Supercomputing in Plain English

Multicore Madness

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OU Supercomputing Center for Education & Research

University of Oklahoma Information Technology

Tuesday April 12 2011

This is an experiment!

It's the nature of these kinds of videoconferences that **FAILURES ARE GUARANTEED TO HAPPEN! NO PROMISES!**

So, please bear with us. Hopefully everything will work out well enough.

If you lose your connection, you can retry the same kind of connection, or try connecting another way.

Remember, if all else fails, you always have the toll free phone bridge to fall back on.

Access Grid

If you aren't sure whether you have AG, you probably don't.

Tue Apr 12	Platinum
Tue Apr 19	Mosaic
Tue Apr 26	Monte Carlo
Tue May 3	Helium

Many thanks to Patrick Calhoun of OU for setting these up for us.

H.323 (Polycom etc)

From an H.323 device (e.g., Polycom, Tandberg, Lifesize, etc):

- If you **ARE** already registered with the OneNet gatekeeper:
  Dial
  2500409
- If you **AREN'T** registered with the OneNet gatekeeper (probably the case):
  1. Dial:
     164.58.250.47
  2. Bring up the virtual keypad.
     On some H.323 devices, you can bring up the virtual keypad by typing:
     #
  3. When asked for the conference ID, enter:
     0409
  4. On some H.323 devices, you indicate the end of conference ID with:
     #

Many thanks to Roger Holder and OneNet for providing this.

H.323 from Internet Explorer

From a Windows PC running Internet Explorer:

1. You **MUST** have the ability to install software on the PC (or have someone install it for you).
2. Download and install the latest Java Runtime Environment (JRE) from here:
   http://www.oracle.com/technetwork/java/javase/downloads/
   (Click on the Java Download icon, because that install package includes both the JRE and other components.)
3. Download and install this video decoder:
   http://164.58.250.47/codian video decoder.msi
4. Start Internet Explorer.
5. Copy-and-paste this URL into your IE window:
   http://164.58.250.47/
6. When that webpage loads, in the upper left, click on "Streaming."
7. In the textbox labeled Sign-in Name, type your name.
8. In the textbox labeled Conference ID, type this:
   0409
9. Click on "Stream this conference."
10. When that webpage loads, you may see, at the very top, a bar offering you options. If so, click on it and choose "Install this add-on."

H.323 from XMeeting (MacOS)

From a Mac running MacOS X:

1. Download XMeeting from
   http://xmeeting.sourceforge.net/
2. Install XMeeting as follows:
   a. Open the .dmg file.
   b. Drag XMeeting into the Applications folder.
3. Open XMeeting from Applications.
4. Skip the setup wizard.
5. In the call box, type
   164.58.250.47
6. Click the **Call** button.
7. From the Remote Control window, when prompted to join the conference, enter :
   0409#

EVO

There's a quick tutorial on the OSCER education webpage.

QuickTime Broadcaster

If you cannot connect via the Access Grid, H.323 or iLinc, then you can connect via QuickTime:

`rtsp://129.15.254.141/test_hpc09.sdp`

We recommend using QuickTime Player for this, because we've tested it successfully.

We recommend upgrading to the latest version at:

`http://www.apple.com/quicktime/`

When you run QuickTime Player, traverse the menus

File -> Open URL

Then paste in the rstp URL into the textbox, and click OK.

Many thanks to Kevin Blake of OU for setting up QuickTime Broadcaster for us.

WebEx

We have only a limited number of WebEx connections, so please avoid WebEx unless you have **NO OTHER WAY TO CONNECT**.

Instructions are available on the OSCER education webpage.

Thanks to Tim Miller of Wake Forest U.

Phone Bridge

If all else fails, you can call into our toll free phone bridge:

US: 1-800-832-0736, *6232874#

International: 303-330-0440, *6232874#

Please mute yourself and use the phone to listen.

Don't worry, we'll call out slide numbers as we go.

Please use the phone bridge **ONLY** if you cannot connect any other way: the phone bridge is charged per connection per minute, so our preference is to minimize the number of connections.

Many thanks to Amy Apon and U Arkansas for providing the previous toll free phone bridge.

Please Mute Yourself

No matter how you connect, please mute yourself, so that we cannot hear you.

At OU, we will turn off the sound on all conferencing technologies.

That way, we won't have problems with echo cancellation.

Of course, that means we cannot hear questions.

So for questions, you'll need to send some kind of text.

Questions via Text: iLinc or E-mail

Ask questions via e-mail to **sipe2011@yahoo.com**.

All questions will be read out loud and then answered out loud.

Thanks for helping!

- OSCER operations staff: Brandon George, Dave Akin, Brett Zimmerman, Josh Alexander
- Horst Severini, OSCER Associate Director for Remote & Heterogeneous Computing
- OU Research Campus staff (Patrick Calhoun, Mark McAvoy)
- Kevin Blake, OU IT (videographer)
- John Chapman, Jeff Pummill and Amy Apon, U Arkansas
- James Deaton and Roger Holder, OneNet
- Tim Miller, Wake Forest U
- Jamie Hegarty Schwettmann, i11 Industries

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Supercomputing Exercises

Want to do the "Supercomputing in Plain English" exercises?

- The first exercise is already posted at:

  http://www.oscer.ou.edu/education.php

- If you don't yet have a supercomputer account, you can get a temporary account, just for the "Supercomputing in Plain English" exercises, by sending e-mail to:

  hneeman@ou.edu

Please note that this account is for doing the **exercises only**, and will be shut down at the end of the series.

- This week's N-Body exercise will give you experience parallelizing using hybrid MPI+OpenMP.

University of Illinois
at Urbana-Champaign

Undergraduate Petascale Internships

- NSF support for undergraduate internships involving high-performance computing in science and engineering.

- Provides a stipend ($5k over the year), a two-week intensive high-performance computing workshop at the National Center for Supercomputing Applications, and travel to the SC11 supercomputing conference in November.

- This support is intended to allow you to work with a faculty mentor on your campus. Have your faculty mentor fill out an intern position description at the link below. There are also some open positions listed on our site.

- Student applications and position descriptions from faculty are due by March 31, 2011. Selections and notifications will be made by April 15.

http://shodor.org/petascale/participation/internships/

Summer Workshops 2011

- In Summer 2011, there will be several workshops on HPC and Computational and Data Enabled Science and Engineering (CDESE) across the US.
- These will be weeklong intensives, running from Sunday evening through Saturday morning.
- We're currently working on where and when those workshops will be held.
- Once we've got that worked out, we'll announce them and open up the registration website.
- One of them will be held at OU.

OK Supercomputing Symposium 2011

2003 Keynote:
Peter Freeman
NSF
Computer & Information Science & Engineering
Assistant Director

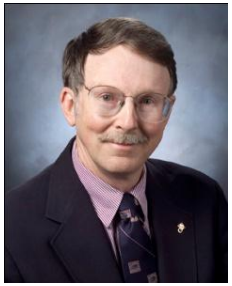
2004 Keynote:
Sangtae Kim
NSF Shared Cyberinfrastructure Division Director

2005 Keynote:
Walt Brooks
NASA Advanced Supercomputing Division Director

2006 Keynote:
Dan Atkins
Head of NSF's Office of Cyberinfrastructure

2007 Keynote:
Jay Boisseau
Director
Texas Advanced Computing Center
U. Texas Austin

2008 Keynote:
José Munoz
Deputy Office Director/ Senior Scientific Advisor
NSF Office of Cyberinfrastructure



2009 Keynote:
Douglass Post
Chief Scientist
US Dept of Defense HPC Modernization Program

2010 Keynote:
Horst Simon
Deputy Director
Lawrence Berkeley National Laboratory

?

2011 Keynote to be announced

FREE! Wed Oct 12 2011 @ OU

http://symposium2011.oscer.ou.edu/

Parallel Programming Workshop
FREE! Tue Oct 11 2011 @ OU
FREE! Symposium Wed Oct 12 2011 @ OU

SC11 Education Program

- At the SC11 supercomputing conference, we'll hold our annual Education Program, Sat Nov 12 – Tue Nov 15.
- You can apply to attend, either fully funded by SC11 or self-funded.
- Henry is the SC11 Education Chair.
- We'll alert everyone once the registration website opens.

Outline

- The March of Progress
- Multicore/Many-core Basics
- Software Strategies for Multicore/Many-core
- A Concrete Example: Weather Forecasting

The March of Progress

OU's TeraFLOP Cluster, 2002

10 racks @ 1000 lbs per rack

270 Pentium4 Xeon CPUs,
2.0 GHz, 512 KB L2 cache

270 GB RAM, 400 MHz FSB

8 TB disk

Myrinet2000 Interconnect

100 Mbps Ethernet Interconnect

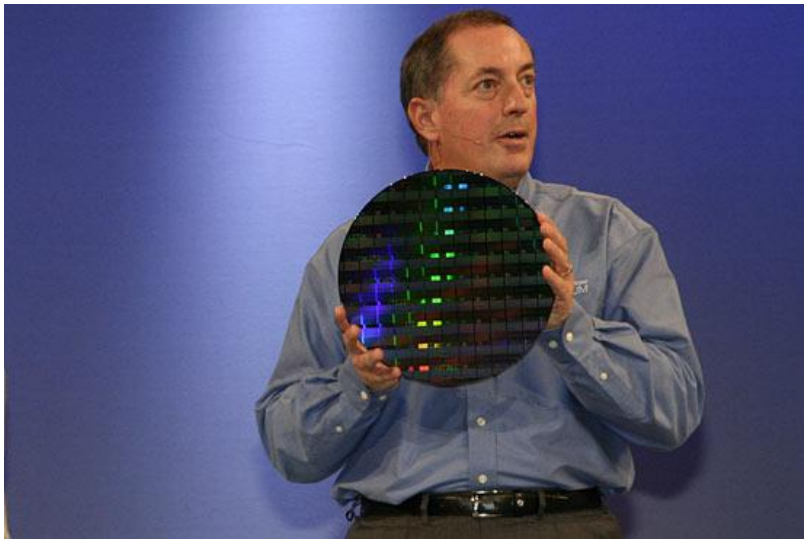
OS: Red Hat Linux

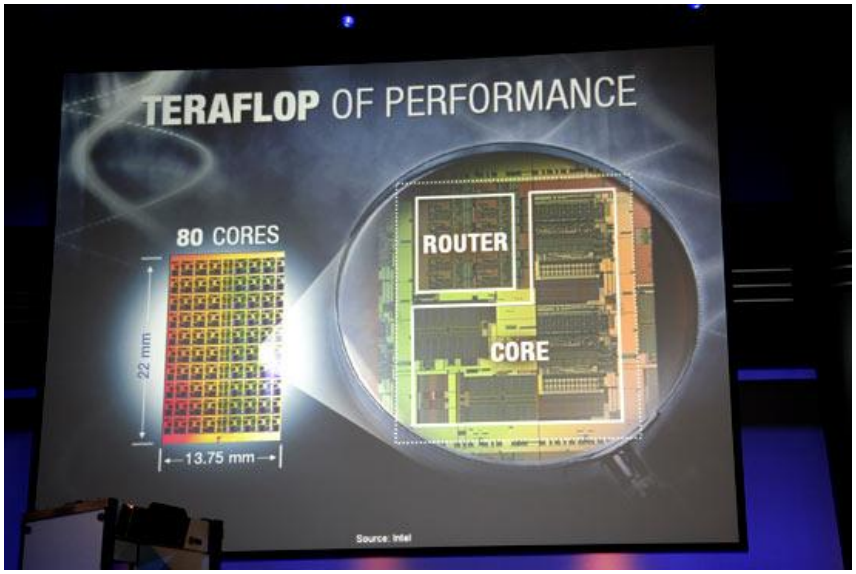
Peak speed: 1.08 TFLOPs
(1.08 trillion calculations per second)

One of the first Pentium4 clusters!

boomer.oscer.ou.edu

TeraFLOP, Prototype 2006





4 years from room to chip!

http://news.com.com/2300-1006_3-6119652.html

Moore's Law

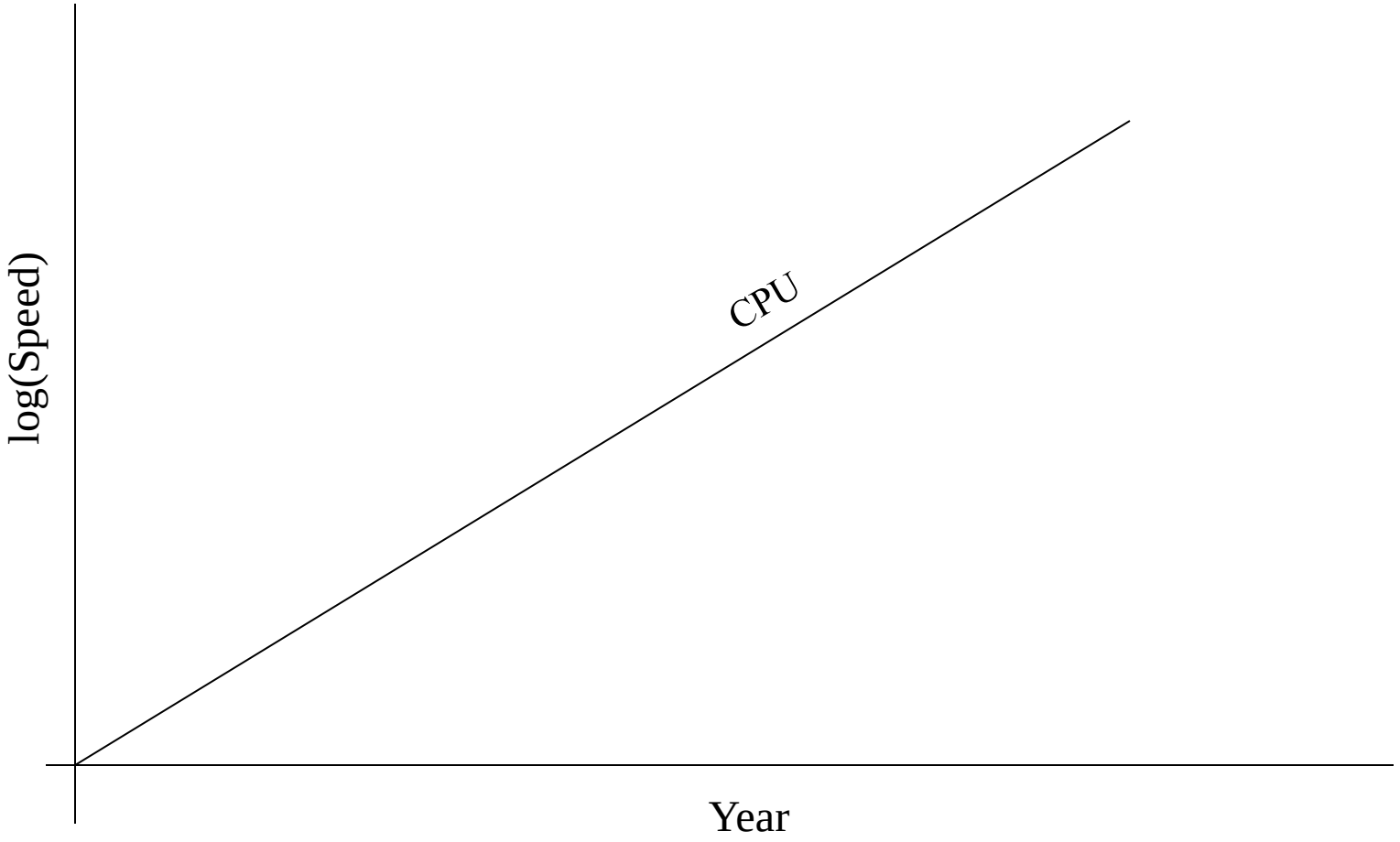
In 1965, Gordon Moore was an engineer at Fairchild Semiconductor.

He noticed that the number of transistors that could be squeezed onto a chip was doubling about every 18 months.

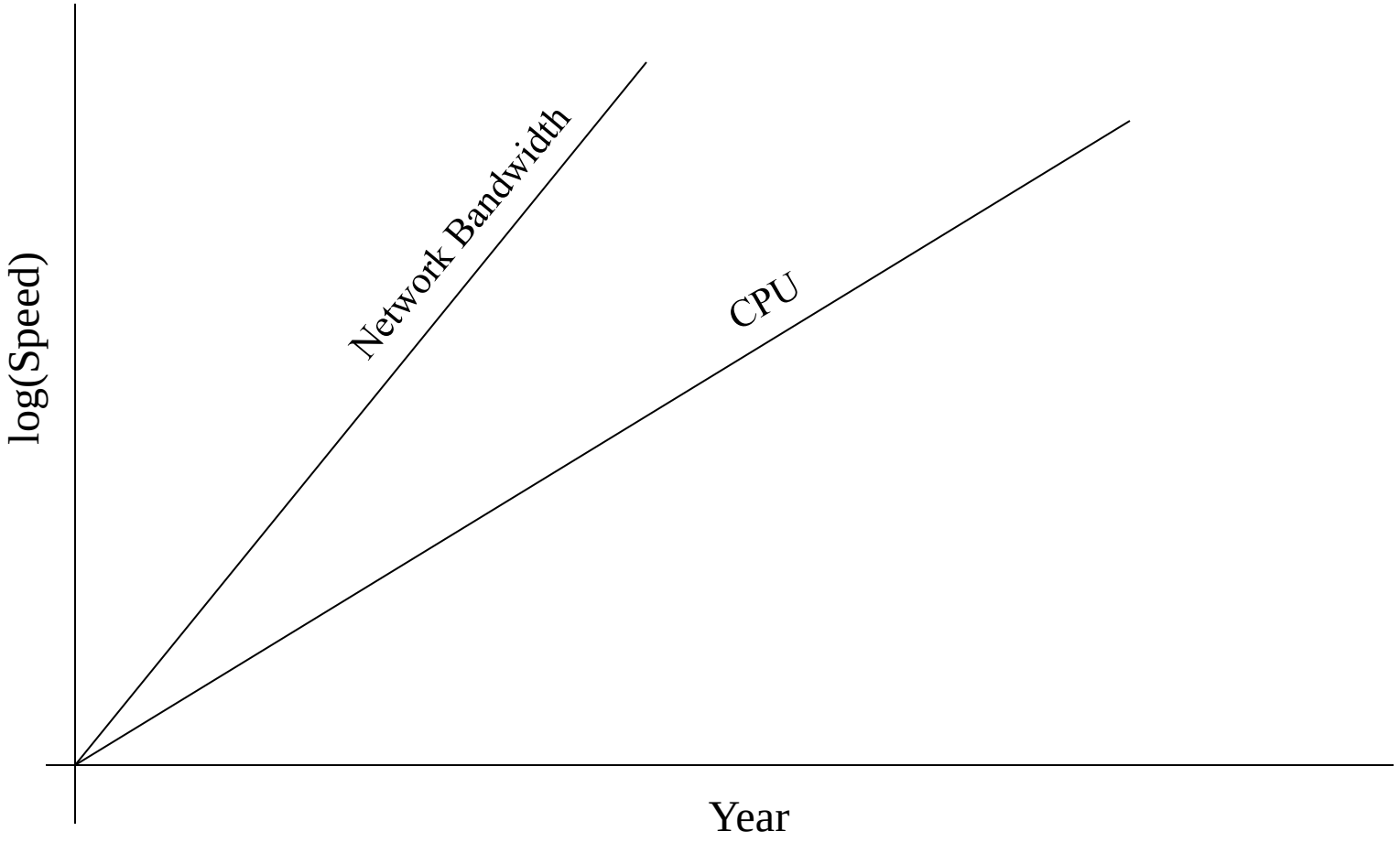
It turns out that computer speed is roughly proportional to the number of transistors per unit area.

Moore wrote a paper about this concept, which became known as ***"Moore's Law."***

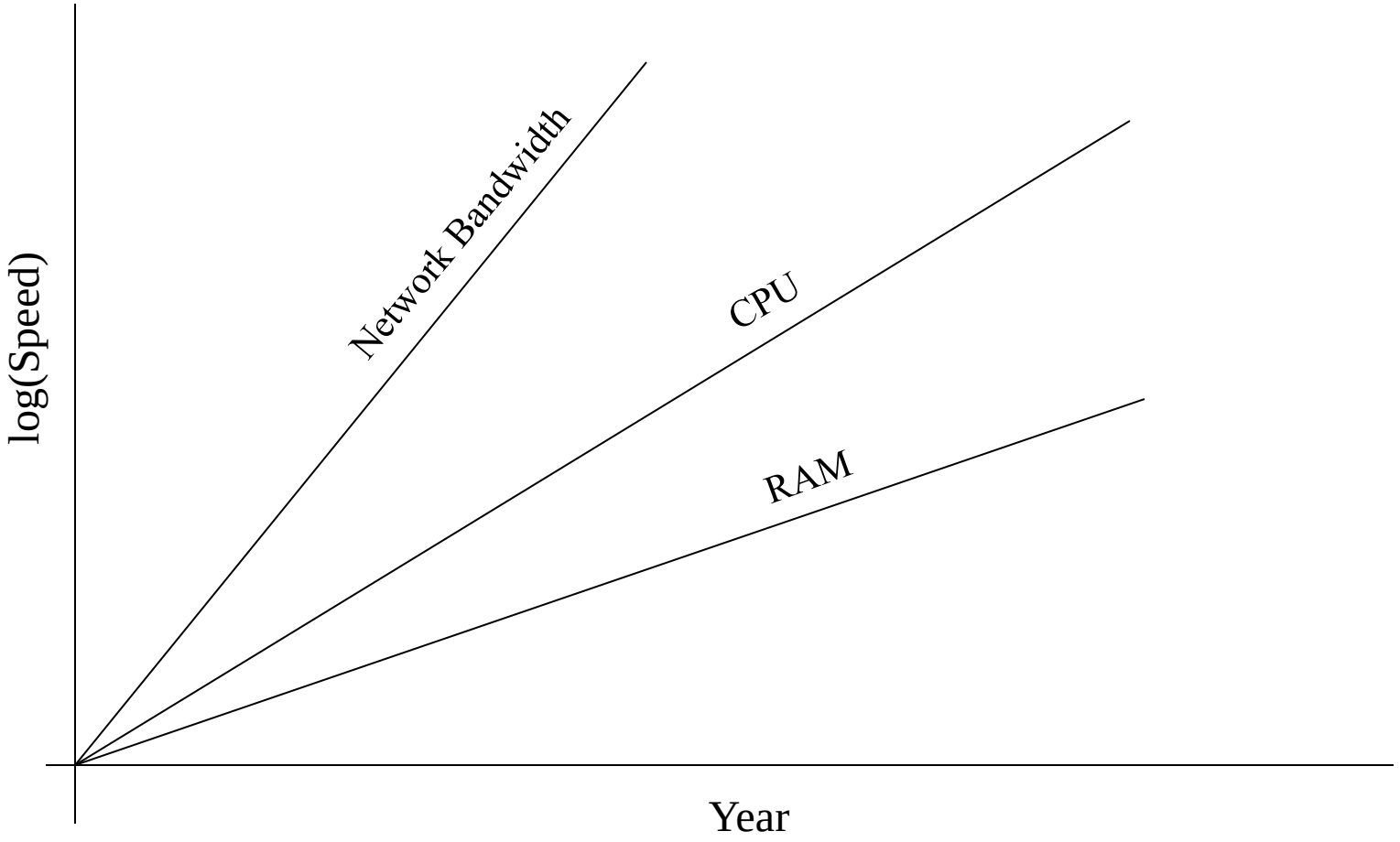
Moore's Law in Practice



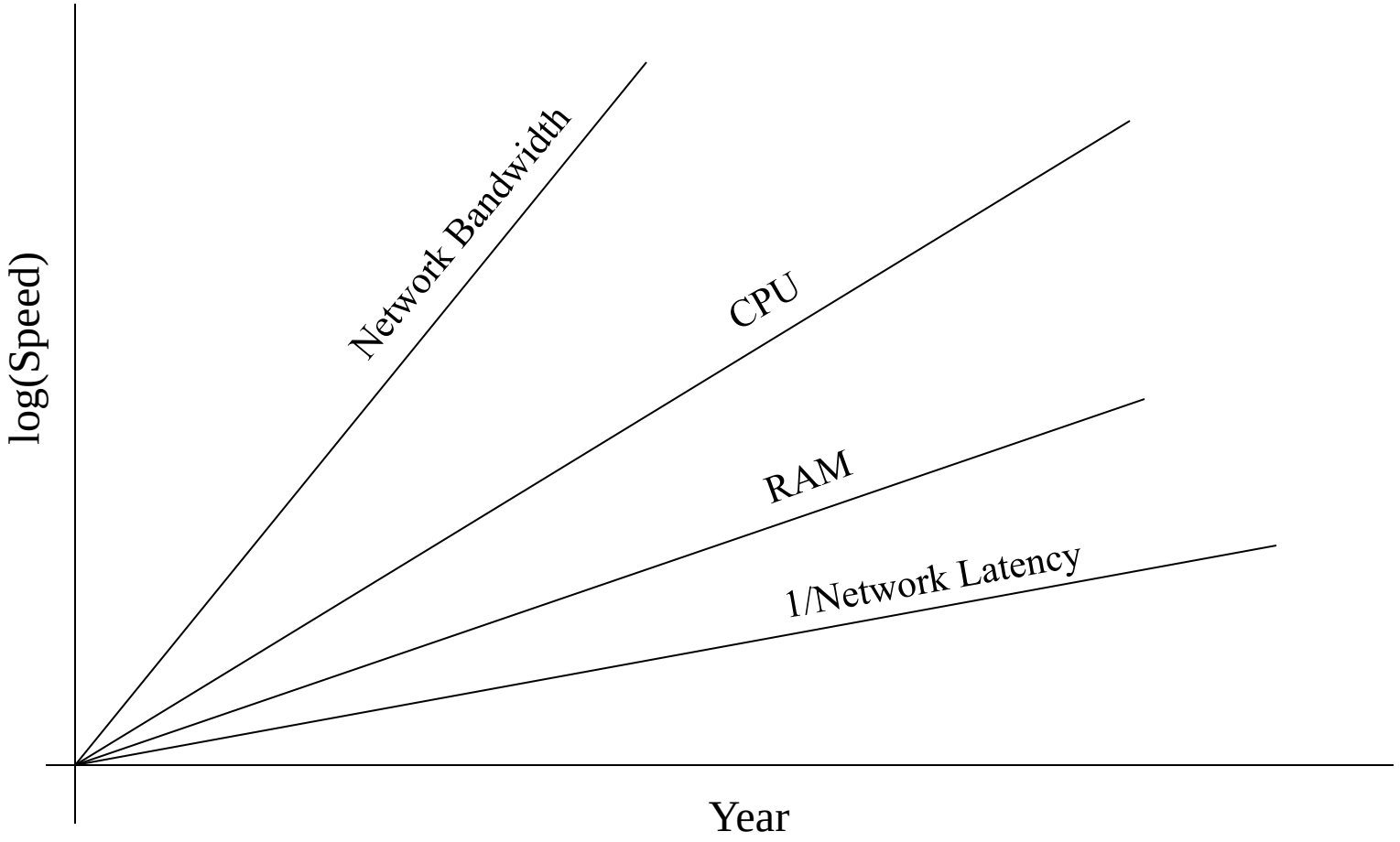
Moore's Law in Practice



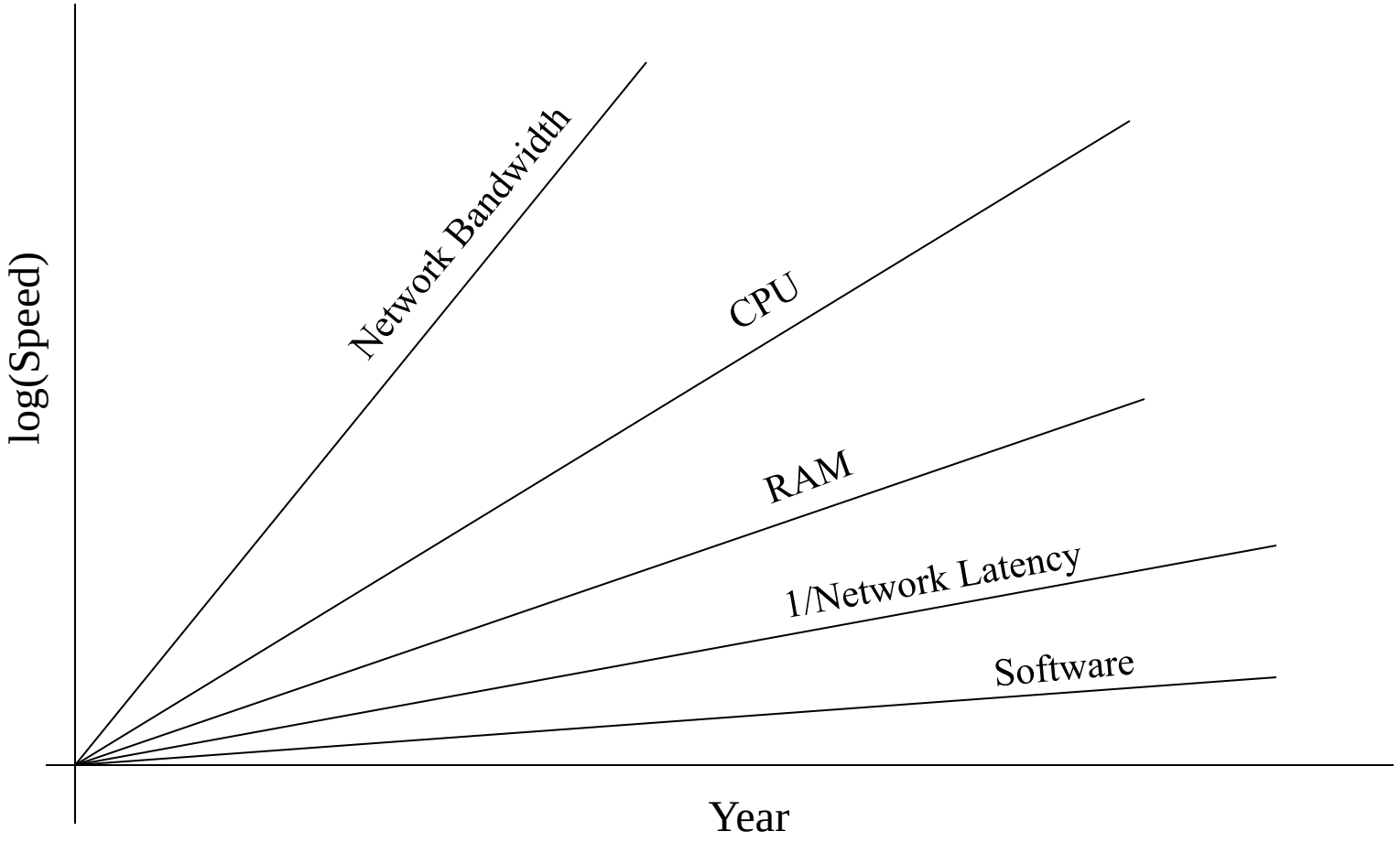
Moore's Law in Practice



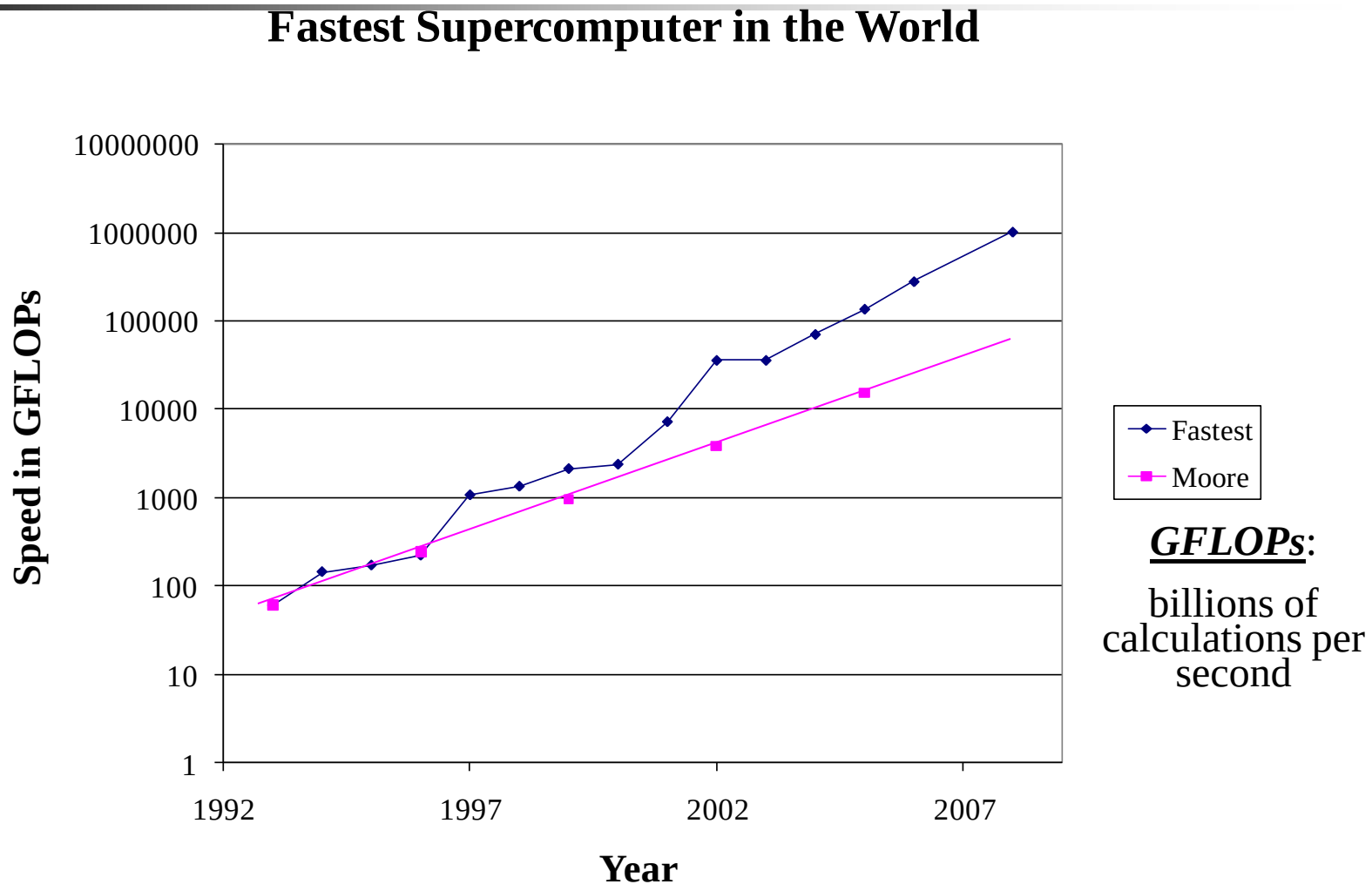
Moore's Law in Practice



Moore's Law in Practice



Fastest Supercomputer vs. Moore

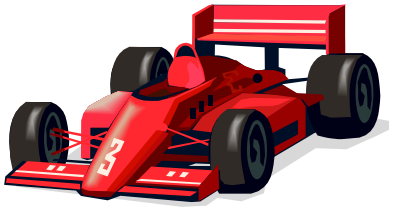


GFLOPs:

billions of calculations per second

The Tyranny of the Storage Hierarchy

The Storage Hierarchy



Fast, expensive, few

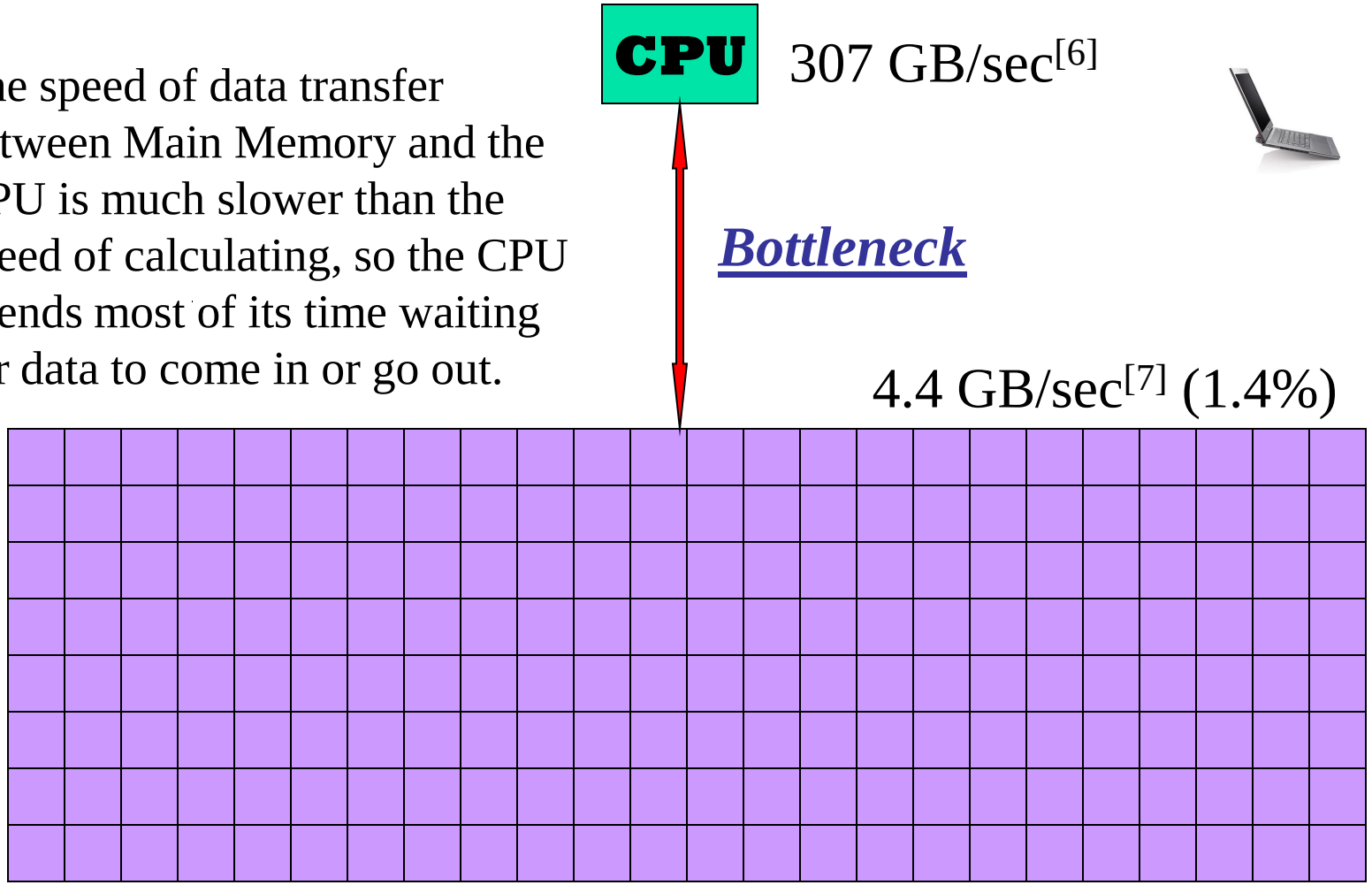
Slow, cheap, a lot

- Registers
- Cache memory
- Main memory (RAM)
- Hard disk
- Removable media (CD, DVD etc)
- Internet

[5]

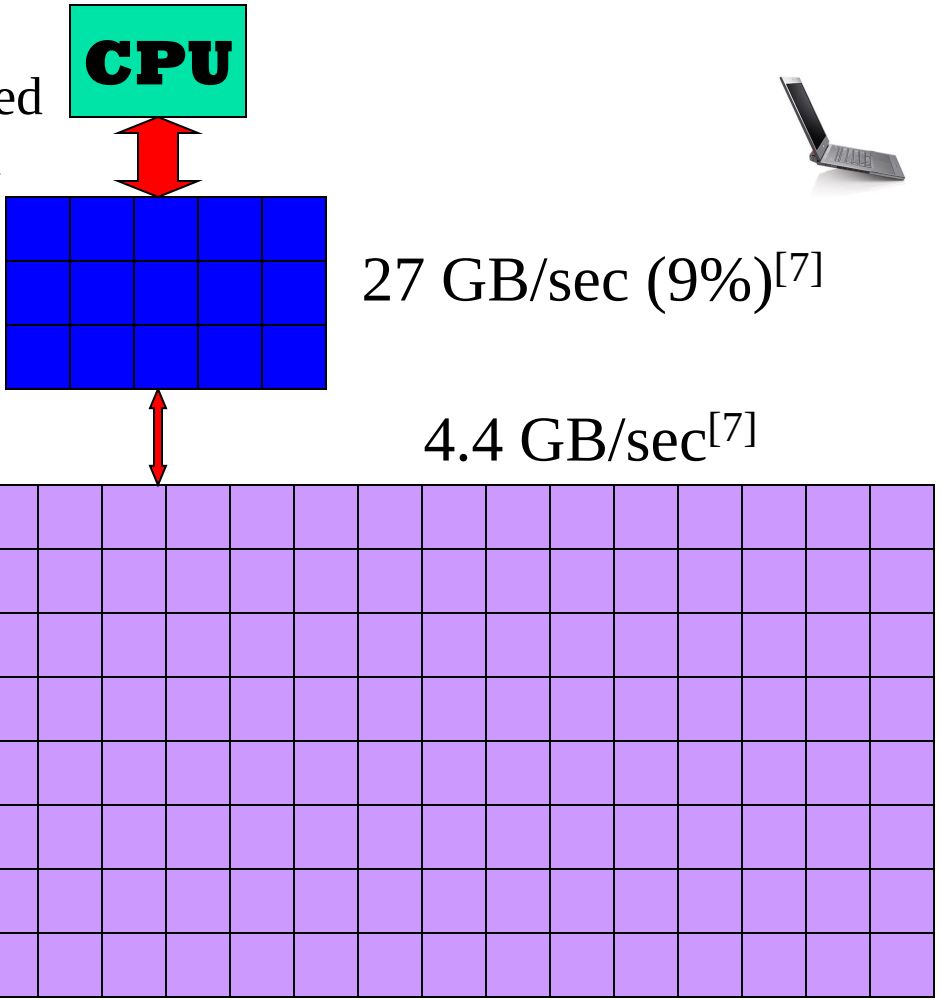
RAM is Slow

The speed of data transfer between Main Memory and the CPU is much slower than the speed of calculating, so the CPU spends most of its time waiting for data to come in or go out.



Why Have Cache?

Cache is much closer to the speed of the CPU, so the CPU doesn't have to wait nearly as long for stuff that's already in cache: it can do more operations per second!



A Laptop

Dell Latitude Z600[4]

- Intel Core2 Duo SU9600
  1.6 GHz w/3 MB L2 Cache
- 4 GB 1066 MHz DDR3 SDRAM
- 256 GB SSD Hard Drive
- DVD±RW/CD-RW Drive (8x)
- 1 Gbps Ethernet Adapter

Storage Speed, Size, Cost

Laptop	Registers (Intel Core2 Duo 1.6 GHz)	Cache Memory (L2)	Main Memory (1066MHz DDR3 SDRAM)	Hard Drive (SSD)	Ethernet (1000 Mbps)	DVD±R (16x)	Phone Modem (56 Kbps)
Speed (MB/sec) [peak]	314,573[6] (12,800 MFLOP/s*)	27,276 [7]	4500 [7]	250 [9]	125	22 [10]	0.007
Size (MB)	464 bytes** [11]	3	4096	256,000	unlimited	unlimited	unlimited
Cost ($/MB)	–	$285 [13]	$0.03 [12]	$0.002 [12]	charged per month (typically)	$0.00005 [12]	charged per month (typically)

* MFLOP/s: millions of floating point operations per second

** 16 64-bit general purpose registers, 8 80-bit floating point registers, 16 128-bit floating point vector registers

Storage Use Strategies

- ***Register reuse***: Do a lot of work on the same data before working on new data.
- ***Cache reuse***: The program is much more efficient if all of the data and instructions fit in cache; if not, try to use what's in cache a lot before using anything that isn't in cache.
- ***Data locality***: Try to access data that are near each other in memory before data that are far.
- **I/O efficiency**: Do a bunch of I/O all at once rather than a little bit at a time; don't mix calculations and I/O.

A Concrete Example

- Consider a cluster with Harpertown CPUs: quad core, 2.0 GHz, 1333 MHz Front Side Bus.
- The theoretical peak CPU speed is 32 GFLOPs (double precision) per CPU chip, and in practice the benchmark per core as 87% of that (93% for a single core). For a dual chip node, the peak is 64 GFLOPs.
- Each double precision calculation is 2 8-byte operands and one 8-byte result, so 24 bytes get moved between RAM and CPU.
- So, in theory each node could transfer up to 1536 GB/sec.
- The theoretical peak RAM bandwidth is 21 GB/sec (but in practice benchmarks have shown 3.4 GB/sec).
- So, even at theoretical peak, any code that does less than 73 calculations **per byte** transferred between RAM and cache has speed limited by RAM bandwidth.

Good Cache Reuse Example

A Sample Application

Matrix-Matrix Multiply

Let A, B and C be matrices of sizes
$nr \times nc$, $nr \times nk$ and $nk \times nc$, respectively:

$$\mathbf{A} = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,nc} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,nc} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,nc} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{nr,1} & a_{nr,2} & a_{nr,3} & \cdots & a_{nr,nc} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & \cdots & b_{1,nk} \\ b_{2,1} & b_{2,2} & b_{2,3} & \cdots & b_{2,nk} \\ b_{3,1} & b_{3,2} & b_{3,3} & \cdots & b_{3,nk} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{nr,1} & b_{nr,2} & b_{nr,3} & \cdots & b_{nr,nk} \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & \cdots & c_{1,nc} \\ c_{2,1} & c_{2,2} & c_{2,3} & \cdots & c_{2,nc} \\ c_{3,1} & c_{3,2} & c_{3,3} & \cdots & c_{3,nc} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_{nk,1} & c_{nk,2} & c_{nk,3} & \cdots & c_{nk,nc} \end{bmatrix}$$

The definition of $A = B \bullet C$ is

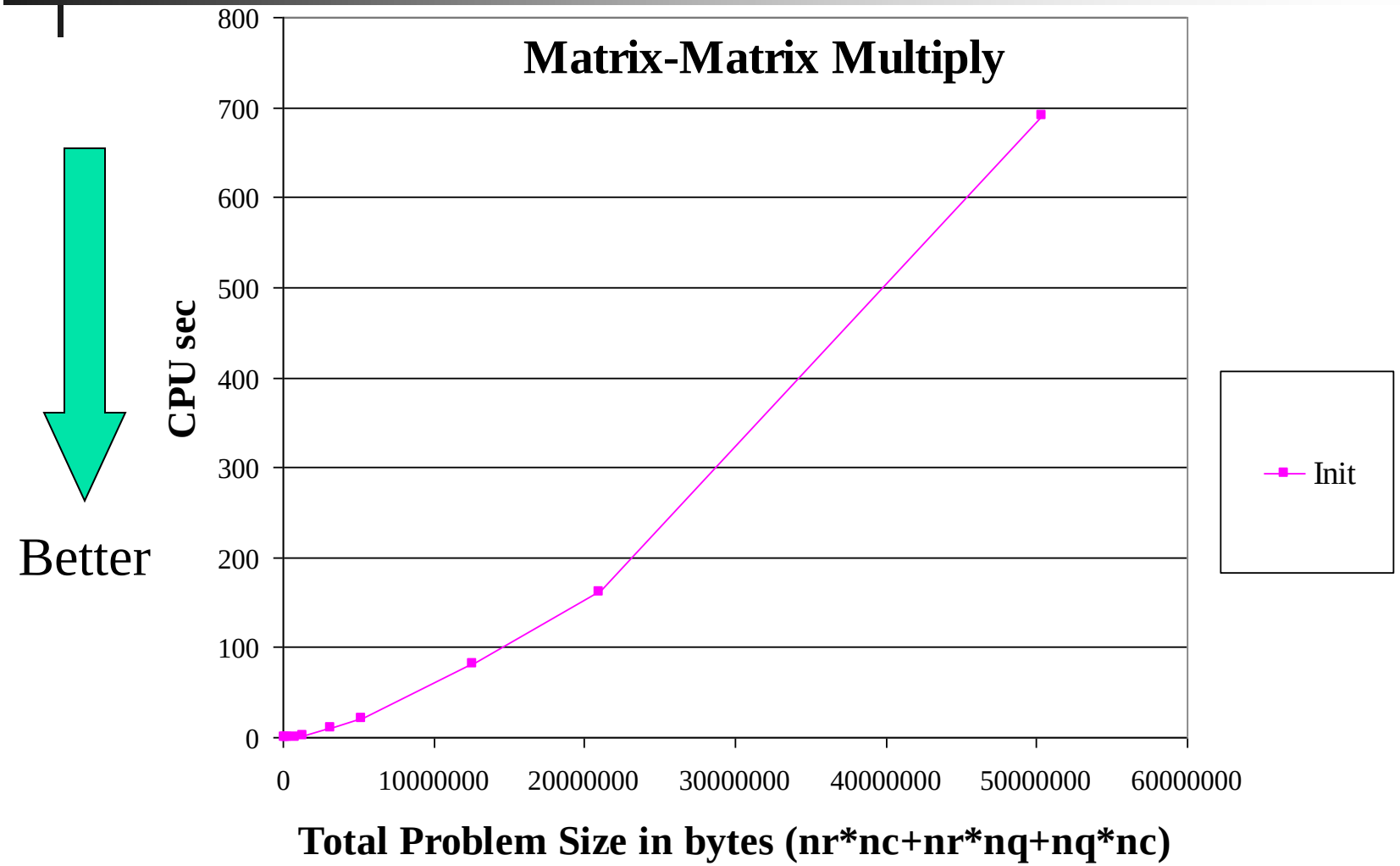
$$a_{r,c} = \sum_{k=1}^{nk} b_{r,k} \cdot c_{k,c} = b_{r,1} \cdot c_{1,c} + b_{r,2} \cdot c_{2,c} + b_{r,3} \cdot c_{3,c} + \ldots + b_{r,nk} \cdot c_{nk,c}$$

for $r \in \{1, nr\}$, $c \in \{1, nc\}$.

Matrix Multiply: Naïve Version

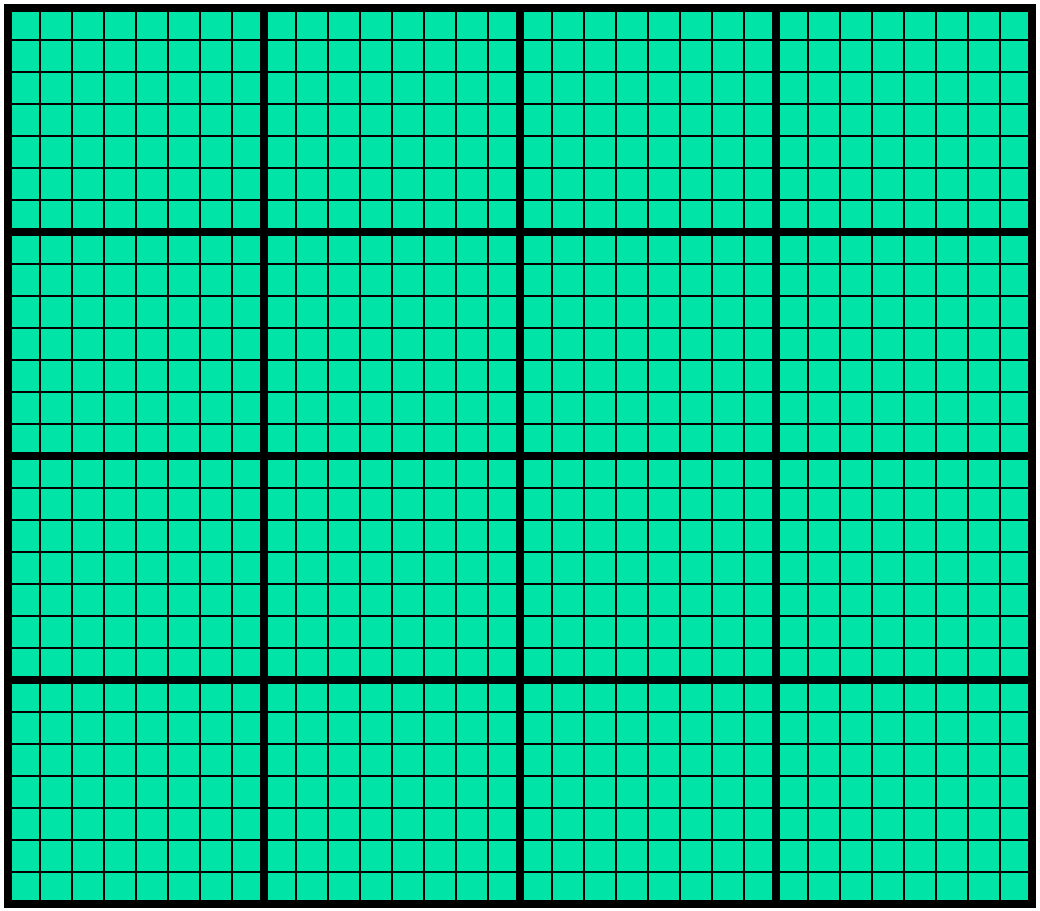
```
SUBROUTINE matrix_matrix_mult_naive (dst, src1, src2, &
 &                                   nr, nc, nq)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2

  INTEGER :: r, c, q

  DO c = 1, nc
    DO r = 1, nr
      dst(r,c) = 0.0
      DO q = 1, nq
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO
    END DO
  END DO
END SUBROUTINE matrix_matrix_mult_naive
```

Performance of Matrix Multiply



Better

Tiling



Tiling

- ***Tile***: A small rectangular subdomain of a problem domain. Sometimes called a ***block*** or a ***chunk***.
- ***Tiling***: Breaking the domain into tiles.
- **Tiling strategy**: Operate on each tile to completion, then move to the next tile.
- **Tile size** can be set at runtime, according to what's best for the machine that you're running on.

Tiling Code

```
SUBROUTINE matrix_matrix_mult_by_tiling (dst, src1, src2, nr, nc, nq, &
 &           rtilesize, ctilesize, qtilesize)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2
  INTEGER,INTENT(IN) :: rtilesize, ctilesize, qtilesize

  INTEGER :: rstart, rend, cstart, cend, qstart, qend

  DO cstart = 1, nc, ctilesize
    cend = cstart + ctilesize - 1
    IF (cend > nc) cend = nc
    DO rstart = 1, nr, rtilesize
      rend = rstart + rtilesize - 1
      IF (rend > nr) rend = nr
      DO qstart = 1, nq, qtilesize
        qend = qstart + qtilesize - 1
        IF (qend > nq) qend = nq
        CALL matrix_matrix_mult_tile(dst, src1, src2, nr, nc, nq, &
 &                                   rstart, rend, cstart, cend, qstart, qend)
      END DO
    END DO
  END DO
END SUBROUTINE matrix_matrix_mult_by_tiling
```

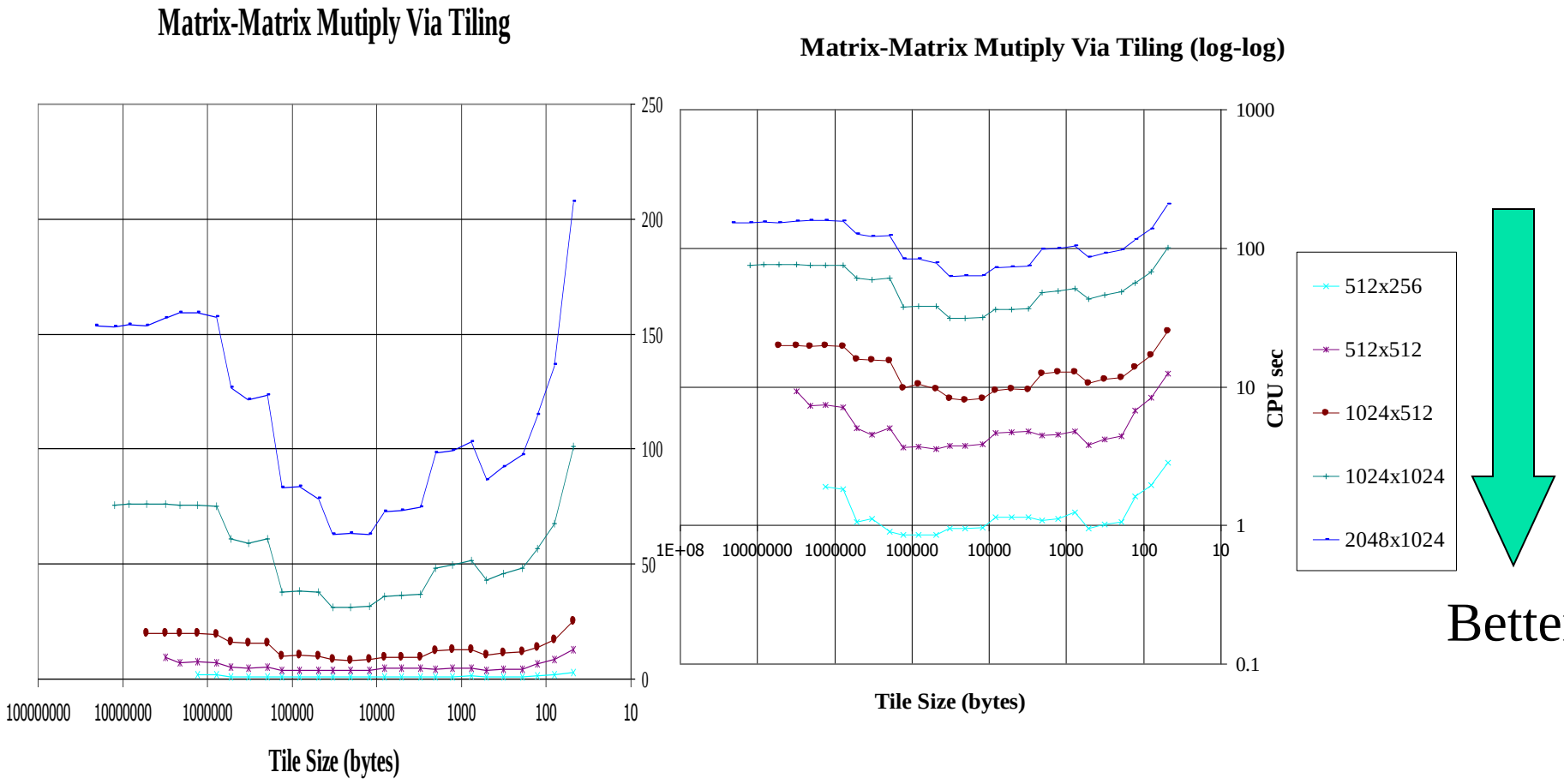
Multiplying Within a Tile

```
SUBROUTINE matrix_matrix_mult_tile (dst, src1, src2, nr, nc, nq, &
 &                 rstart, rend, cstart, cend, qstart, qend)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2
  INTEGER,INTENT(IN) :: rstart, rend, cstart, cend, qstart, qend

  INTEGER :: r, c, q

  DO c = cstart, cend
    DO r = rstart, rend
      IF (qstart == 1) dst(r,c) = 0.0
      DO q = qstart, qend
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO
    END DO
  END DO
END SUBROUTINE matrix_matrix_mult_tile
```

Reminder: Naïve Version, Again

```
SUBROUTINE matrix_matrix_mult_naive (dst, src1, src2, &
 &                                   nr, nc, nq)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2

  INTEGER :: r, c, q

  DO c = 1, nc
    DO r = 1, nr
      dst(r,c) = 0.0
      DO q = 1, nq
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO
    END DO
  END DO
END SUBROUTINE matrix_matrix_mult_naive
```

Performance with Tiling



The Advantages of Tiling

- It allows your code to **exploit data locality** better, to get much more cache reuse: your code runs faster!
- It's a relatively **modest amount of extra coding** (typically a few wrapper functions and some changes to loop bounds).
- **If you don't need** tiling – because of the hardware, the compiler or the problem size – then you can **turn it off by simply** setting the tile size equal to the problem size.

Why Does Tiling Work Here?

Cache optimization works best when the number of calculations per byte is large.

For example, with matrix-matrix multiply on an $n \times n$ matrix, there are $\mathbf{O}(n^3)$ calculations (on the order of n^3), but only $\mathbf{O}(n^2)$ bytes of data.

So, for large n, there are a huge number of calculations per byte transferred between RAM and cache.

Will Tiling Always Work?

Tiling **WON'T** always work. Why?

Well, tiling works well when:

- the order in which calculations occur doesn't matter much, AND
- there are lots and lots of calculations to do for each memory movement.

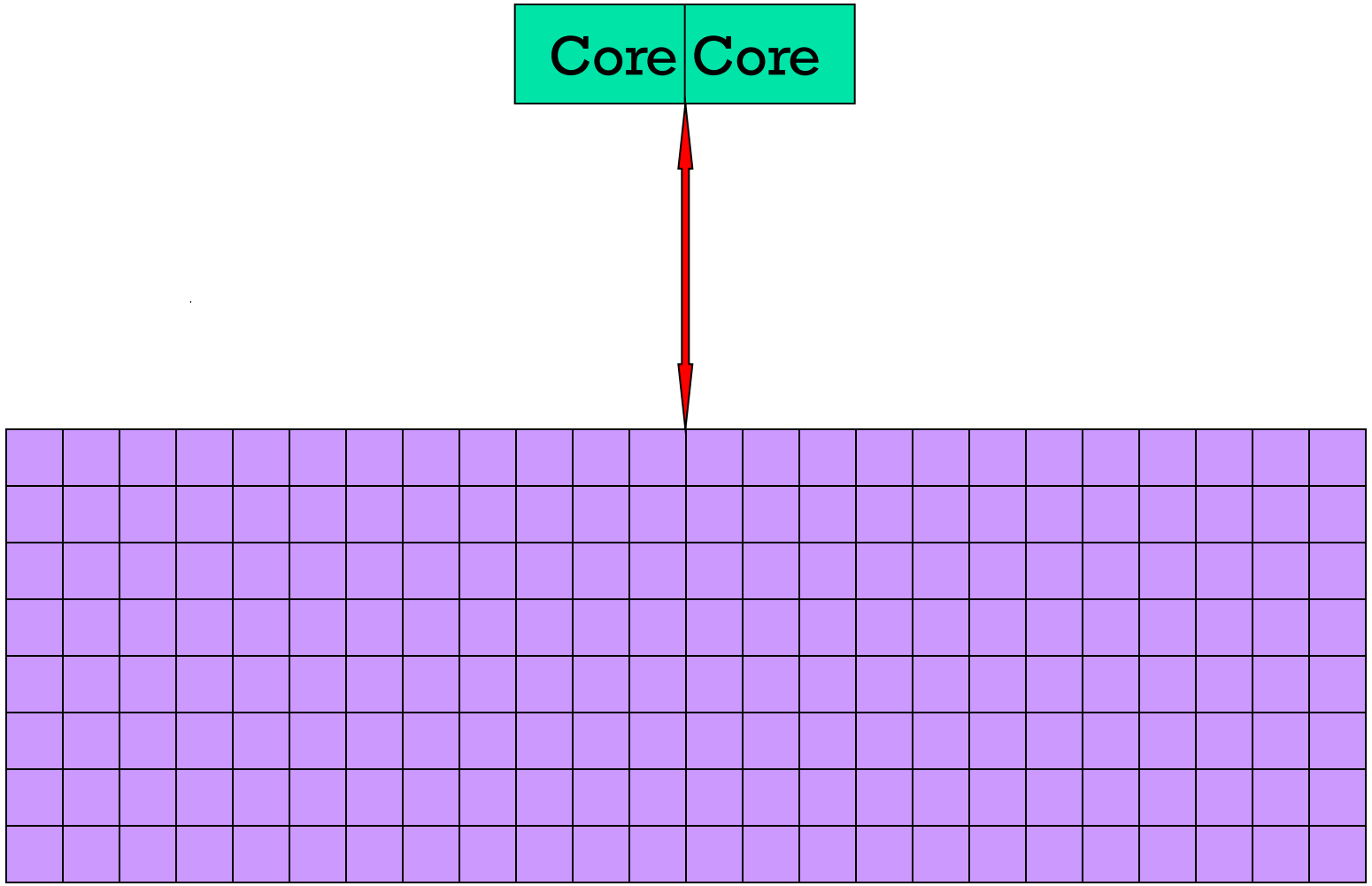
If either condition is absent, then tiling won't help.

Multicore/Many-core Basics

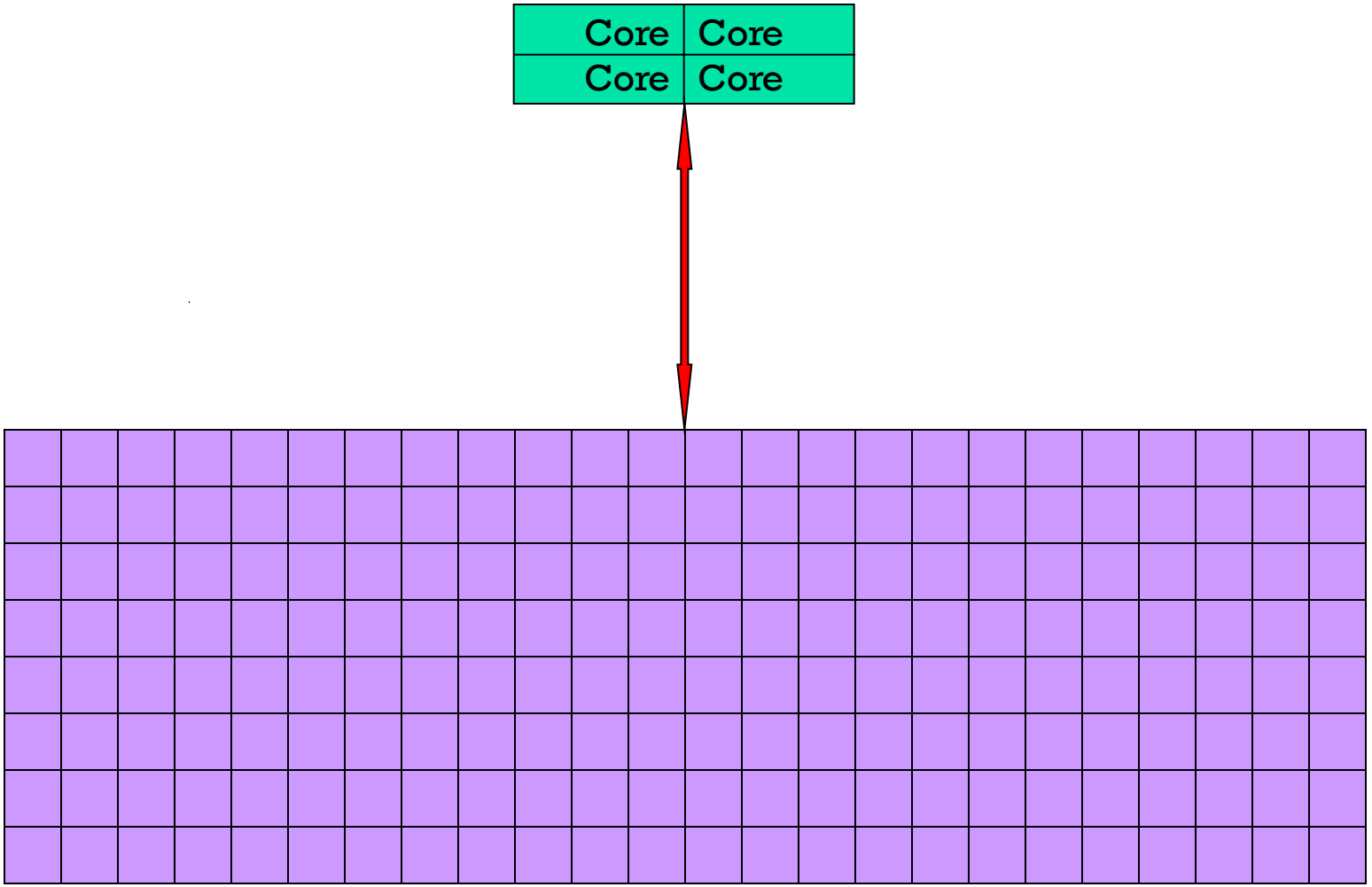
What is Multicore?

- In the olden days (that is, the first half of 2005), each CPU chip had one "brain" in it.
- Starting the second half of 2005, each CPU chip can have up to 2 ***cores*** (brains); starting in late 2006, 4 cores; starting in late 2008, 6 cores; in early 2010, 8 cores; in mid 2010, 12 cores.
- **Jargon**: Each CPU chip plugs into a ***socket***, so these days, to avoid confusion, people refer to **sockets** and **cores**, rather than CPUs or processors.
- Each core is just like a full blown CPU, except that it shares its socket (and maybe some of its cache) with one or more other cores – and therefore shares its bandwidth to RAM with them.

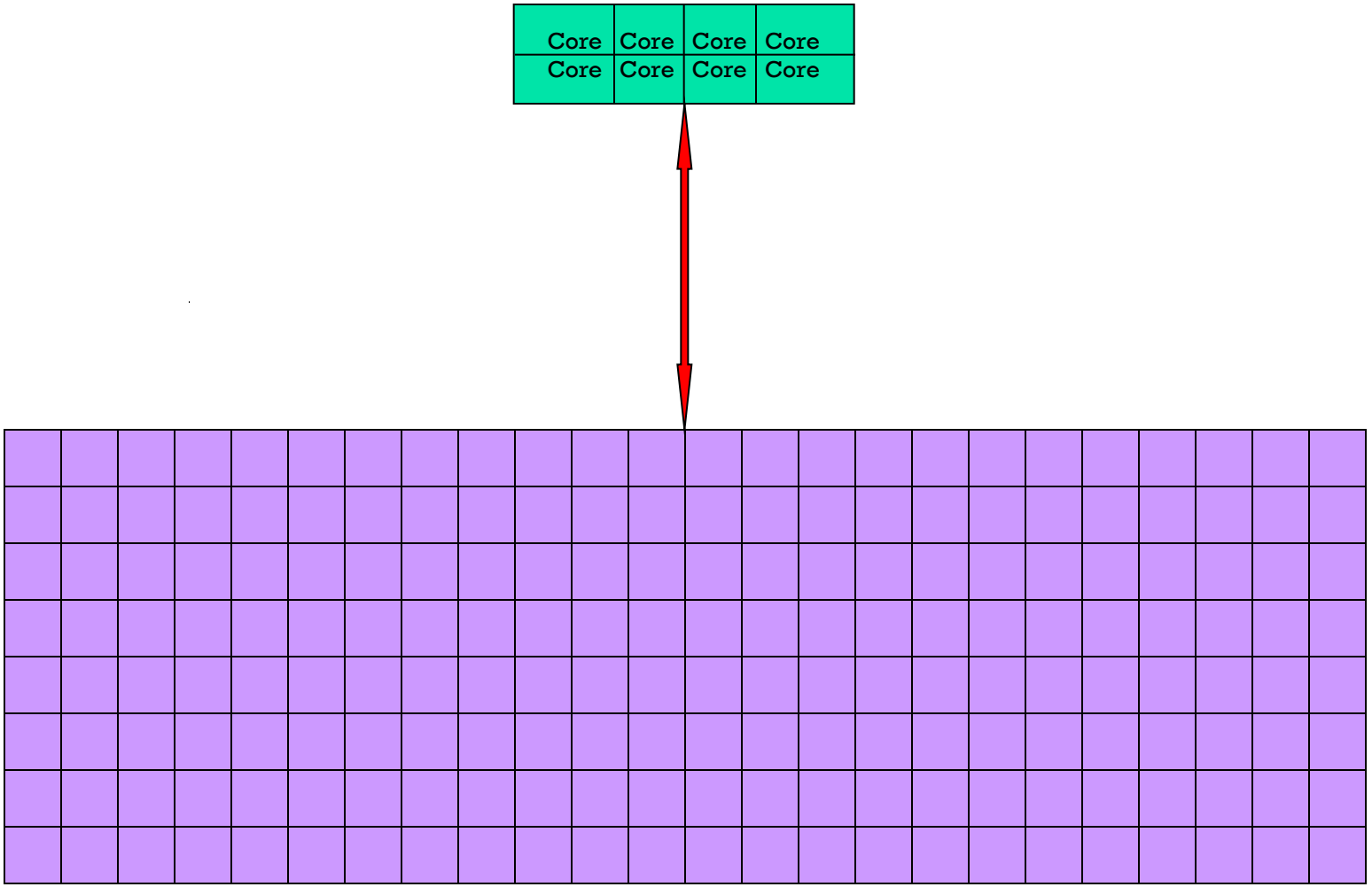
Dual Core



Quad Core



Oct Core



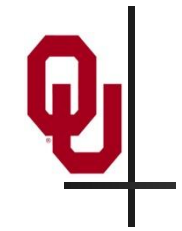
The Challenge of Multicore: RAM

- Each socket has access to a certain amount of RAM, at a **fixed RAM bandwidth per SOCKET** – or even per node.
- As the number of cores per socket increases, the **contention for RAM bandwidth increases** too.
- At 2 or even 4 cores in a socket, this problem isn't too bad. But at 16 or 32 or 80 cores, it's **a huge problem**.
- So, applications that **are cache optimized** will get **big speedups**.
- But, applications whose performance is **limited by RAM bandwidth** are going to speed up only as fast as RAM bandwidth speeds up.
- RAM bandwidth **speeds up much slower** than CPU speeds up.

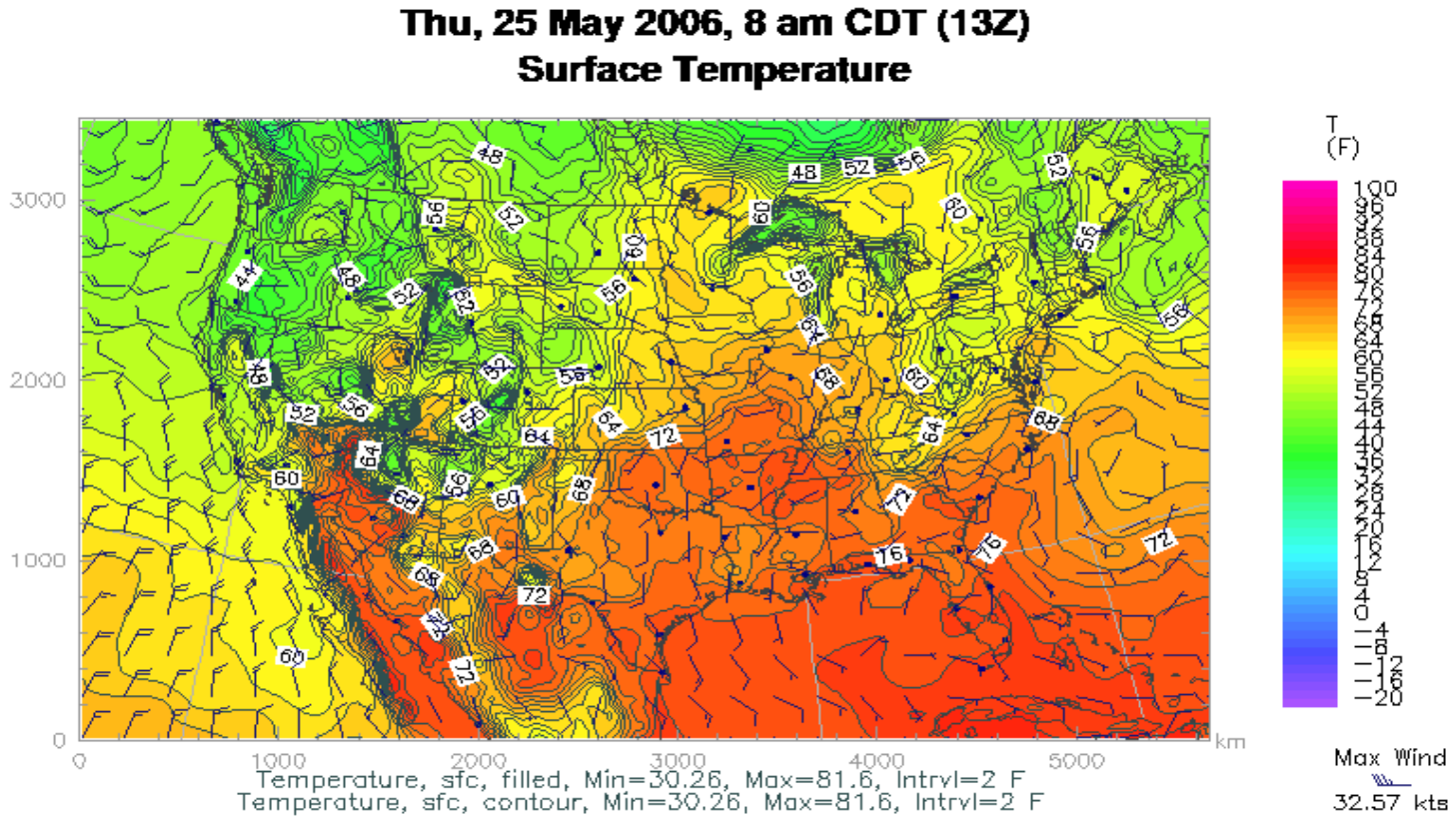
The Challenge of Multicore: Network

- Each node has access to a certain number of network ports, at a **fixed number of network ports per NODE**.
- As the number of cores per node increases, the **contention for network ports increases** too.
- At 2 or 4 cores in a socket, this problem isn't too bad. But at 16 or 32 or 80 cores, it's **a huge problem**.
- So, applications that **do minimal communication** will get **big speedups**.
- But, applications whose performance is **limited by the number of MPI messages** are going to speed up very very little – and may even crash the node.

A Concrete Example: Weather Forecasting



Weather Forecasting

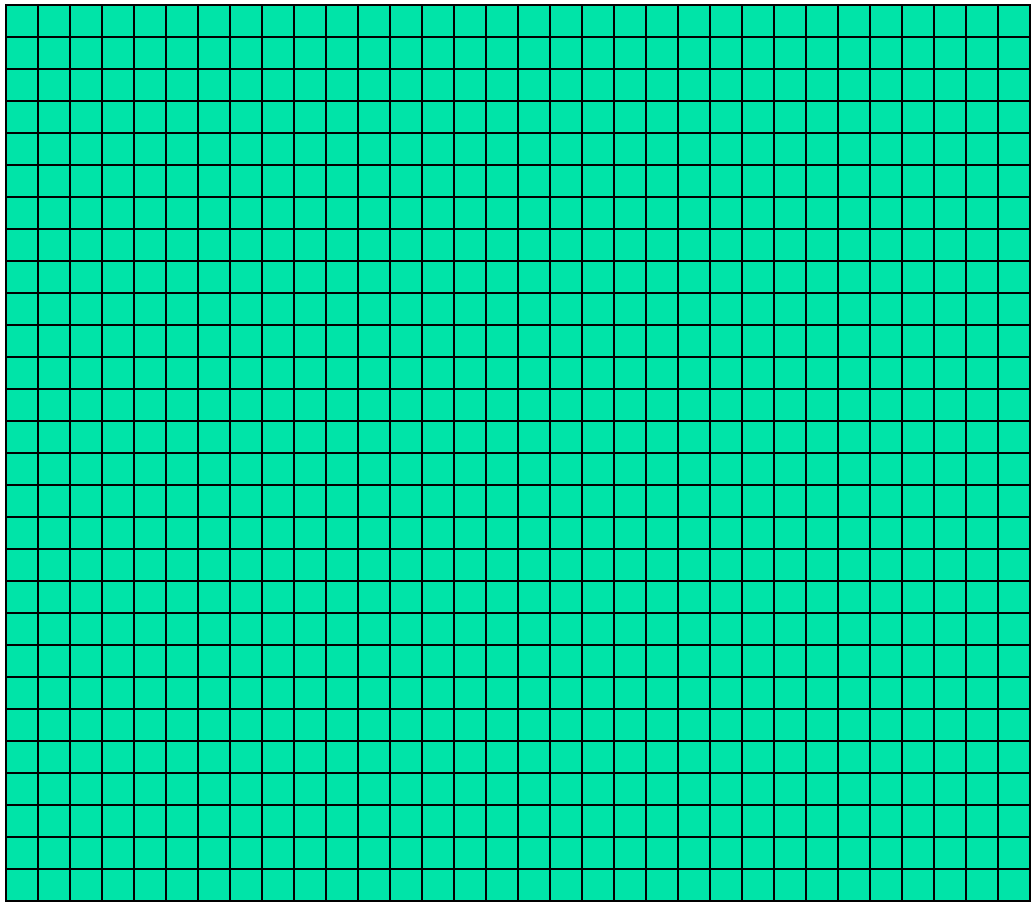


http://www.caps.ou.edu/wx/p/r/conus/fcst/

Weather Forecasting

- Weather forecasting is a **transport** problem.
- The goal is to predict future weather conditions by simulating the movement of fluids in Earth's atmosphere.
- The physics is the Navier-Stokes Equations.
- The numerical method is Finite Difference.

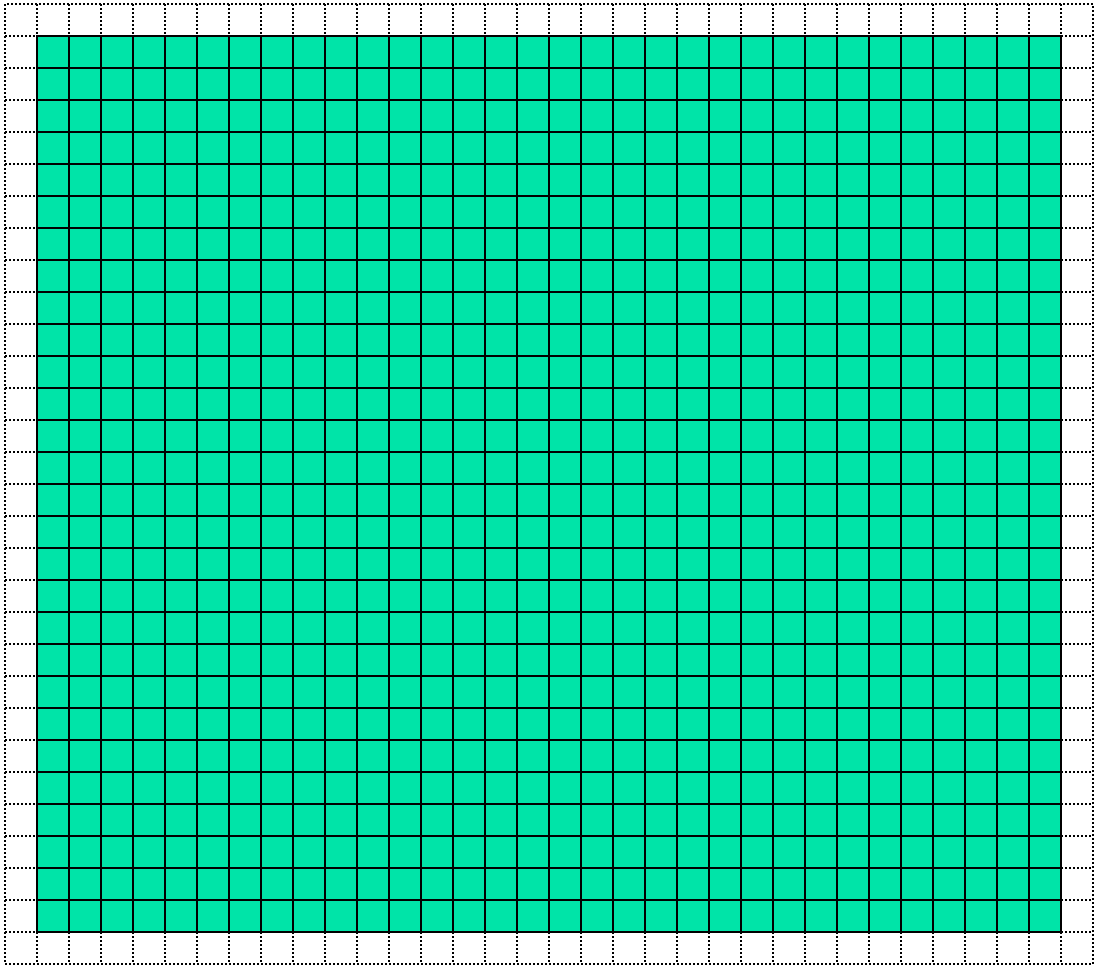
Cartesian Mesh



Finite Difference

$$unew(i,j,k) = F(uold, i, j, k, \Delta t) =$$
$$F(uold(i,j,k),$$
$$uold(i\text{-}1,j,k), uold(i\text{+}1,j,k),$$
$$uold(i,j\text{-}1,k), uold(i,j\text{+}1,k),$$
$$uold(i,j,k\text{-}1), uold(i,j,k\text{+}1), \Delta t)$$

Ghost Boundary Zones



Virtual Memory

Virtual Memory

- Typically, the amount of main memory (RAM) that a CPU can ***address*** is larger than the amount of data physically present in the computer.
- For example, consider a laptop that can address 16 GB of main memory (roughly 16 billion bytes), but only contains 2 GB (roughly 2 billion bytes).

Virtual Memory (cont'd)

- **Locality**: Most programs don't jump all over the memory that they use; instead, they work in a particular area of memory for a while, then move to another area.
- So, you can offload onto hard disk much of the ***memory image*** of a program that's running.

Virtual Memory (cont'd)

- Memory is chopped up into many ***pages*** of modest size (e.g., 1 KB – 32 KB; typically 4 KB).
- Only pages that have been recently used actually reside in memory; the rest are stored on hard disk.
- Hard disk is typically 0.1% as fast as main memory, so you get better performance if you rarely get a ***page fault***, which forces a read from (and maybe a write to) hard disk: **exploit data locality!**

Cache vs. Virtual Memory

- Lines (cache) vs. pages (VM)
- Cache faster than RAM (cache) vs. RAM faster than disk (VM)

Virtual Memory

- Every CPU family today uses ***virtual memory***, in which disk pretends to be a bigger RAM.
- Virtual memory capability **can't be turned off**.
- RAM is split up into ***pages***, typically **4 KB** each.
- Each page is either **in RAM** or **out on disk**.
- To keep track of the pages, a ***page table*** notes whether each table is in RAM, where it is in RAM (that is, physical address and virtual address are different), and some other information.
- So, a 4 GB physical RAM would need over a million ***page table entries***.

Why Virtual Memory is Slow

- When you want to access a byte of memory, you have to find out whether it's in physical memory (RAM) or virtual disk (disk) – and the page table is in RAM!
- A page table of a million entries can't fit in a 2 MB cache.
- So, each memory access (load or store) is actually 2 memory accesses: the first for the page table entry, and the second for the data itself.
- This is slow!
- And notice, this is assuming that you don't need more memory than your physical RAM.

The Notorious T.L.B.

- To speed up memory accesses, CPUs today have a special cache just for page table entries, known as the ***Translation Lookaside Buffer*** (TLB).
- The size of TLBs varies from 64 entries to 1024 entries, depending on chip families.
- At 4 KB pages, this means that the size of cache covered by the TLB varies from 256 KB to 4 MB.

The T.L.B. on a Recent Chip

On Intel Core Duo ("Yonah"):

- Cache size is 2 MB per core.
- Page size is 4 KB.
- A core's data TLB size is 128 page table entries.
- Therefore, D-TLB only covers 512 KB of cache.

The T.L.B. on a Recent Chip

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- Cache size is 2 MB per core.
- Page size is 4 KB.
- A core's data TLB size is 128 page table entries.
- Therefore, D-TLB only covers 512 KB of cache.
- Mesh: At 100 vertical levels of 150 single precision variables, 512 KB is a 3 x 3 vertical domain – **nothing but ghost zones**!
- The cost of a TLB miss is 49 cycles, equivalent to as many as **196 calculations**! (4 FLOPs per cycle)

http://www.digit-life.com/articles2/cpu/rmma-via-c7.html

Software Strategies for Weather Forecasting on Multicore/Many-core

Tiling NOT Good for Weather Codes

- Weather codes typically have on the order of 150 3D arrays used in each timestep (some transferred multiple times in the same timestep, but let's ignore that for simplicity).
- These arrays typically are single precision (4 bytes per floating point value).
- So, a typical weather code uses about 600 bytes per mesh zone per timestep.
- Weather codes typically do 5,000 to 10,000 calculations per mesh zone per timestep.
- So, the ratio of calculations to data is less than 20 to 1 – much less than the 73 to 1 needed (on mid-2008 hardware).

Weather Forecasting and Cache

- On current weather codes, data decomposition is per process. That is, each process gets one subdomain.
- As CPUs speed up and RAM sizes grow, the size of each processor's subdomain grows too.
- However, given RAM bandwidth limitations, this means that performance can only grow with RAM speed – which increases slower than CPU speed.
- If the codes were optimized for cache, would they speed up more?
- First: How to optimize for cache?

How to Get Good Cache Reuse?

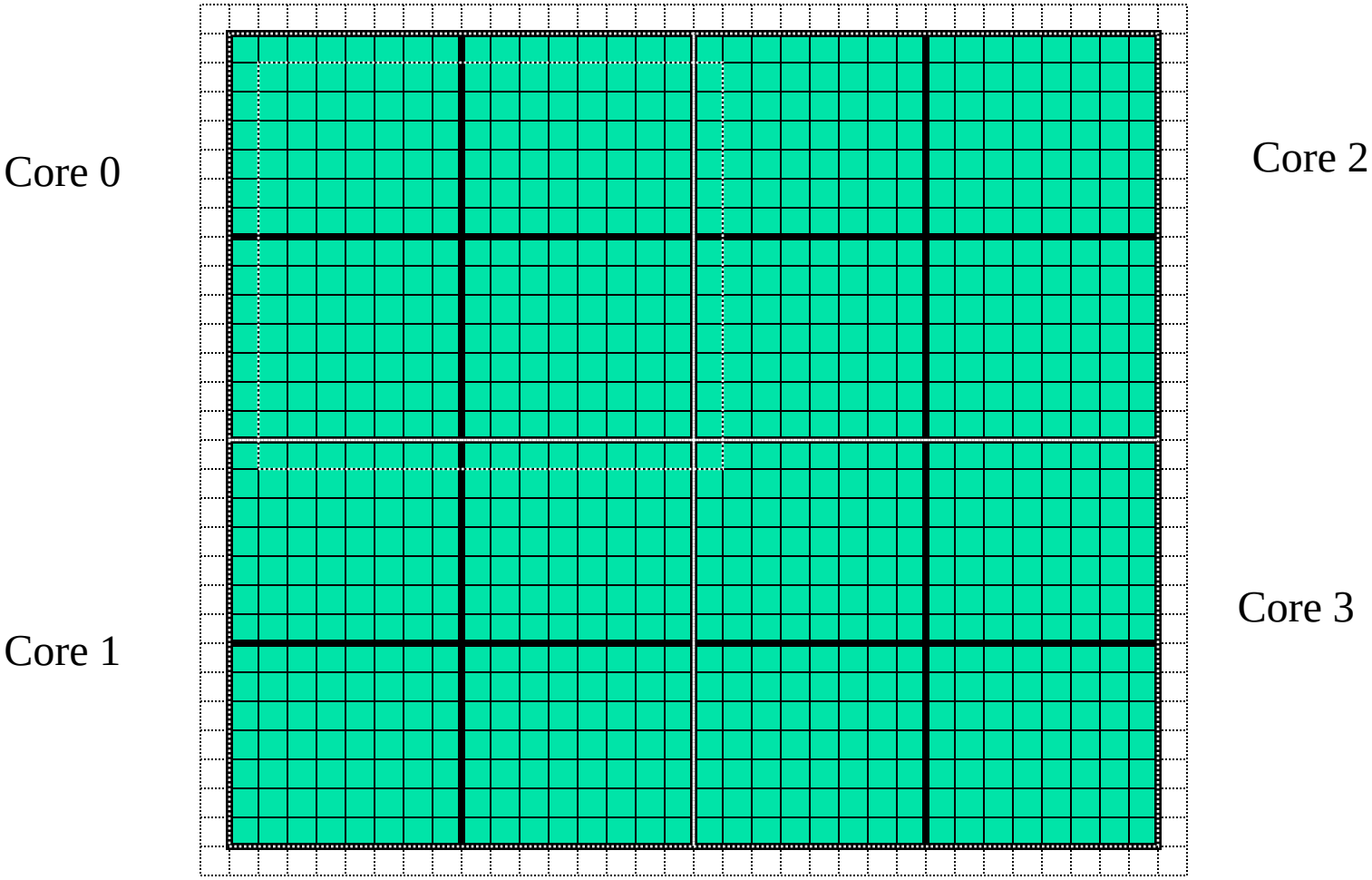
- Multiple independent subdomains per processor.
- Each subdomain fits entirely in L2 cache.
- Each subdomain's page table entries fit entirely in the TLB.
- Expanded ghost zone stencil allows multiple timesteps before communicating with neighboring subdomains.
- Parallelize along the Z-axis as well as X and Y.
- Use higher order numerical schemes.
- Reduce the memory footprint as much as possible.

Coincidentally, this also reduces communication cost.

Cache Optimization Strategy: Tiling?

Would tiling work as a cache optimization strategy for weather forecasting codes?

Multiple Subdomains Per Core



Why Multiple Subdomains?

- If each subdomain fits in cache, then the CPU can bring all the data of a subdomain into cache, chew on it for a while, then move on to the next subdomain: lots of cache reuse!
- Oh, wait, what about the TLB? Better make the subdomains smaller! (So more of them.)
- But, doesn't tiling have the same effect?

Why Independent Subdomains?

- Originally, the point of this strategy was to hide the cost of communication.
- When you finish chewing up a subdomain, send its data to its neighbors non-blocking (**`MPI_Isend`**).
- While the subdomain's data is flying through the interconnect, work on other subdomains, which hides the communication cost.
- When it's time to work on this subdomain again, collect its data (**`MPI_Waitall`**).
- If you've done enough work, then the communication cost is zero.

Expand the Array Stencil

- If you expand the array stencil of each subdomain beyond the numerical stencil, then you don't have to communicate as often.
- When you communicate, instead of sending a slice along each face, send a slab, with extra stencil levels.
- In the first timestep after communicating, do extra calculations out to just inside the numerical stencil.
- In subsequent timesteps, calculate fewer and fewer stencil levels, until it's time to communicate again – less total communication, and more calculations to hide the communication cost underneath!

An Extra Win!

- If you do all this, there's an amazing side effect: you get better cache reuse, because you stick with the same subdomain for a longer period of time.
- So, instead of doing, say, 5000 calculations per zone per timestep, you can do 15000 or 20000.
- So, you can better amortize the cost of transferring the data between RAM and cache.

New Algorithm (F90)

```
DO timestep = 1, number_of_timesteps, extra_stencil_levels
    DO subdomain = 1, number_of_local_subdomains
        CALL receive_messages_nonblocking(subdomain,
                 timestep)
        DO extra_stencil_level=0, extra_stencil_levels - 1
            CALL calculate_entire_timestep(subdomain,
                     timestep + extra_stencil_level)
        END DO
        CALL send_messages_nonblocking(subdomain,
                 timestep + extra_stencil_levels)
    END DO
END DO
```

New Algorithm (C)

```
for (timestep = 0;
     timestep < number_of_timesteps;
     timestep += extra_stencil_levels) {
    for (subdomain = 0;
         subdomain < number_of_local_subdomains;
         subdomain++) {
        receive_messages_nonblocking(subdomain, timestep);
        for (extra_stencil_level = 0;
             extra_stencil_level < extra_stencil_levels;
             extra_stencil_level++) {
            calculate_entire_timestep(subdomain,
                timestep + extra_stencil_level);
        } /* for extra_stencil_level */
        send_messages_nonblocking(subdomain,
            timestep + extra_stencil_levels);
    } /* for subdomain */
} /* for timestep */
```

Higher Order Numerical Schemes

- Higher order numerical schemes are great, because they require more calculations per mesh zone per timestep, which you need to amortize the cost of transferring data between RAM and cache. Might as well!
- Plus, they allow you to use a larger time interval per timestep (`dt`), so you can do fewer total timesteps for the same accuracy – or you can get higher accuracy for the same number of timesteps.

Parallelize in Z

- Most weather forecast codes parallelize in X and Y, but not in Z, because gravity makes the calculations along Z more complicated than X and Y.
- But, that means that each subdomain has a high number of zones in Z, compared to X and Y.
- For example, a 1 km CONUS run will probably have 100 zones in Z (25 km at 0.25 km resolution).

Multicore/Many-core Problem

- Most multicore chip families have relatively small cache per core (for example, 1 - 4 MB per core at the highest/slowest cache level) – and this problem seems likely to remain.
- Small TLBs make the problem worse: 512 KB per core rather than 1 - 4 MB.
- So, to get good cache reuse, you need subdomains of no more than 512 KB.
- If you have 150 3D variables at single precision, and 100 zones in Z, then your horizontal size will be 3 x 3 zones – just enough for your stencil!

What Do We Need?

- We need much bigger caches!
  - 16 MB cache ➔ 16 x 16 horizontal including stencil
  - 32 MB cache ➔ 23 x 23 horizontal including stencil
- TLB must be big enough to cover the entire cache.
- It'd be nice to have RAM speed increase as fast as core counts increase, but let's not kid ourselves.

Keep this in mind when we get to GPGPU!

University of Illinois
at Urbana-Champaign

Undergraduate Petascale Internships

- NSF support for undergraduate internships involving high-performance computing in science and engineering.

- Provides a stipend ($5k over the year), a two-week intensive high-performance computing workshop at the National Center for Supercomputing Applications, and travel to the SC11 supercomputing conference in November.

- This support is intended to allow you to work with a faculty mentor on your campus. Have your faculty mentor fill out an intern position description at the link below. There are also some open positions listed on our site.

- Student applications and position descriptions from faculty are due by March 31, 2011. Selections and notifications will be made by April 15.

http://shodor.org/petascale/participation/internships/

Summer Workshops 2011

- In Summer 2011, there will be several workshops on HPC and Computational and Data Enabled Science and Engineering (CDESE) across the US.
- These will be weeklong intensives, running from Sunday evening through Saturday morning.
- We're currently working on where and when those workshops will be held.
- Once we've got that worked out, we'll announce them and open up the registration website.
- One of them will be held at OU.

OK Supercomputing Symposium 2011

2003 Keynote:
Peter Freeman
NSF
Computer & Information Science & Engineering
Assistant Director

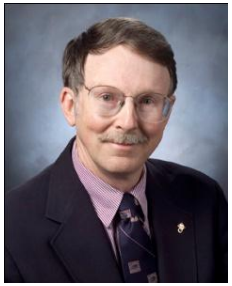
2004 Keynote:
Sangtae Kim
NSF Shared Cyberinfrastructure Division Director

2005 Keynote:
Walt Brooks
NASA Advanced Supercomputing Division Director

2006 Keynote:
Dan Atkins
Head of NSF's Office of Cyberinfrastructure

2007 Keynote:
Jay Boisseau
Director
Texas Advanced Computing Center
U. Texas Austin

2008 Keynote:
José Munoz
Deputy Office Director/ Senior Scientific Advisor
NSF Office of Cyberinfrastructure



2009 Keynote:
Douglass Post
Chief Scientist
US Dept of Defense HPC Modernization Program

2010 Keynote:
Horst Simon
Deputy Director
Lawrence Berkeley National Laboratory

?

2011 Keynote to be announced

FREE! Wed Oct 12 2011 @ OU

http://symposium2011.oscer.ou.edu/

Parallel Programming Workshop
FREE! Tue Oct 11 2011 @ OU
FREE! Symposium Wed Oct 12 2011 @ OU

SC11 Education Program

- At the SC11 supercomputing conference, we'll hold our annual Education Program, Sat Nov 12 – Tue Nov 15.
- You can apply to attend, either fully funded by SC11 or self-funded.
- Henry is the SC11 Education Chair.
- We'll alert everyone once the registration website opens.

Thanks for your attention!

Questions?

www.oscer.ou.edu

References

[1] Image by Greg Bryan, Columbia U.

[2] "Update on the Collaborative Radar Acquisition Field Test (CRAFT): Planning for the Next Steps." Presented to NWS Headquarters August 30 2001.

[3] See http://hneeman.oscer.ou.edu/hamr.html for details.

[4] http://www.dell.com/

[5] http://www.vw.com/newbeetle/

[6] Richard Gerber, The Software Optimization Cookbook: High-performance Recipes for the Intel Architecture. Intel Press, 2002, pp. 161-168.

[7] RightMark Memory Analyzer. http://cpu.rightmark.org/

[8] ftp://download.intel.com/design/Pentium4/papers/24943801.pdf

[9] http://www.seagate.com/cda/products/discsales/personal/family/0,1085,621,00.html

[10] http://www.samsung.com/Products/OpticalDiscDrive/SlimDrive/OpticalDiscDrive_SlimDrive_SN_S082D.asp?page=Specifications

[11] ftp://download.intel.com/design/Pentium4/manuals/24896606.pdf

[12] http://www.pricewatch.com/