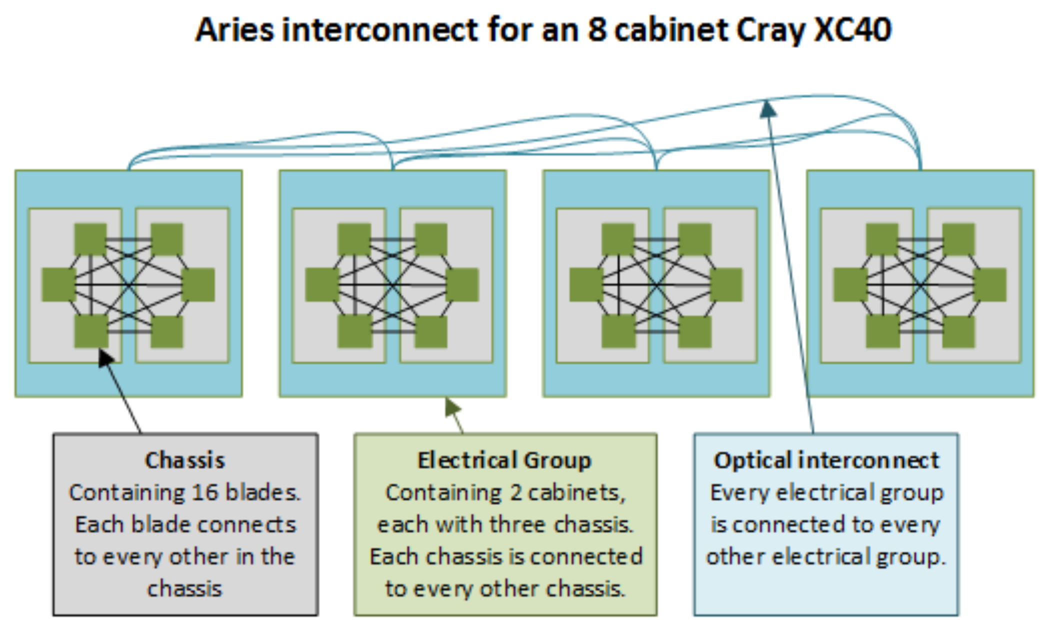
° **Uses a randomized routing algorithm**

° **Outcome:** programmer can (usually) ignore topology, get good performance

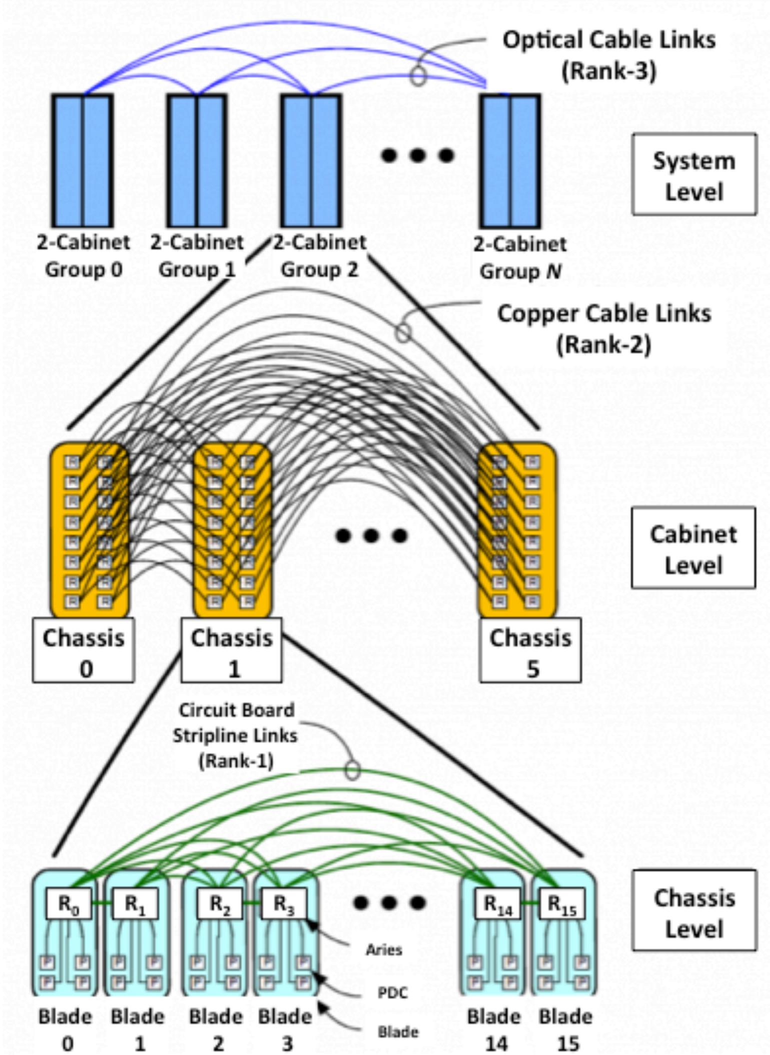
- Important in virtualized, dynamic environment
- Drawback: variable performance

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

Dragonfly in practice



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/

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

$$\text{Time} = \text{latency} + n*\text{cost\_per\_word}$$
$$= \text{latency} + n/\text{bandwidth}$$

- Topology is assumed irrelevant.
- Often called "$\alpha-\beta$ model" and written

$$\text{Time} = \alpha + n*\beta$$

- 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.

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

- 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

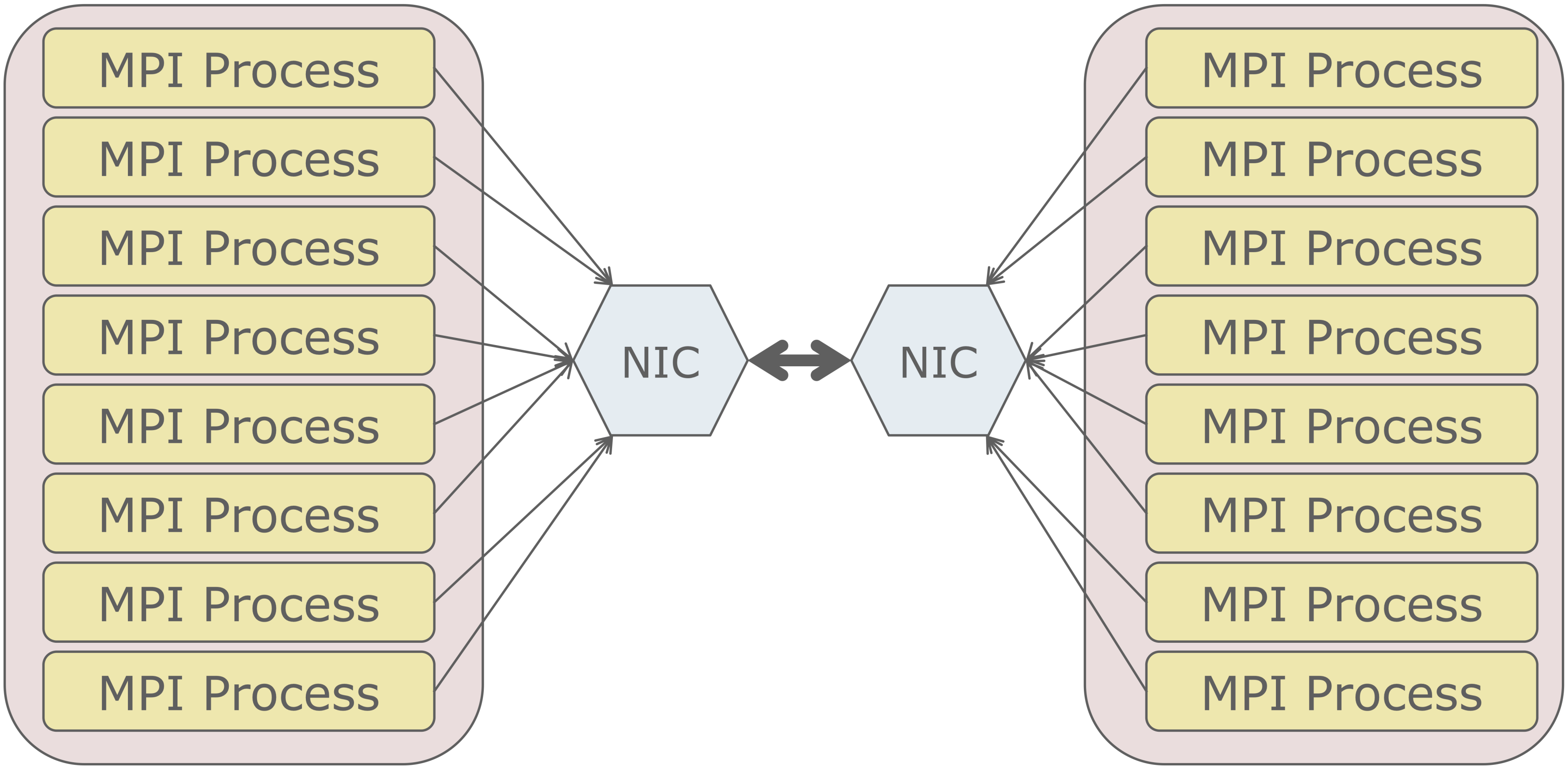
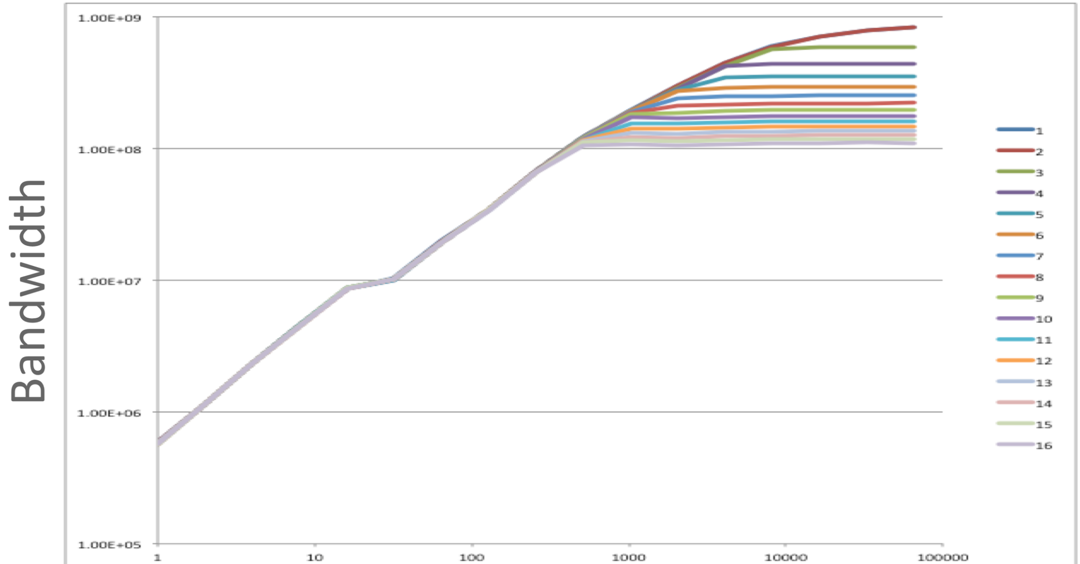
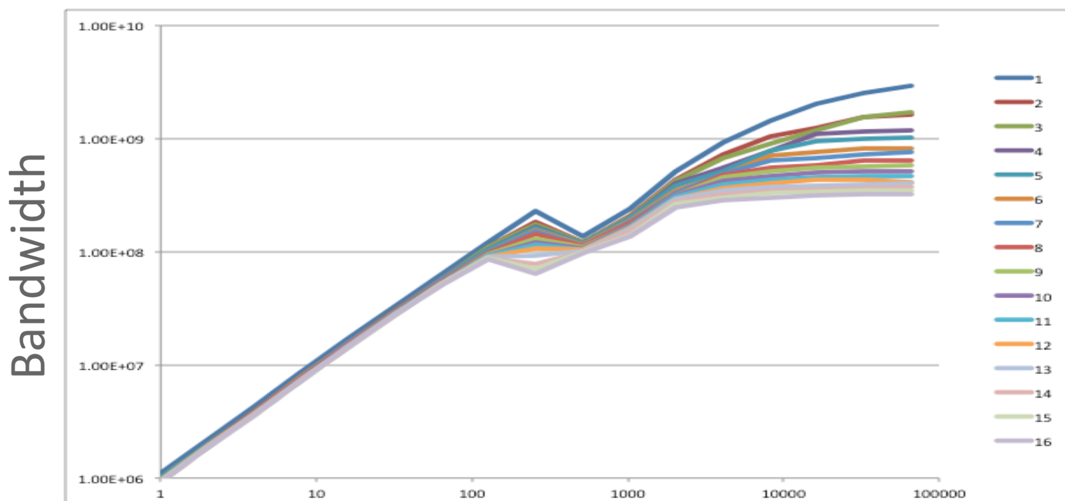


Figure source: Balaji, Gropp, Thakur

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

Figure source: Balaji, Gropp, Thakur

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**
- **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

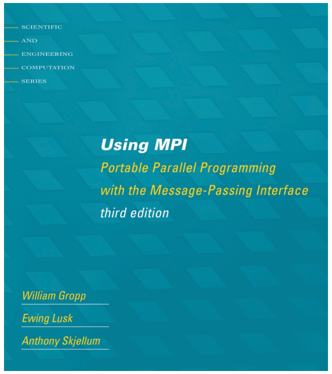
- Communicators encapsulate communication spaces for library safety
- Datatypes reduce copying costs and permit heterogeneity
- Multiple communication modes allow precise buffer management
- Extensive collective operations for scalable global communication
- Process topologies permit efficient process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

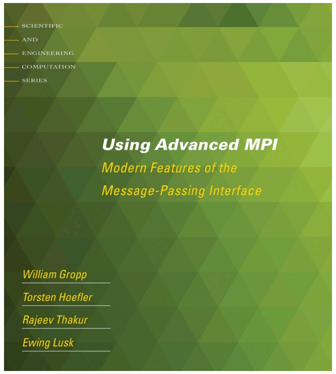
MPI References

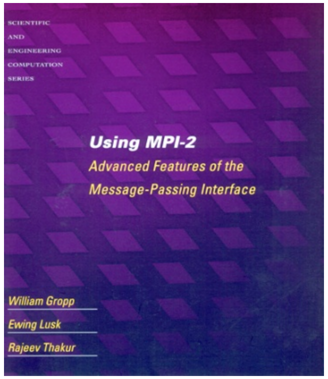
- **The Standard itself:**
  - at http://www.mpi-forum.org
  - All MPI official releases, in both postscript and HTML
  - Latest version MPI 3.1, released June 2015
- **Other information on Web:**
  - at http://www.mcs.anl.gov/research/projects/mpi/index.htm
  - pointers to lots of stuff, including other 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.
- ***MPI: The Complete Reference - Vol 1 The MPI Core*,** by Snir, 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)

```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;
}
```

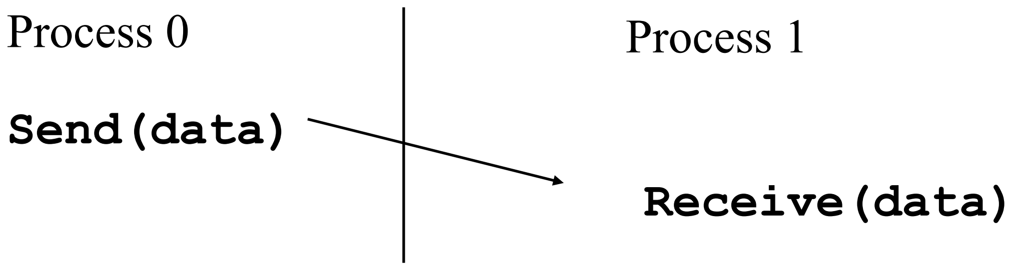
Notes on Hello World

- 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
```

MPI Basic Send/Receive

- 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 context, and must be received in the same context
  - Provides necessary support for libraries
- A group and context together form a communicator
- A process is identified by its rank in the group associated with a communicator
- There is a default communicator whose group contains all initial processes, called `MPI_COMM_WORLD`

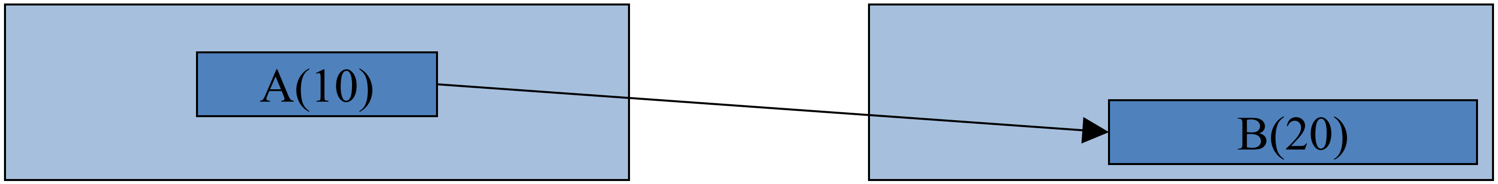
MPI Datatypes

- 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 user-defined 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



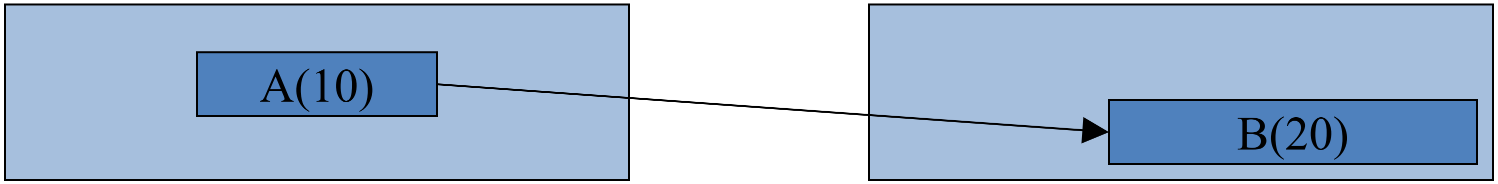
MPI_Send(A, 10, MPI_DOUBLE, 1, …)

MPI_Recv(B, 20, MPI_DOUBLE, 0, …)

`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_Send(A, 10, MPI_DOUBLE, 1, …)

MPI_Recv(B, 20, MPI_DOUBLE, 0, …)

`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)**

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;
}
```

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 );
```

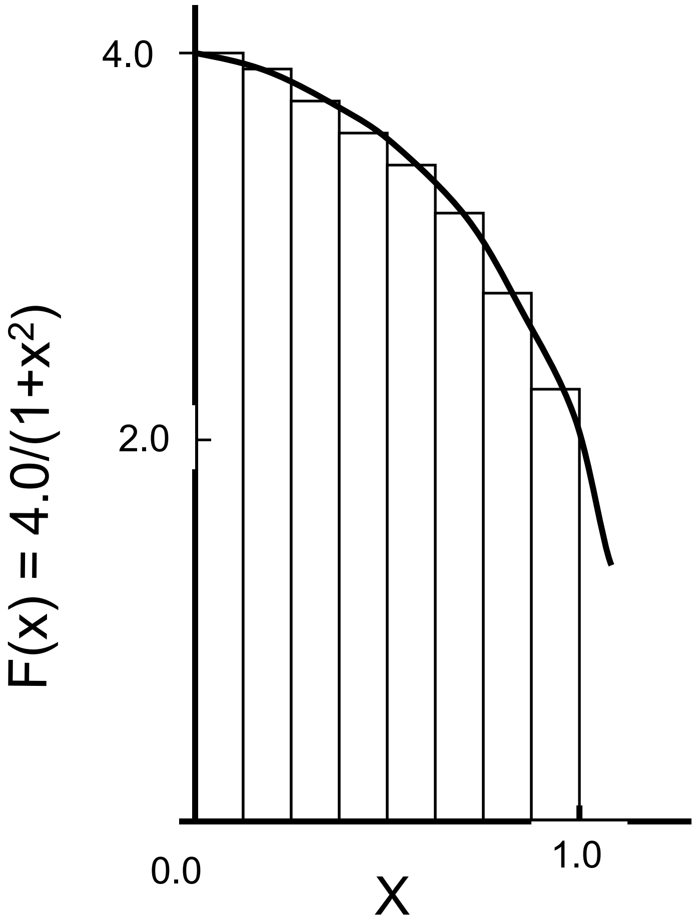
MPI can be simple

- **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**

PI redux: Numerical integration



Mathematically, we know that:

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

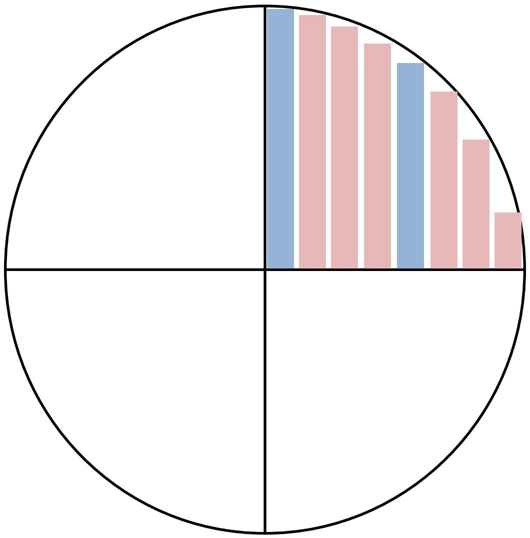
We can approximate the integral as a sum of rectangles:

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

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

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 "tricks with trees" 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)

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 <= 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;

}
```