Computing & Information Science 4205

Effective Use of High Performance Computing

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www.cac.cornell.edu/~slantz

Course Overview

Goals for CIS 4205

- Introduction to HPC – Practical experience for your research
- Finding the parallelism in your work
- Measuring speedup & efficiency and the factors that affect it
- Writing & debugging parallel code (MPI & OpenMP)
- Exposure to using production HPC systems at Cornell
- Effective techniques for inherently (“embarrassingly”) parallel codes
- Critical analysis of current & future HPC solutions

A Little About Me

- **Role at the Cornell Center for Advanced Computing**
  - Senior Research Associate: consulting, training, advising, & participating
  - Involved in HPC around 25 years
- **Background**
  - Education
  - Experience
- **Research interests**
  - Numerical modeling and simulation
  - Fluid and plasma dynamics
  - Parallel computing

A Little About You*

- **Fields of study and/or research interests**
- **Programming experience**
  – C, C++, Fortran, Others…
  – Scripting languages
- **Practical experiences**
  – Ever written a program from scratch for your research?
  – Ever had to work with someone else's code?
  – Which was harder? Why?
- **HPC experience**
- **Your goals for this course**

*** - ("A Little Bit Me, A Little Bit You" – Monkees, 1967)**

Assignments

- **Check the course website before every class**
  - http://www.cac.cornell.edu/~slantz/CIS4205
- **Assignments are due on date specified**
- **Assignments should be emailed to me**
  - slantz@cac.cornell.edu
- **Assignments can be done on any HPC system**
  - Windows, Linux, Macintosh OS X
  - HPC system must have MPI, OpenMP & batch scheduling system
- **Access to CAC HPC systems is available**

Connecting to CAC Resources

- **All students' Cornell NetIDs will be added the course account**
  - Everyone will have the option to use CAC resources for assignments
- **Accessing CAC machines**
  - http://www.cac.cornell.edu/Documentation/Linux.asx
  - http://www.cac.cornell.edu/Documentation/Linux
- **Poll: what's your background?**
  - Familiar with Linux?
  - Familiar with ssh and X Windows?
  - Comfortable with text editors (emacs, vi)?

Where and How to Find Me

- **Physical and and virtual whereabouts**
  - Office: 533 Frank H. T. Rhodes Hall
  - Phone: 4-8887
  - Email: slantz@cac.cornell.edu

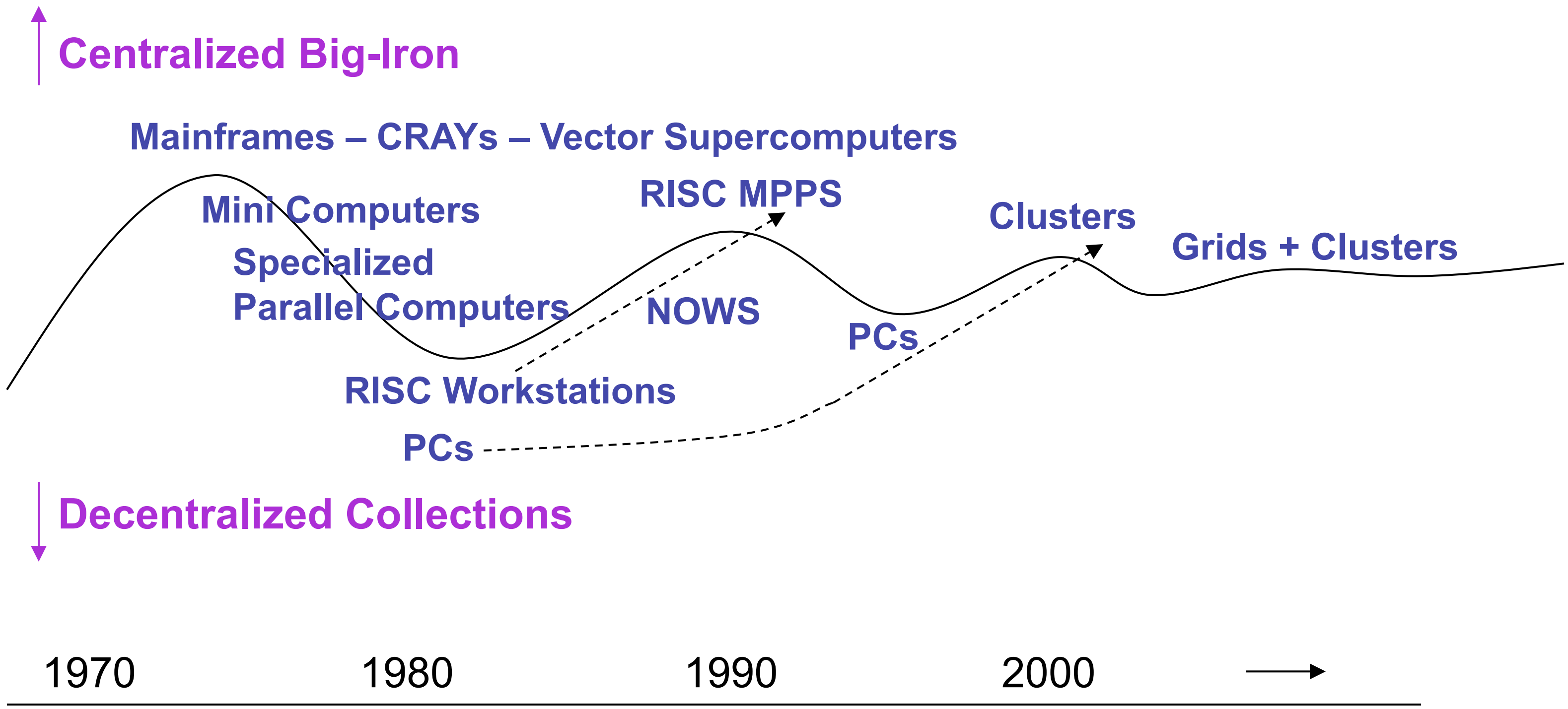
- **Office hours by appointment**

Introduction to High Performance Computing

Why HPC? Why Parallel Computing?

- **Want to have best possible time-to-solution, minimize waiting**
- **Want to gain a competitive advantage**
- **As expected, processor clock speeds have flattened out**
  - Not the end of Moore's law: transistor densities are still doubling every 1.5 years
  - Clock speeds limited by power consumption, heat dissipation, current leakage
  - Bad news for mobile computers!
- **Parallelism will be the path toward future performance gains**
  - Trend is toward multi-core: put a cluster on a chip (in a laptop)
  - Goes well beyond microarchitectures that have multiple functional units

Evolution of HPC



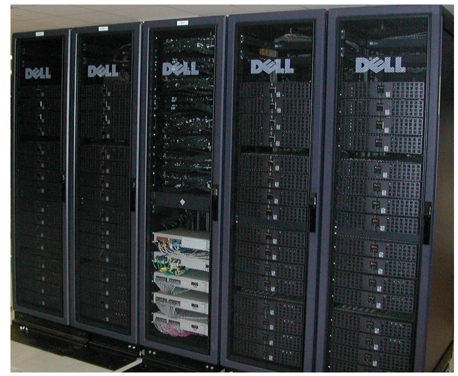
The Cornell Programmer's View

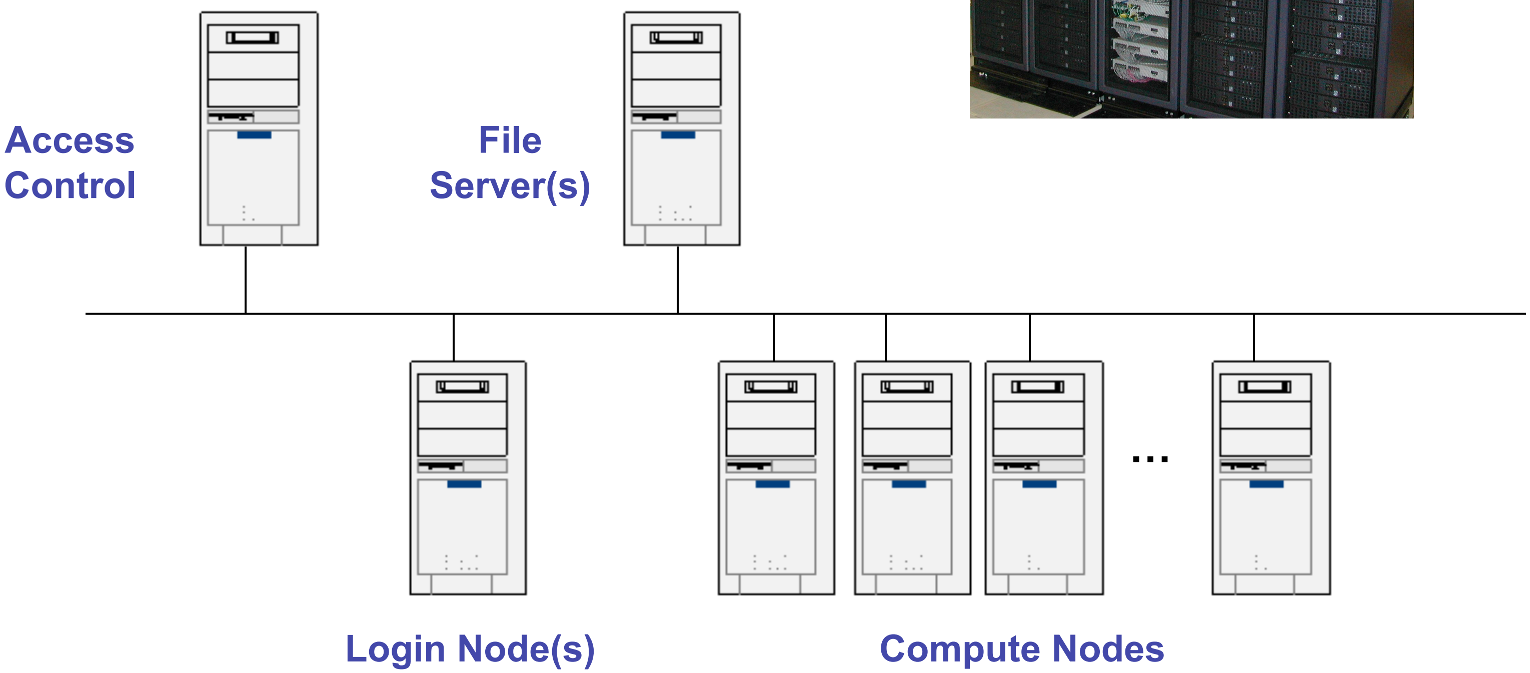
Timeframe *– hardware – parallel programming model*

- **Mid '80's** – IBM mainframe with attached Floating Point Systems array processors – IBM and FPS compiler extensions
- **Late '80's** – Interconnected IBM 3090 mainframes featuring internal vector processors – Parallel VS FORTRAN and APF compilers
- **Early '90's** – IBM SP1, rack-mounted RS6000 workstations with POWER RISC processors networked via multistage crossbar switch; KSR-1 from Kendall Square Research – PVM, MPL, MPI message passing libraries; HPF/KAP directives; KSR compiler for ALLCACHE "virtual shared memory"
- **Mid '90's** – IBM SP2 featuring POWER2 and P2SC – MPI (not a compiler)
- **Late '90's to present** – Several generations of Dell HPC clusters (Velocity 1, 1+, 2, 3), quad or dual Intel Pentiums running Windows, Red Hat Linux – MPI plus OpenMP compiler directives for multithreading

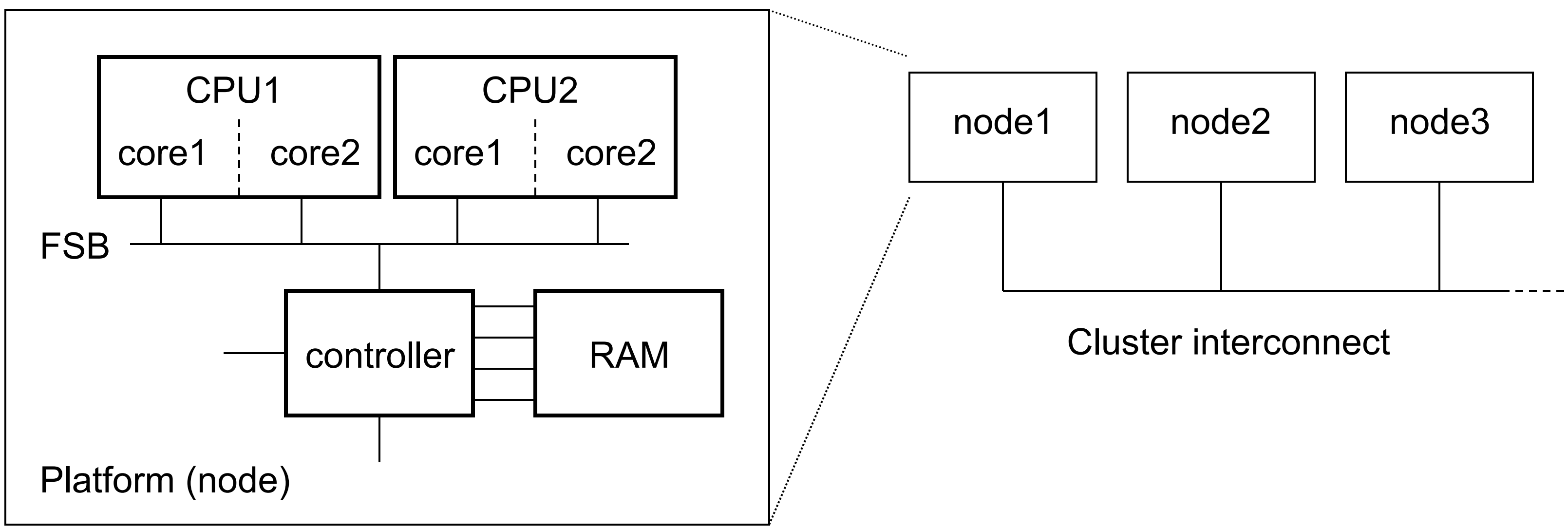
Current HPC Platforms: COTS-Based Clusters

COTS = Commercial off-the-shelf





Shared and Distributed Memory

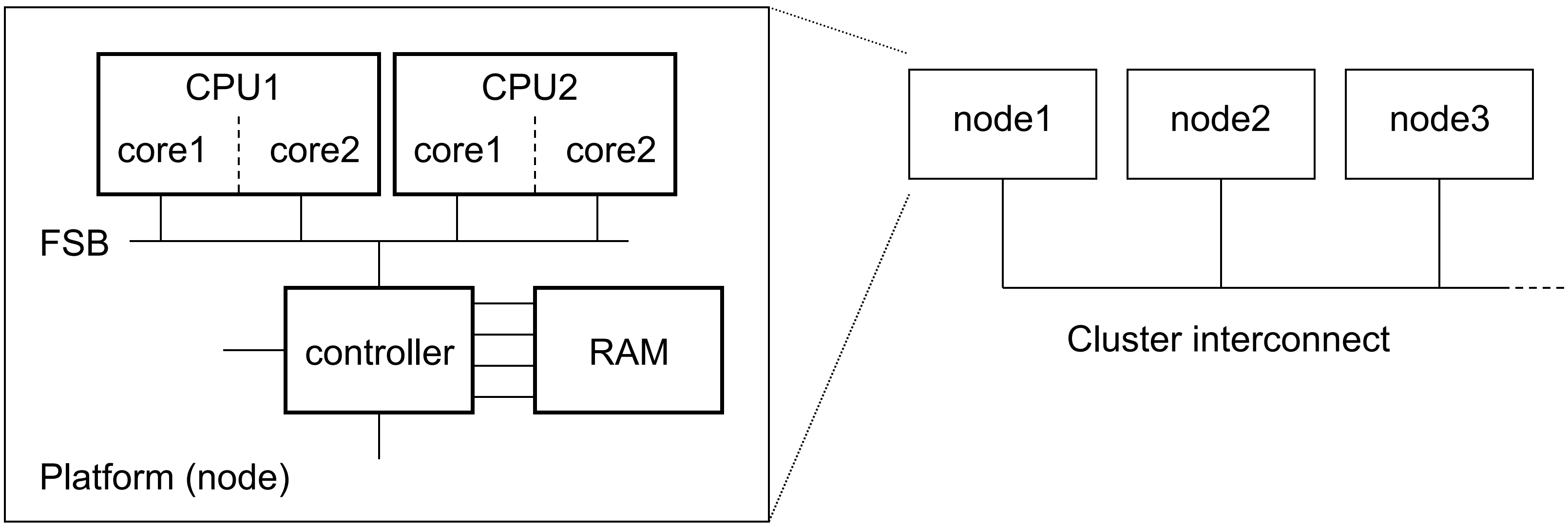


Shared memory on each node…

Distributed memory across cluster

Multi-core CPUs in clusters – two types of parallelism to consider

Shared and Distributed Memory



Shared memory on each node…

OpenMP
Pthreads
MPI

Distributed memory across cluster

MPI

OpenMP and MPI? In 2009?

Strengths:

- Adherence to carefully defined specifications (not standards per se)
- Specifications still under active development
- Cross-platform, multi-OS, multi-language (e.g., pypar in Python)
- Wide acceptance
- Time-tested with large existing code base
- Useful for both data and task (functional) parallelism

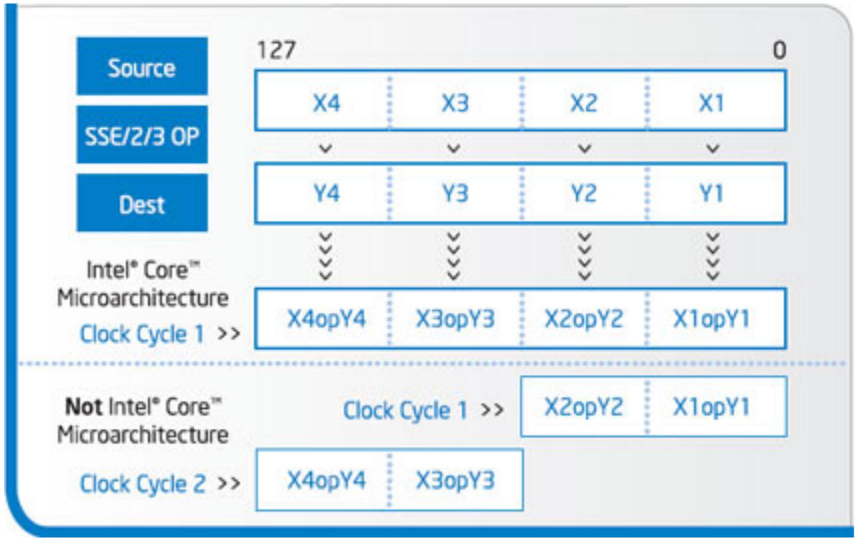
Weaknesses:

- Relatively low-level programming (though not as low as pthreads)
- Mindset taken from procedural languages (C, Fortran)

Where's My Parallel Compiler?

- **You've had it for years! "Serial" compilers produce code that takes advantage of parallelism at the *top* of the memory hierarchy**

Example: SSE(2/3/4) instructions operate on several floats or doubles simultaneously using special 128-bit-wide registers in Intel Xeons (vector processing)

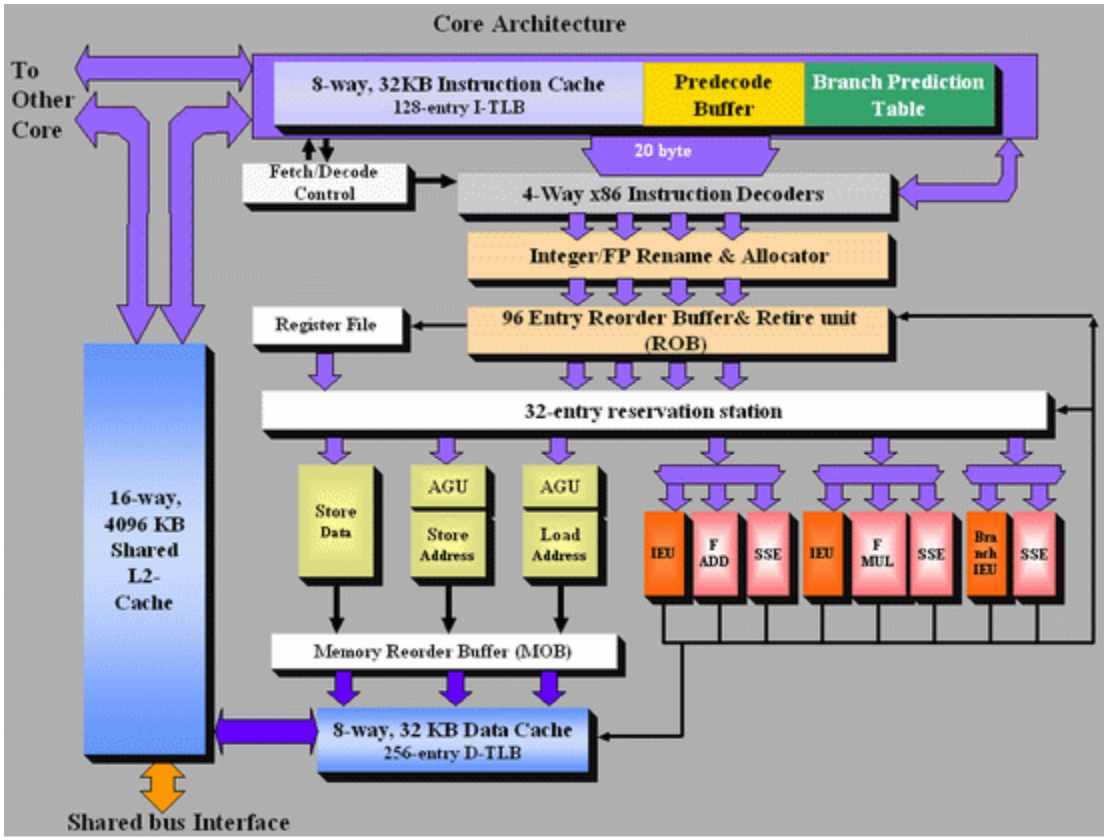


http://www.tomshardware.com/2006/06/26/xeon_woodcrest_preys_on_opteron/page9.html

Parallelism Inside the Intel Core

In the Intel Core microarchitecture:

- **4 instructions per cycle**
- Branch prediction
- Out-of-order execution
- 5 prefetchers
- 4MB L2 cache
- 3 128-bit SSE registers
- 1 SSE / cycle

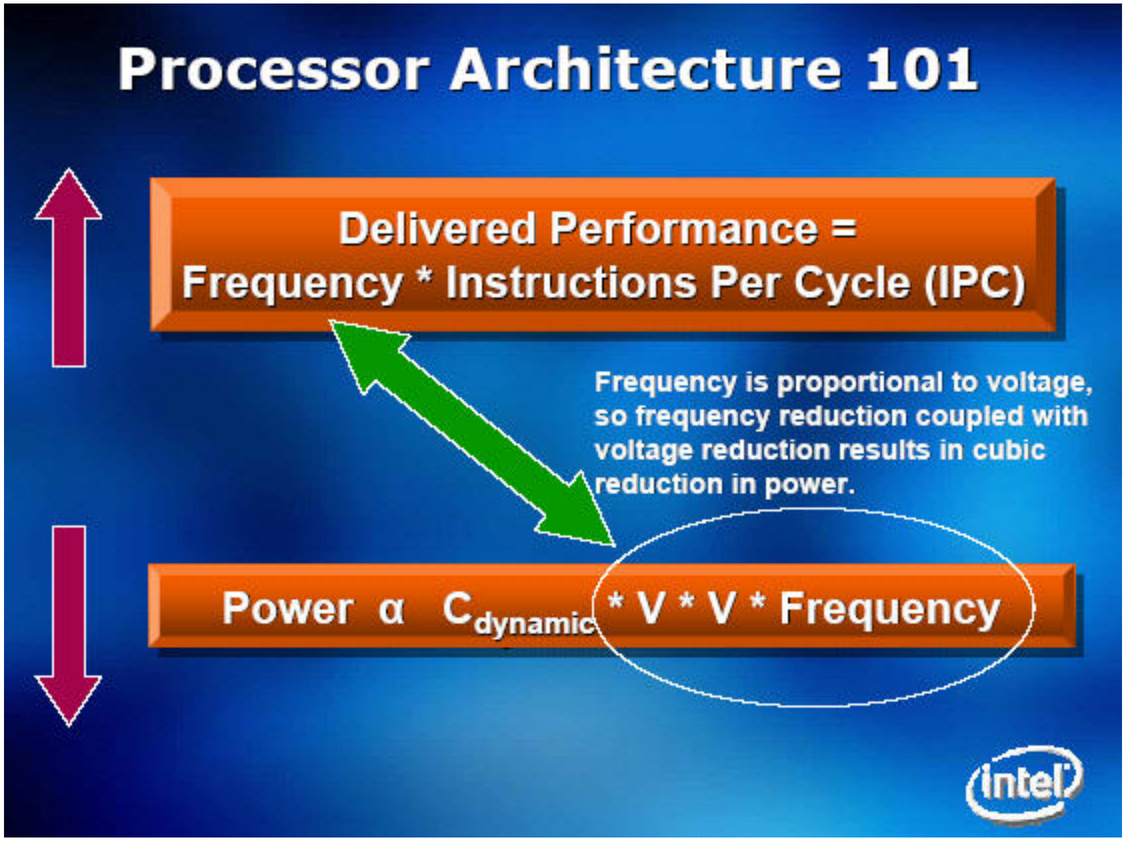


http://www.anandtech.com/cpuchipsets/showdoc.aspx?i=2748&p=4

Why Not Crank Up the Clock?

Because the CPU's power consumption goes up like the cube of frequency!

No wonder Intel tries so hard to boost the IPC…



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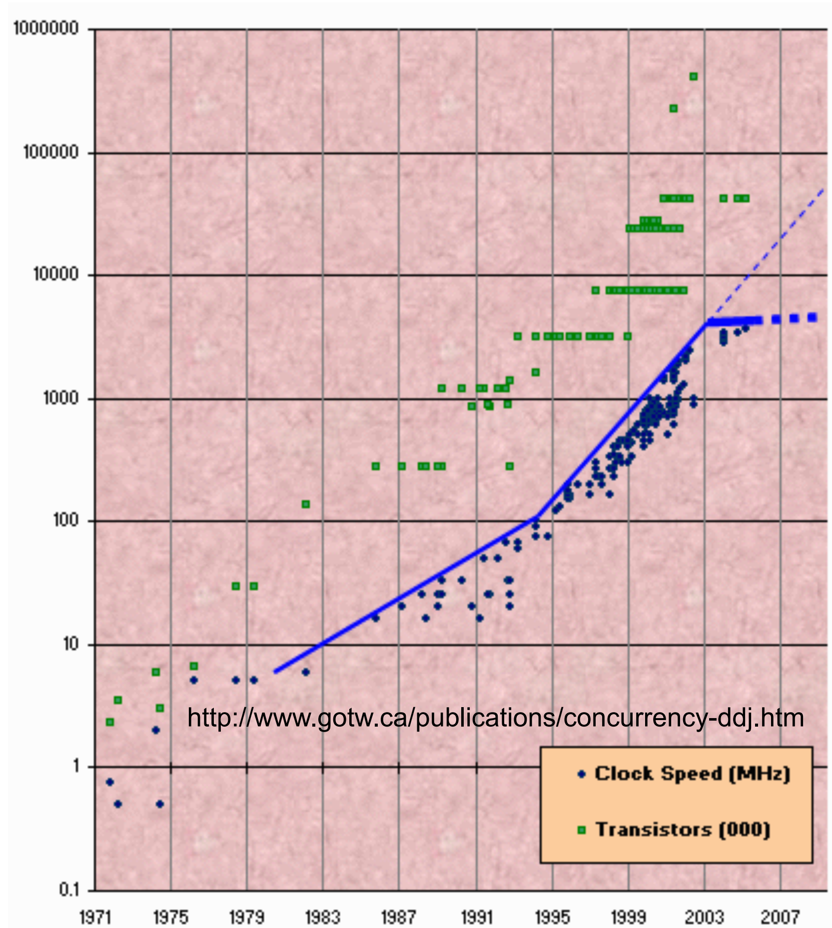
OK, What's Next?

Trend toward growing numbers of cores per processor die

- **Moore's Law still holds; transistor densities are still increasing**
- **Higher densities don't translate into faster speeds due to:**
  - Problems with heat dissipation
  - Hefty power requirements
  - Leakage current
- **The "free lunch" of ever-increasing clock speeds is *over!***



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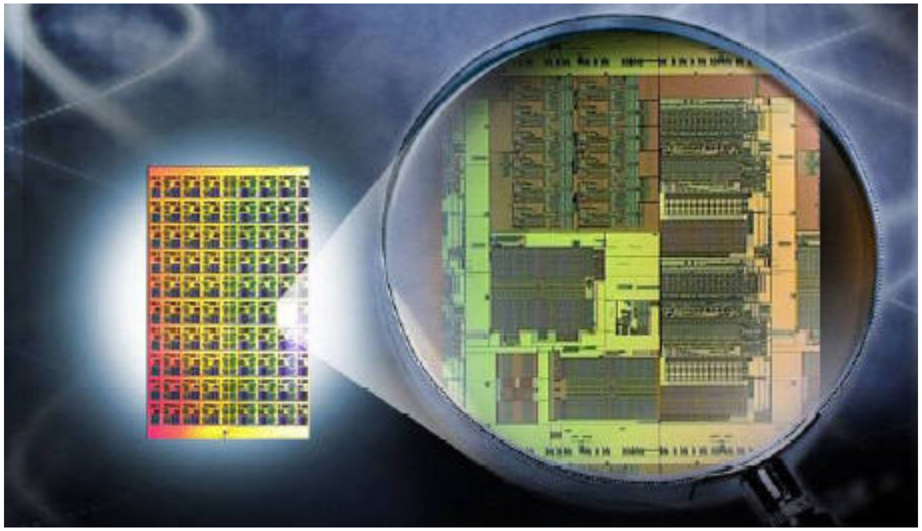
Signs of the Times…

- **IBM promotes BlueGene HPC line with 1000's of low-frequency, low-power chips (700 MHz PowerPCs)**
- **On 2/11/07, Intel announces successful tests of an 80-core research processor – "teraflops on a chip"**



Implications for Programmers

- **Concurrency will no longer be just desirable, it will be essential**
  - Previously it was the economical path to greater performance
  - Now it has become the physically reasonable path
- **Compilers (still) aren't the answer**
  - Degree of concurrency depends on algorithm choices
  - Need for high-level creation (as opposed to mere identification) of concurrent code sections
- **Improved programming languages could make life easier, but nothing has caught on yet**
- **Some newer languages (Java, C++) do have mechanisms for concurrency built in… but kind of clumsy to use…**
- **In the final analysis: TANSTAAFL**

Conclusions

- **Future processor technology will drive programmers to *create* and *exploit* concurrency in their software to get performance**
- **Some problems are inherently not parallelizable; what then?**
  - “9 women can't produce a baby in one month”
  - …But… what if the goal isn't just to produce one baby, but many?
  - “Embarrassing parallelism” isn’t so embarrassing any more
  - Examples: optimization of a design; high-level Monte Carlo simulation
- **Coding for efficiency and performance optimization will get more, not less, important**
  - Not all performance gains need to come from high-level parallelism
  - Nevertheless, parallelism needs to be designed into codes, preferably from the beginning

Parallel Computing: Types of Parallelism

Parallel Computing: Definitions

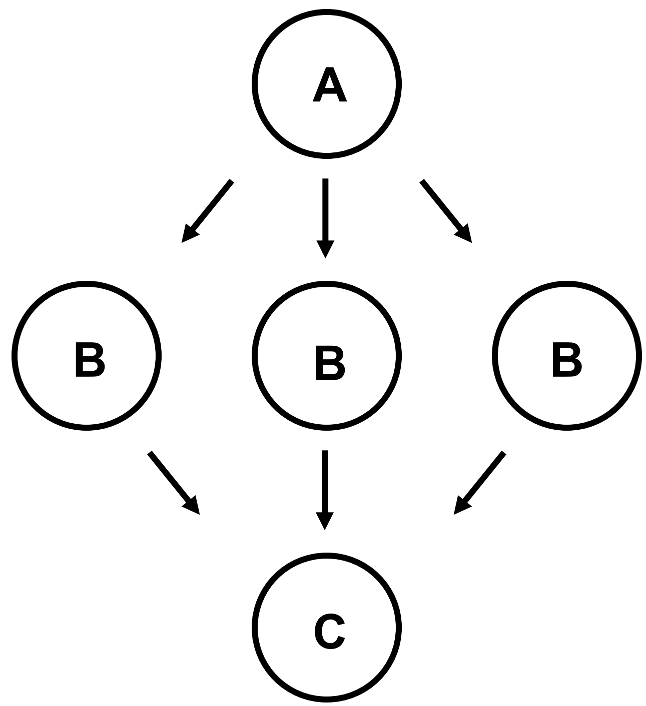
- **As we have seen, HPC necessarily relies on parallel computing**
- ***Parallel computing…***
  - Involves the use of multiple processors simultaneously to reduce the time needed to solve a single computational problem.
- **Examples of fields where this is important:**
  - Climate modeling, weather forecasting
  - Aircraft and ship design
  - Cosmology, simulations of the evolution of stars and galaxies
  - Molecular dynamics and electronic (quantum) structure
- ***Parallel programming…***
  - Is writing code in a language (plus extensions) that allows you to explicitly indicate how different portions of the computation may be executed concurrently
- **Therefore, the first step in parallel programming is to identify the parallelism in the way your problem is being solved (algorithm)**

Data Parallelism

Definition: when independent tasks can apply the same operation to different elements of the data set at the same time.

Examples:

- 2 brothers mow the lawn
- 8 farmers paint a barn



Data Parallelism

Partitions of the Data Can Be Processed Simultaneously

```
// initialize array values to 1
   a[]=1;
   b[]=1;
   c[]=1;

   for (i=0; i<3; i++)
    {
     a[i] = b[i] + c[i];
    }

// Serial Execution
   i=0 (a[0] = 2)
   a[0] = b[0] + c[0];
   i=1 (a[1] = 2)
   a[1] = b[1] + c[1];
   i=2 (a[2] = 2)
   a[2] = b[2] + c[2];

// Parallel Execution
   i=0 (a[0] = 2)            i=1 (a[1] = 2)            i=2 (a[2] = 2)
   a[0] = b[0] + c[0];       a[1] = b[1] + c[1];       a[2] = b[2] + c[2];
```

Data Parallelism
MPI Example

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

void main(int argc, char **argv )
 {
  int myid, numprocs;
  int i;
  int *a,*b,*c;
  MPI_Status status;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD,&myid);

  a = (int *) malloc(numprocs*sizeof(int));
  b = (int *) malloc(numprocs*sizeof(int));
  c = (int *) malloc(numprocs*sizeof(int));

  for (i=0;i<numprocs;i++)
   {
    // initialize array values to i
    a[i]=i;
    b[i]=i;
    c[i]=i;
   }
  a[myid] = b[myid] + c[myid];
  printf("a[%d] = %d\n",myid,a[myid]);
  MPI_Finalize();
 }
```

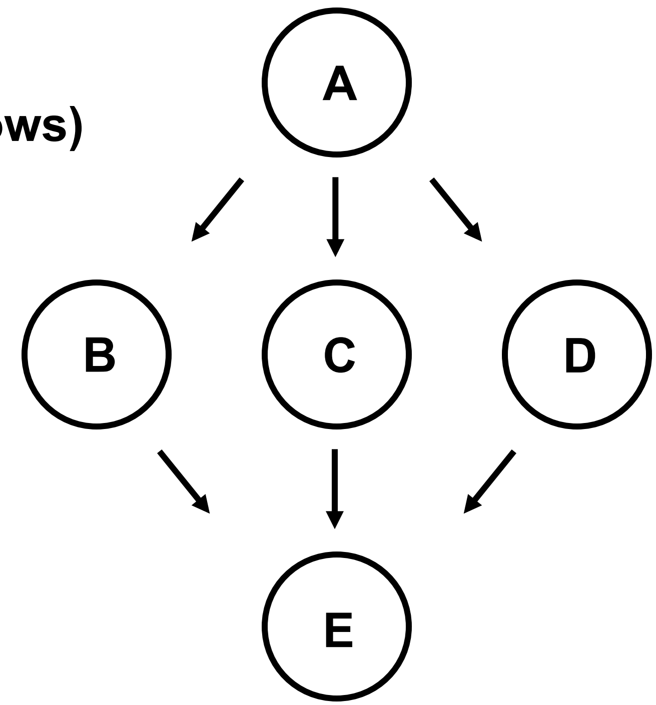
```
mpiexec -n 8 dp1.exe
3: a[3] = 6
4: a[4] = 8
5: a[5] = 10
7: a[7] = 14
0: a[0] = 0
2: a[2] = 4
6: a[6] = 12
1: a[1] = 2
```

Functional Parallelism

Definition: when independent tasks can apply different operations to the same (or different) data elements at the same time.

Examples:

- **2 brothers do yard work (1 rakes, 1 mows)**
- **8 farmers build a barn**



Functional Parallelism
Partitions of the Program Can Execute Simultaneously

```
// initialize values 0-9
   a[]=i;
   b[]=i;

// These different operations can happen at the same time
   for (i=0; i<10; i++)
    {
     c[i] = a[i] + b[i];
    }
   for (i=0; i<10; i++)
    {
     d[i] = a[i] * b[i];
    }

// This part requires solutions from above
   for (i=0; i<10; i++)
    {
     e[i] = d[i] - c[i];
    }
```

Functional Parallelism
MPI Example

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

void main(int argc, char **argv )
 {
  int myid, numprocs;
  int i;
  int iter=10;
  int *a,*b,*c,*d,*e;
  MPI_Status status;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD,&myid);

  if (numprocs < 3)
   {
    printf("ERROR: This example requires 3 processes\n");
   }
  else
   {
    a = (int *) malloc(iter*sizeof(int));
    b = (int *) malloc(iter*sizeof(int));
    c = (int *) malloc(iter*sizeof(int));
    d = (int *) malloc(iter*sizeof(int));
    for (i=0; i<iter; i++)
     {
      a[i] = i;
      b[i] = i;
     }
    if (myid == 0)
     {
      MPI_Recv(c,10,MPI_INT,1,0,MPI_COMM_WORLD,&status);
      MPI_Recv(d,10,MPI_INT,2,0,MPI_COMM_WORLD,&status);
      e = (int *) malloc(iter*sizeof(int));
      for (i=0; i<iter; i++)
       {
        e[i] = d[i] - c[i];
        printf("e[%d] = %d\n",i,e[i]);
       }
     }
    else if (myid == 1)
     {
      for (i=0; i<iter; i++) { c[i] = a[i] + b[i]; }
      MPI_Send(c,10,MPI_INT,0,0,MPI_COMM_WORLD);
     }
    else if (myid == 2)
     {
      for (i=0; i<iter; i++) { d[i] = a[i] * b[i]; }
      MPI_Send(d,10,MPI_INT,0,0,MPI_COMM_WORLD);
     }
    else
     {
      printf("Process id %d not needed\n",myid);
     }
   }
  MPI_Finalize();
 }
```

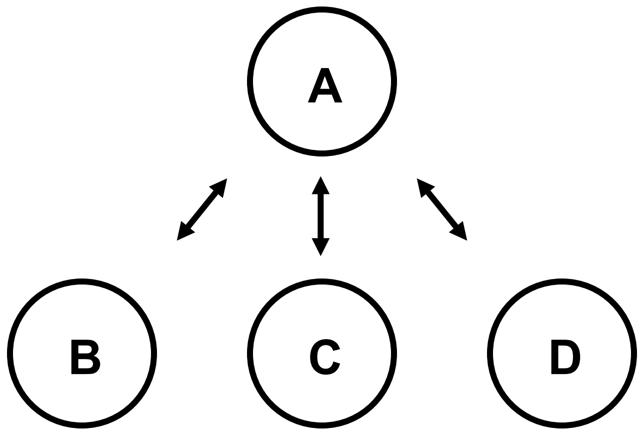
Task Parallelism

Definition: when independent "Worker" tasks can perform functions that do not need to communicate with each other, only with a "Master" or "Manager" process.

Such tasks are often called "Embarrassingly Parallel" because they can be parallelized with little extra work or thought.

Examples:

- Independent Monte Carlo Simulations
- ATM Transactions



Task Parallelism
Independent Tasks are Distributed as Workers are Available

```
// initialize values 0-99
    a[]=i;
    b[]=i;

// Send each idle worker an index of a[] & b[] to add and return the sum
// and continue while there is still work to be done

    while (i<100)
     {
      // find an idle worker & send it value of i (index) to add
      // receive back summed values
     }
```

Pipeline Parallelism

Definition: each task works on one stage in a sequence of stages. The output of one stage is the input of the next. (Note: This works best when each stage takes the same amount of time to complete)

Examples:

- Assembly lines
- Computing partial sums

	T_0	T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8	T_9
A	i	i+1	i+2	i+3	i+4	i+5	i+6			
↓ B		i	i+1	i+2	i+3	i+4	i+5	i+6		
↓ C			i	i+1	i+2	i+3	i+4	i+5	i+6	
				i	i+1	i+2	i+3	i+4	i+5	i+6

Pipeline Parallelism

```
// Process 0 initializes a[] & b[]
   for (i=0; i<=3; i++)
     {
      a[i] = i;
      b[i] = 0;
     }
   b[0] = a[0];
// Process 0 sends a & b to Process 1

// Process 1 receives a & b from Process 0
   b[1] = b[0] + a[1];
// Process 1 sends a & b to Process 2

// Process 2 receives a & b from Process 1
   b[2] = b[1] + a[2];
// Process 2 sends a & b to Process 3

// Process 3 receives a & b from Process 2
   b[3] = b[2] + a[3];
```

Tightly vs. Loosely Coupled Parallelism

Tightly Coupled Parallel Approaches

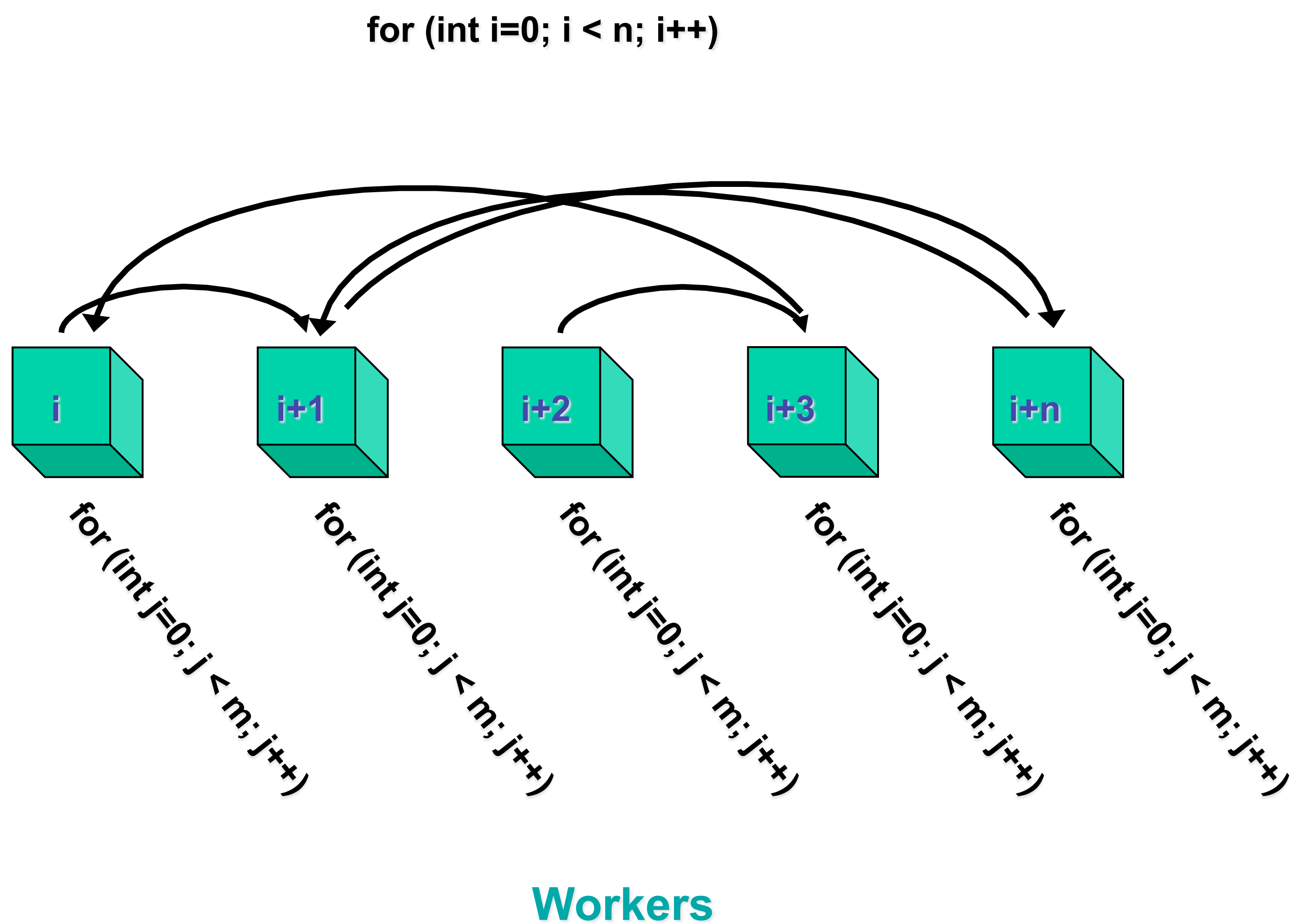
Parallel tasks must exchange data during the computation

Loosely Coupled Parallel Approaches

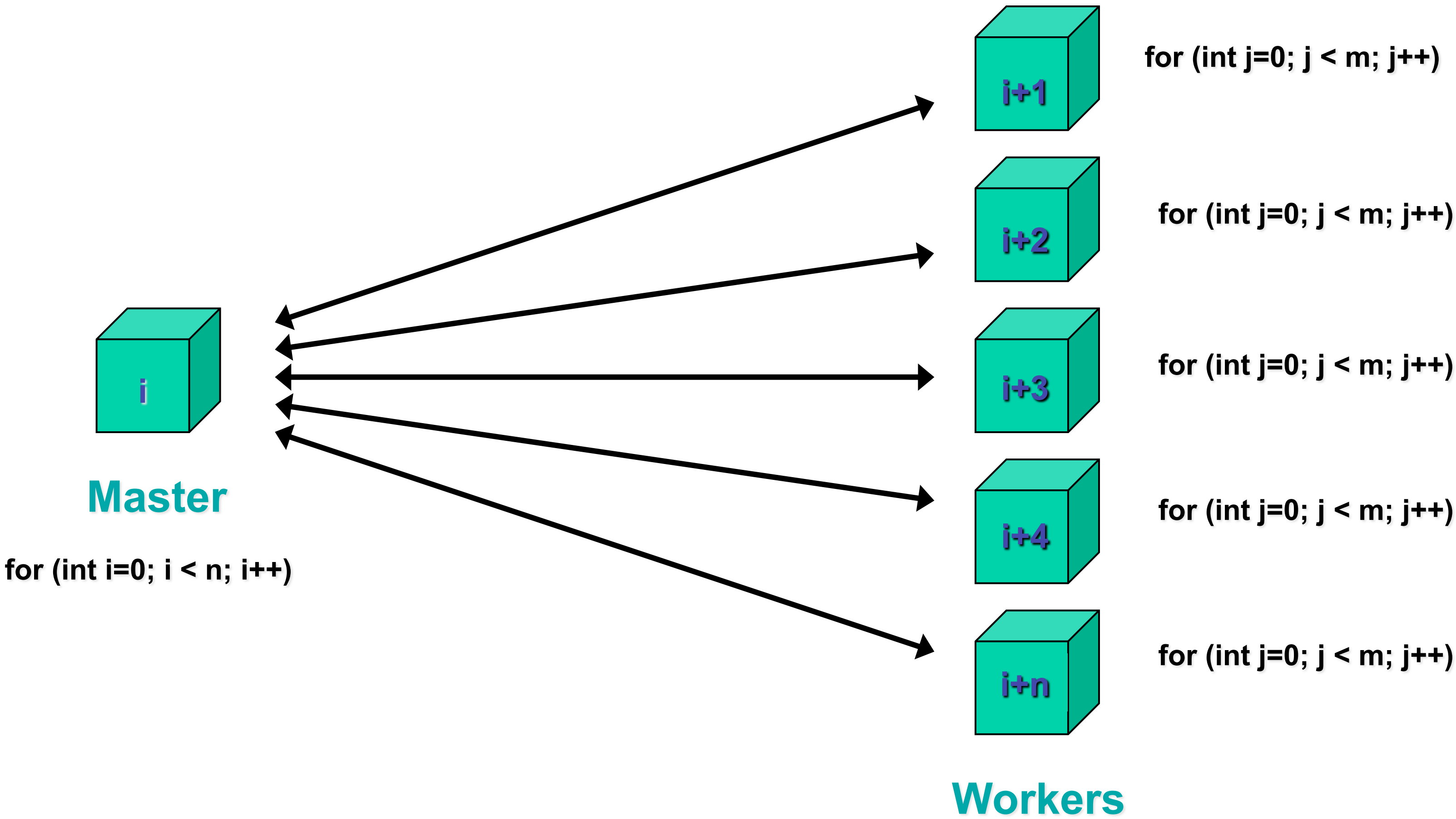
Parallel tasks can complete independent of each other

```
for (int i=0; i < n; i++)
 {
  for (int j=0; j < m; j++)
   {
    //Perform Calculation Here
   } // for j
 } // for i
```

Tightly Coupled Example: Strong Data Dependencies

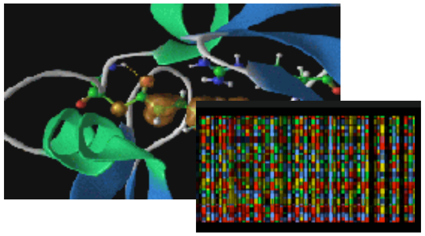


Loosely Coupled Example: Master-Worker Codes

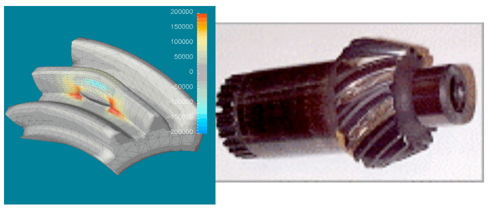


HPC Examples at Cornell: Parallel Computing and Data Intensive Computing

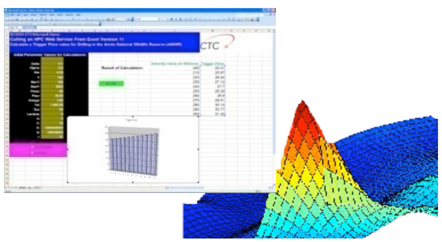
Parallel Computing Examples



Computational Biology Service Unit
http://cbsu.tc.cornell.edu/index.htm



Cornell Fracture Group
http://www.cfg.cornell.edu



Computational Finance
http://www.orie.cornell.edu/orie/manhattan/

Cornell Institute for Social and Economic Research
http://www.ciser.cornell.edu/

Data Intensive Computing Applications

Modern Research is Producing Massive Amounts of Data

- Microscopes
- Telescopes
- Gene Sequencers
- Mass Spectrometers
- Satellite & Radar Images
- Distributed Weather Sensors
- High Performance Computing (especially HPC Clusters)

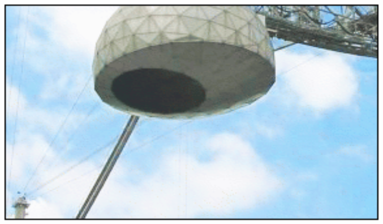
Research Communities Rely on Distributed Data Sources

- Collaboration
- Virtual Laboratories
- Laboratory Information Management Systems (LIMS)

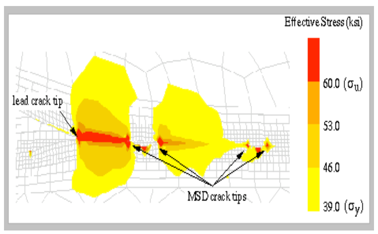
New Management and Usage Issues

- Security
- Reliability/Availability
- Manageability
- Data Locality – You can't ftp a petabyte to your laptop….

Data Intensive Computing Examples



Arecibo - World's Largest Radiotelescope
Johannes Gehrke, Jim Cordes, David Lifka
Serving Astronomy Data via SQL Server and Web Services
http://arecibo.tc.cornell.edu/PALFA
http://www.cs.cornell.edu/johannes/



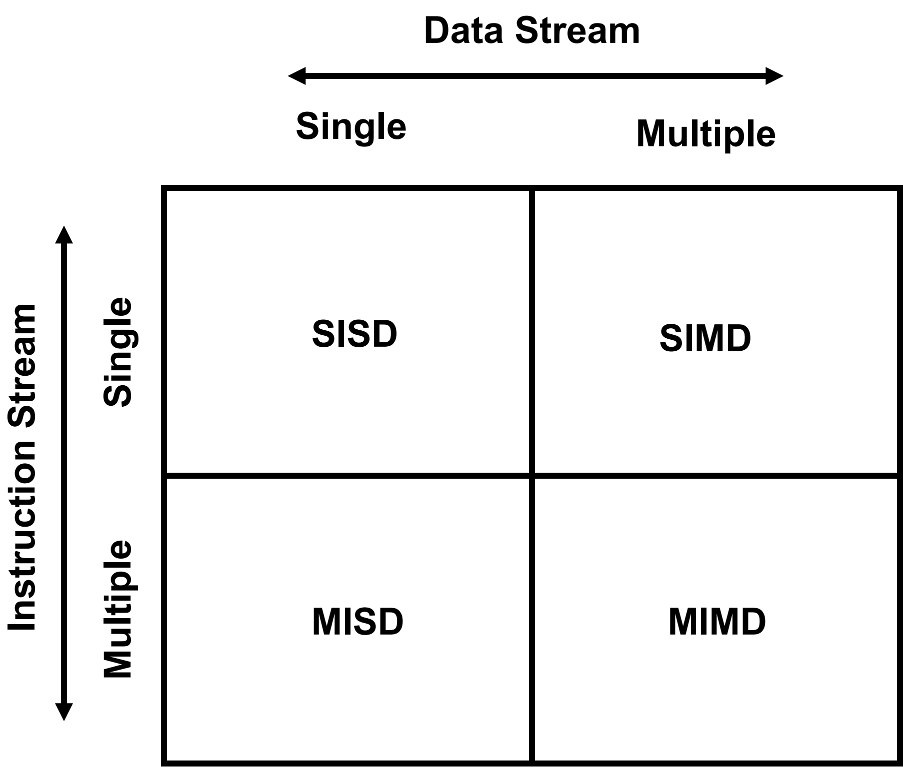
Cornell Fracture Group
Tony Ingraffea
Serving Finite Element Models via SQL Server & Web Services
http://www.cfg.cornell.edu/

Physically Accurate Imagery
Steve Marschner
http://www.cs.cornell.edu/~srm/

The Structure and Evolution of the Web
William Arms
http://www.cs.cornell.edu/wya/

High Performance Computing Architectures

Flynn's Taxonomy
Classification Scheme for Parallel Computers

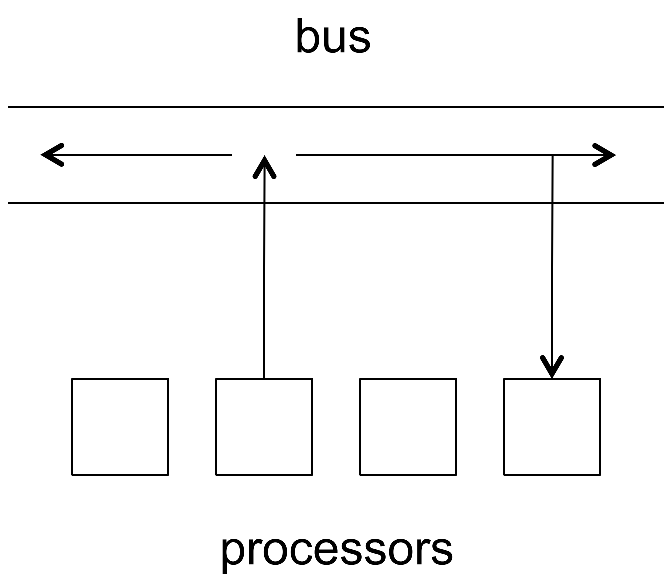


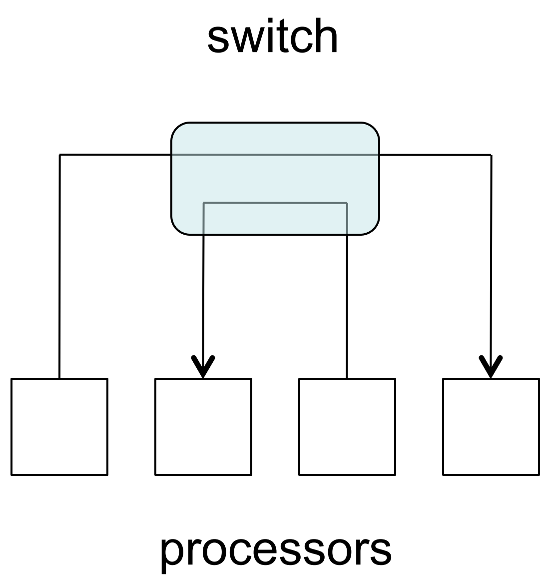
Examples from Flynn's Categories

- **SISD – Single Instruction Stream, Single Data Stream**
  - Common uniprocessor machines
- **SIMD – Single Instruction Stream, Multiple Data Streams**
  - Processor arrays (including GPUs) & pipelined vector processors
- **MISD – Multiple Instruction Streams, Single Data Stream**
  - Systolic arrays: think data pump or pumping-heart model (not many built)
- **MIMD – Multiple Instruction Streams, Multiple Data Streams**
  - Multiprocessors and multicomputers

- **Multiprocessor: multi-CPU computer with shared memory**
  - SMP: Symmetric MultiProcessor (uniform memory access)
  - NUMA: Non Uniform Memory Access multiprocessor
- **Multicomputer: team of computers with distributed CPUs and memory**
  - Must have external *interconnect* between "nodes"

Shared vs. Switched Media





SMP: not scalable,
bus becomes congested
as processors are added

NUMA, Multicomputer:
switch can grow with
number of processors

2D Mesh and Torus Topologies

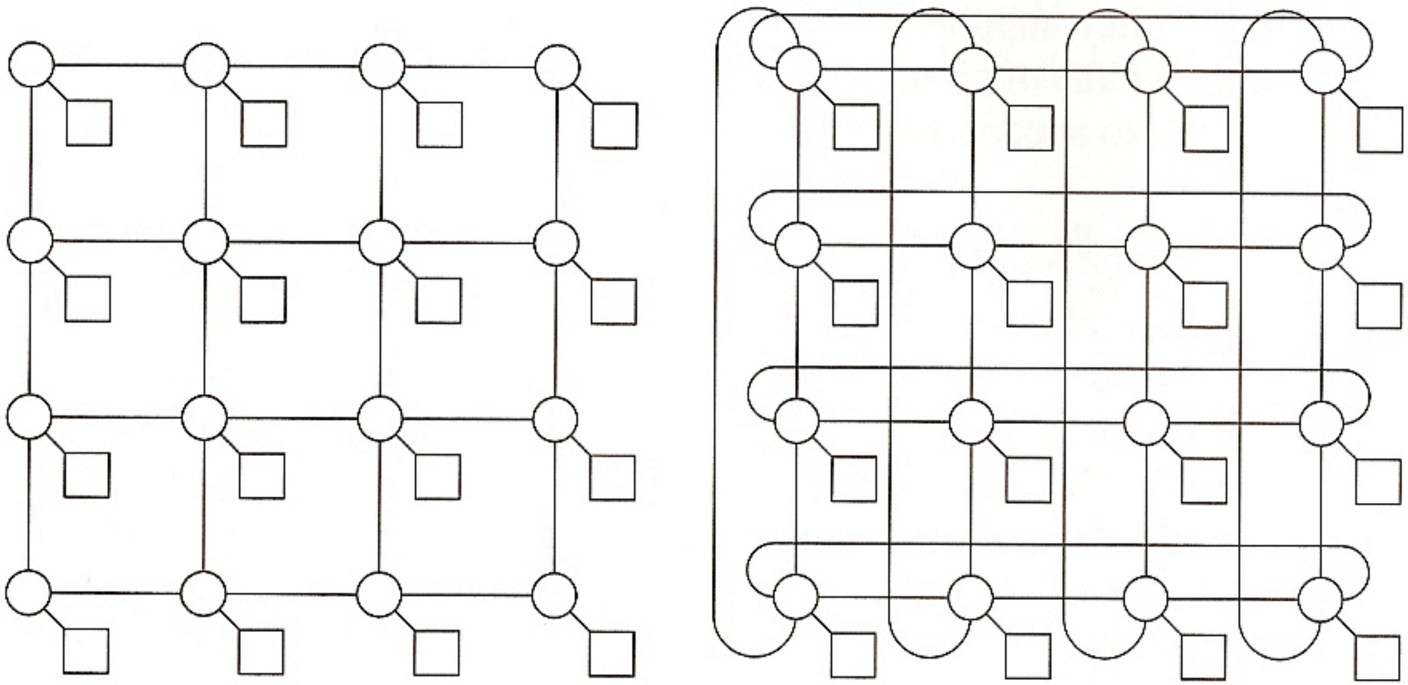


Figure 2.2 Variants of the 2-D mesh network. Circles represent switches, while squares represent processors. (a) Without wraparound connections. (b) With wraparound connections.

Hypercube Topology

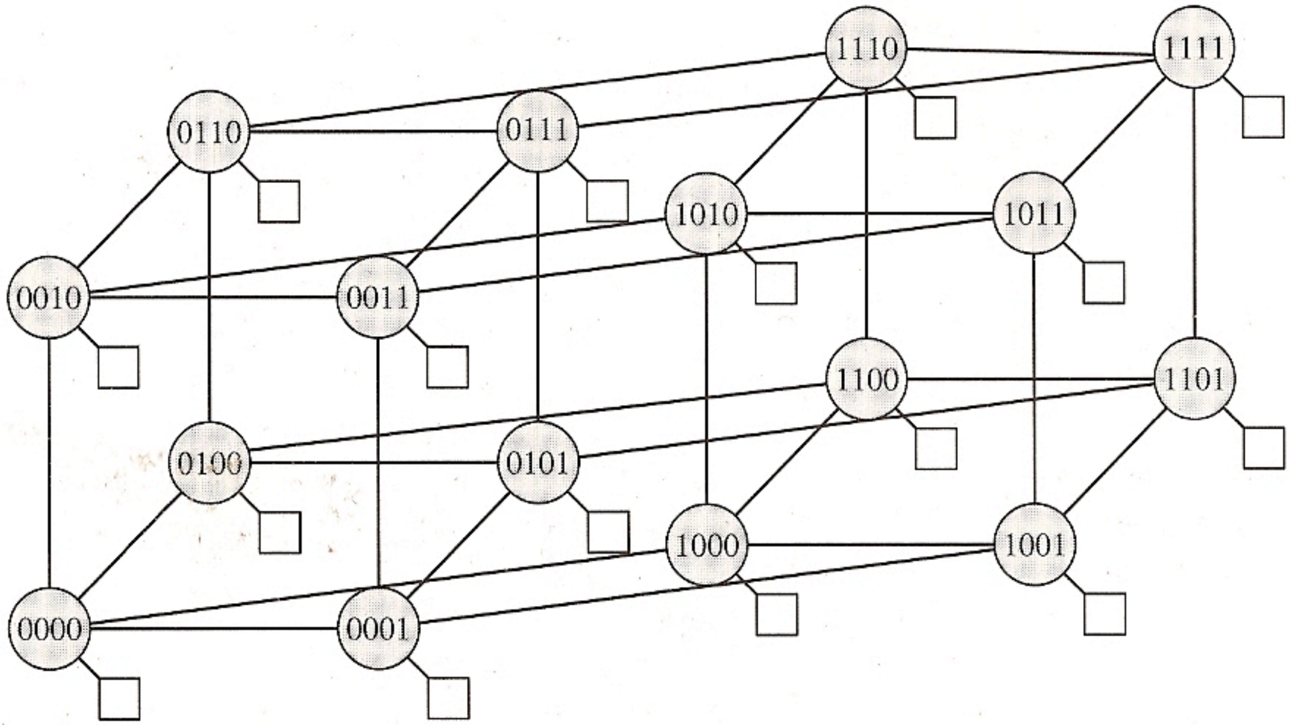


Figure 2.7 A hypercube network with 16 processor nodes and an equal number of switch nodes. Circles represent switches, and squares represent processors. Processor/switch pairs share addresses.

Tree, Fat Tree, and Hypertree Topologies

Fat tree if links get wider toward the top…

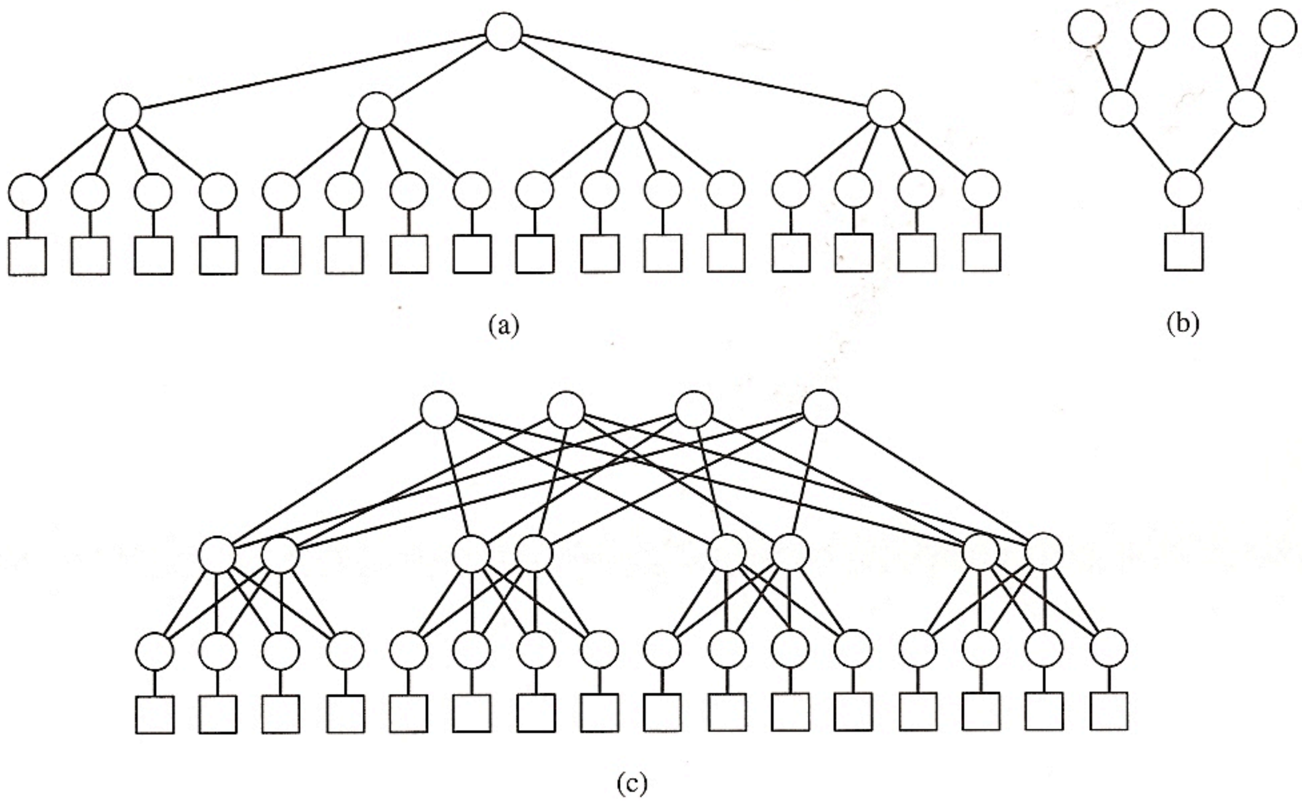
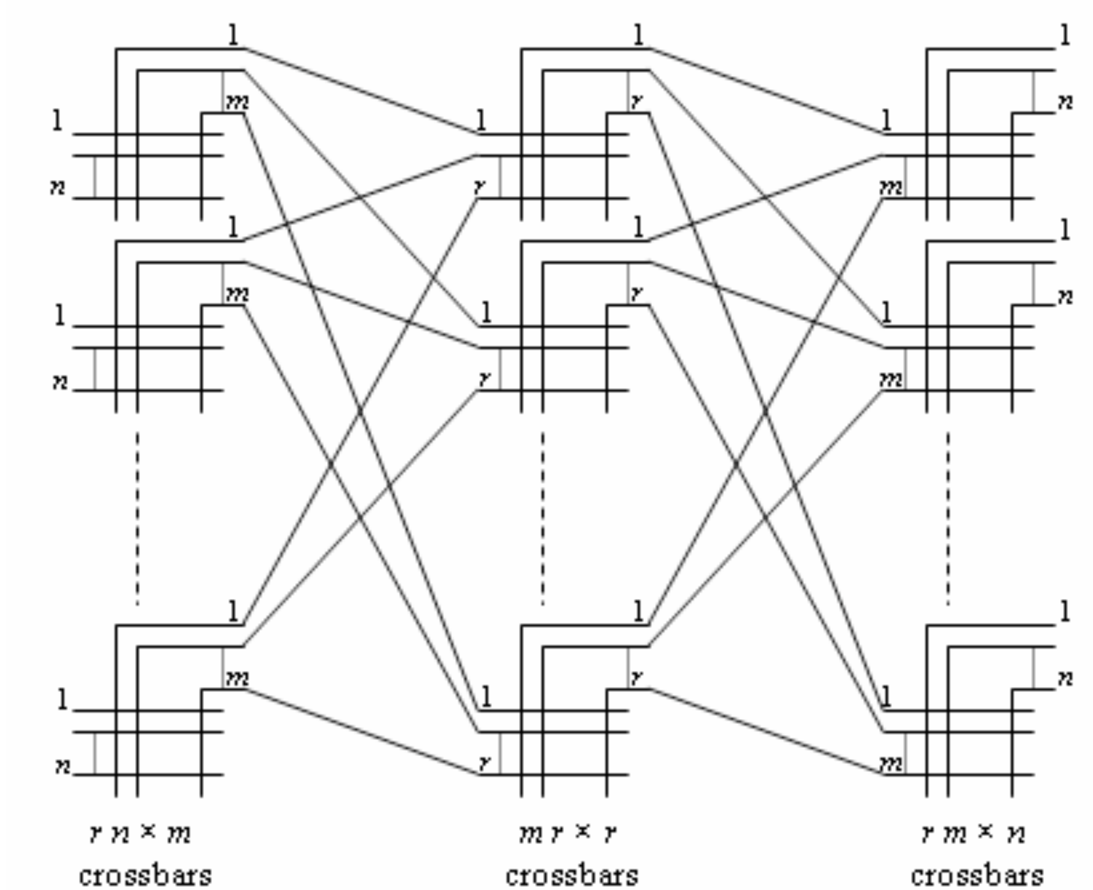


Figure 2.4 Hypertree network of degree 4 and depth 2. Circles represent switches, and squares represent processors. (a) Front view. (b) Side view. (c) Complete network.

Clos Network: Equal to a Full Crossbar Switch, Better Than a Hypertree (Fewer Hops)



Generally *n* = *m*, so inputs and outputs can be bundled into the same cable and plug into a single *switch port*

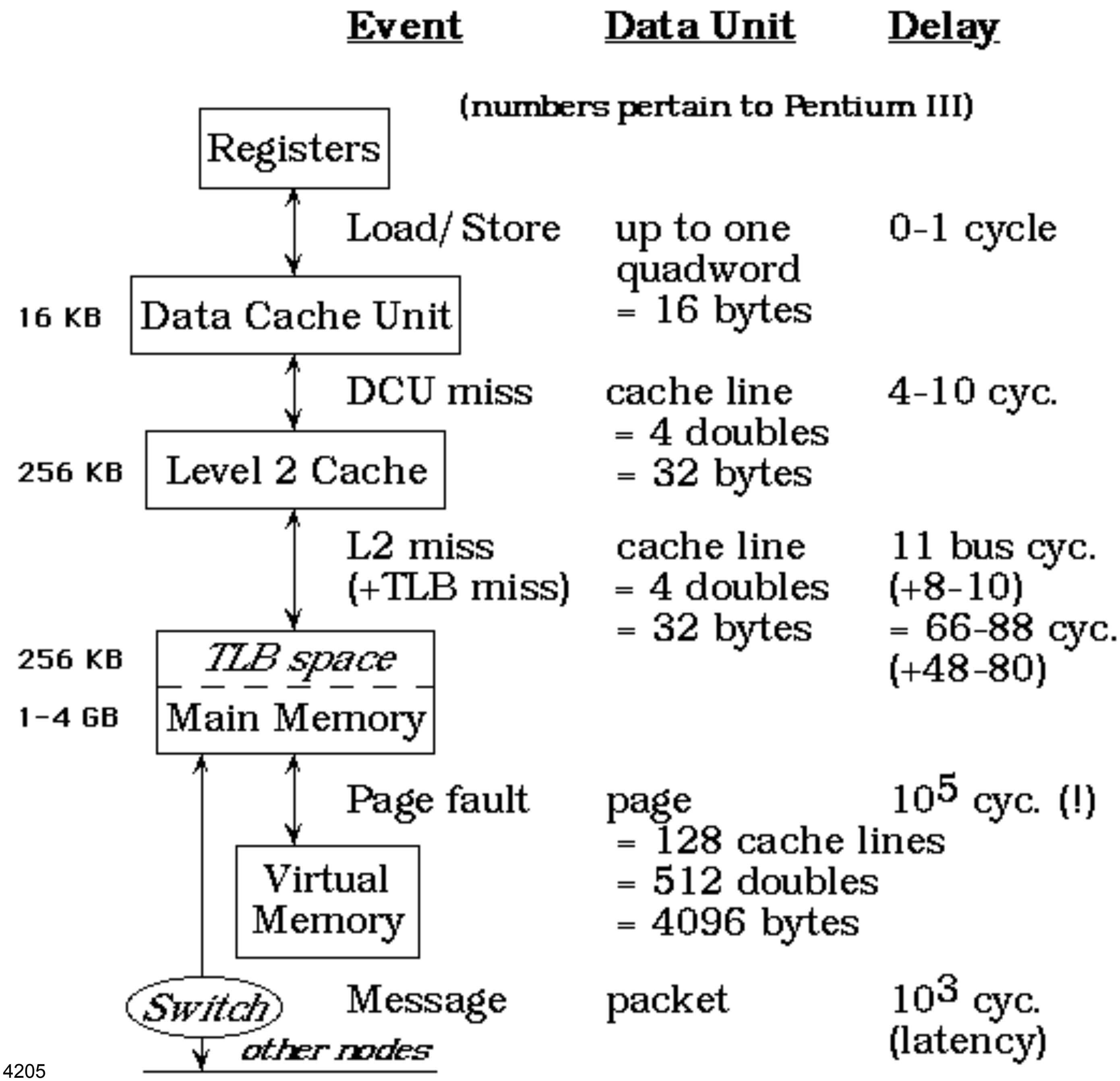
Comparison of Switched Media

Type	Latency	Bandwidth	Cost
Gigabit Ethernet	~1 msec	0.1 gigabyte/sec	$
10 Gigabit Ethernet	~100 μsec	1.0 gigabyte/sec	$$
QDR InfiniBand	~1μsec	3.6 gigabyte/sec	$$$

Mellanox 36-port InfiniBand switch

Computing Concepts

Single Processor Memory Hierarchy



Creating and Running Software

- **Compiler**
  - Produces object code: from myprog.c, creates myprog.o (Windows: .obj)
- **Linker**
  - Produces complete executable, including object code imported from libraries
- **Shared Objects (.so) and Dynamic Load Libraries (Windows DLLs)**
  - These are loaded at runtime: the link step inserts instructions on what to import
  - If a shared object is loaded, a single copy can be used by multiple processes
- **Process**
  - A running executable: the OS controls multitasking of processes via scheduling
- **Virtual Memory**
  - "Address space" available to a running process, addresses can be 32- or 64-bit
- **Paging (to Disk)**
  - Physical RAM has been exceeded: requested data are not in any cache (*cache miss*) or in RAM (*page fault*) must be loaded from swap space on a hard drive