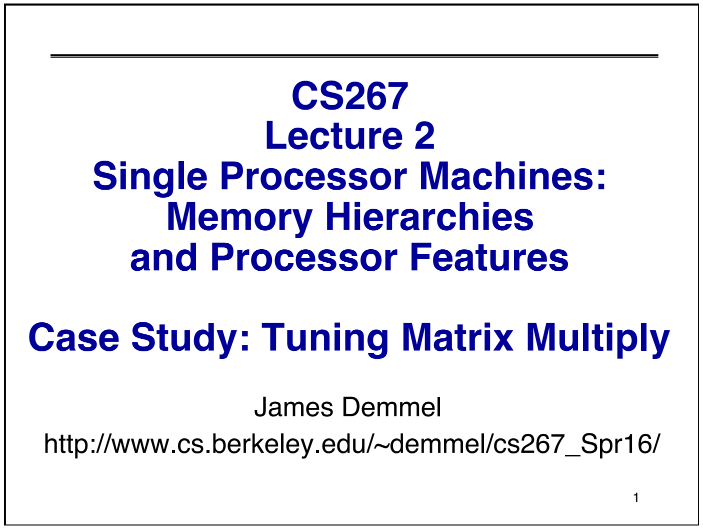
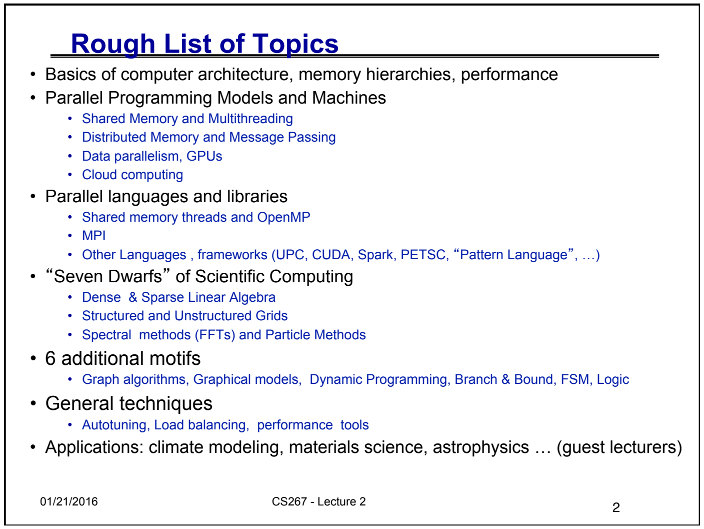


CS267
Lecture 2
Single Processor Machines: Memory Hierarchies and Processor Features

Case Study: Tuning Matrix Multiply

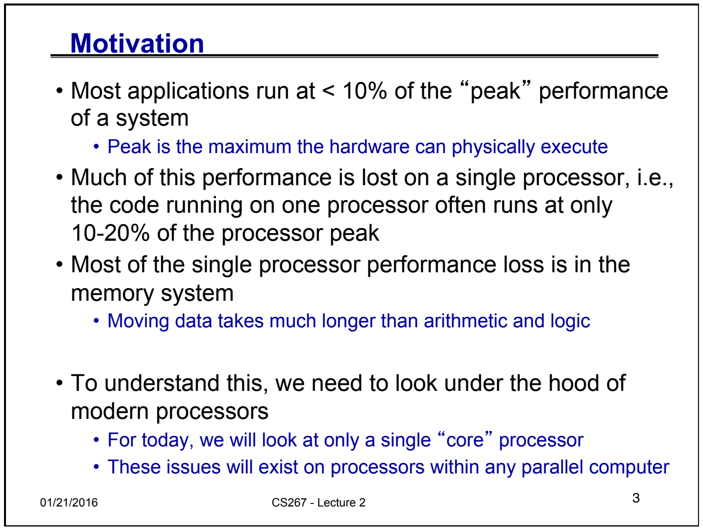
James Demmel

http://www.cs.berkeley.edu/~demmel/cs267_Spr16/



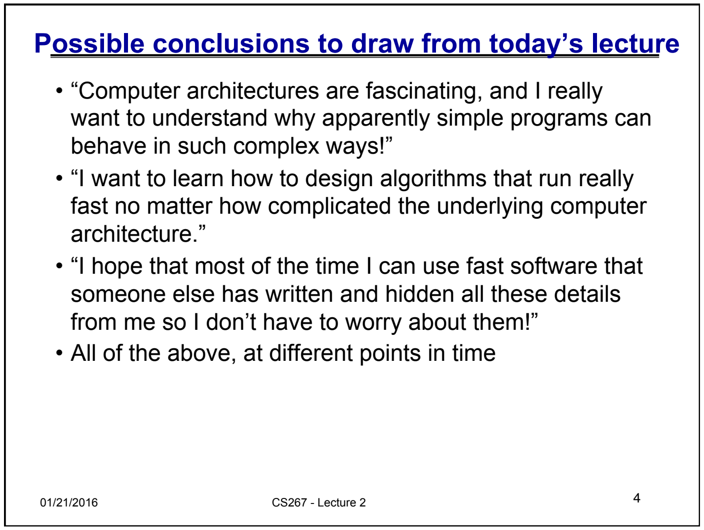
Rough List of Topics

- Basics of computer architecture, memory hierarchies, performance
- Parallel Programming Models and Machines
  - Shared Memory and Multithreading
  - Distributed Memory and Message Passing
  - Data parallelism, GPUs
  - Cloud computing
- Parallel languages and libraries
  - Shared memory threads and OpenMP
  - MPI
  - Other Languages , frameworks (UPC, CUDA, Spark, PETSC, "Pattern Language", …)
- "Seven Dwarfs" of Scientific Computing
  - Dense & Sparse Linear Algebra
  - Structured and Unstructured Grids
  - Spectral methods (FFTs) and Particle Methods
- 6 additional motifs
  - Graph algorithms, Graphical models, Dynamic Programming, Branch & Bound, FSM, Logic
- General techniques
  - Autotuning, Load balancing, performance tools
- Applications: climate modeling, materials science, astrophysics … (guest lecturers)



Motivation

- Most applications run at < 10% of the "peak" performance of a system
  - Peak is the maximum the hardware can physically execute
- Much of this performance is lost on a single processor, i.e., the code running on one processor often runs at only 10-20% of the processor peak
- Most of the single processor performance loss is in the memory system
  - Moving data takes much longer than arithmetic and logic
- To understand this, we need to look under the hood of modern processors
  - For today, we will look at only a single "core" processor
  - These issues will exist on processors within any parallel computer



Possible conclusions to draw from today's lecture

- "Computer architectures are fascinating, and I really want to understand why apparently simple programs can behave in such complex ways!"
- "I want to learn how to design algorithms that run really fast no matter how complicated the underlying computer architecture."
- "I hope that most of the time I can use fast software that someone else has written and hidden all these details from me so I don't have to worry about them!"
- All of the above, at different points in time

Outline

- Idealized and actual costs in modern processors
- Memory hierarchies
  - Use of microbenchmarks to characterized performance
- Parallelism within single processors
- Case study: Matrix Multiplication
  - Use of performance models to understand performance
  - Attainable lower bounds on communication

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Idealized Uniprocessor Model

- **Processor names bytes, words, etc. in its address space**
  - **These represent integers, floats, pointers, arrays, etc.**
- **Operations include**
  - **Read and write into very fast memory called registers**
  - **Arithmetic and other logical operations on registers**
- **Order specified by program**
  - **Read returns the most recently written data**
  - **Compiler and architecture translate high level expressions into "obvious" lower level instructions**

```
                    Read address(B) to R1
                    Read address(C) to R2
A = B + C ⇒         R3 = R1 + R2
                    Write R3 to Address(A)
```

  - **Hardware executes instructions in order specified by compiler**
- ***Idealized Cost***
  - **Each operation has roughly the same cost**

    (read, write, add, multiply, etc.)

Uniprocessors in the Real World

- **Real processors have**
  - **registers and caches**
    - **small amounts of fast memory**
    - **store values of recently used or nearby data**
    - **different memory ops can have very different costs**
  - **parallelism**
    - **multiple "functional units" that can run in parallel**
    - **different orders, instruction mixes have different costs**
  - **pipelining**
    - **a form of parallelism, like an assembly line in a factory**
- **Why is this your problem?**
    - **In theory, compilers and hardware "understand" all this and can optimize your program; in practice they don't.**
    - **They won't know about a different algorithm that might be a much better "match" to the processor**

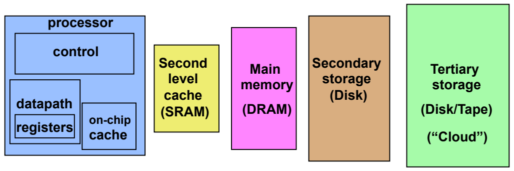
In theory there is no difference between theory and practice.
But in practice there is. - Yogi Berra

Outline

- Idealized and actual costs in modern processors
- Memory hierarchies
  - Temporal and spatial locality
  - Basics of caches
  - Use of microbenchmarks to characterized performance
- Parallelism within single processors
- Case study: Matrix Multiplication
  - Use of performance models to understand performance
  - Attainable lower bounds on communication

Memory Hierarchy

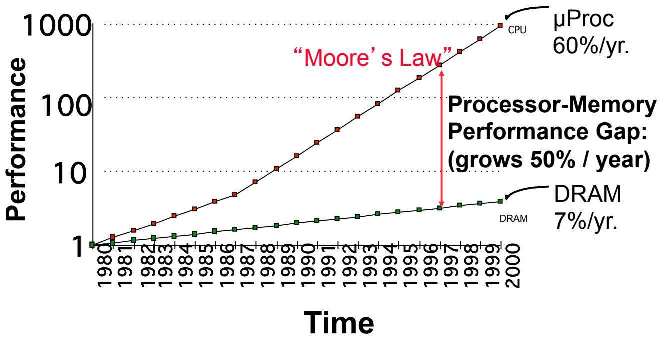
- Most programs have a high degree of locality in their accesses
  - **spatial locality:** accessing things nearby previous accesses
  - **temporal locality:** reusing an item that was previously accessed
- Memory hierarchy tries to exploit locality to improve average



Speed	1ns	10ns	100ns	10ms	10sec
Size	KB	MB	GB	TB	PB

Processor-DRAM Gap (latency)

- Memory hierarchies are getting deeper
  - Processors get faster more quickly than memory



Approaches to Handling Memory Latency

- Eliminate memory operations by saving values in small, fast memory (cache) and reusing them
  - **need temporal locality in program**
- Take advantage of better bandwidth by getting a chunk of memory and saving it in small fast memory (cache) and using whole chunk
  - **bandwidth improving faster than latency: 23% vs 7% per year**
  - **need spatial locality in program**
- Take advantage of better bandwidth by allowing processor to issue multiple reads to the memory system at once
  - **concurrency in the instruction stream, e.g. load whole array, as in vector processors; or prefetching**
- Overlap computation & memory operations
  - **prefetching**

Cache Basics

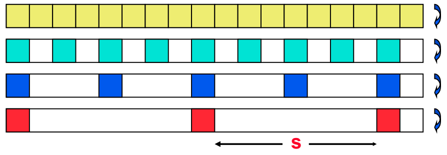
- Cache is fast (expensive) memory which keeps copy of data in main memory; it is hidden from software
  - Simplest example: data at memory address xxxxx1101 is stored at cache location 1101
- Cache hit: in-cache memory access—cheap
- Cache miss: non-cached memory access—expensive
  - Need to access next, slower level of cache
- Cache line length: # of bytes loaded together in one entry
  - Ex: If either xxxxx1100 or xxxxx1101 is loaded, both are
- Associativity
  - direct-mapped: only 1 address (line) in a given range in cache
    - Data stored at address xxxxx1101 stored at cache location 1101, in 16 word cache
  - *n*-way: $n \geq 2$ lines with different addresses can be stored
    - Up to $n \leq 16$ words with addresses xxxxx1101 can be stored at cache location 1101 (so cache can store 16n words)

Why Have Multiple Levels of Cache?

- On-chip vs. off-chip
  - On-chip caches are faster, but limited in size
- A large cache has delays
  - Hardware to check longer addresses in cache takes more time
  - Associativity, which gives a more general set of data in cache, also takes more time
- Some examples:
  - Cray T3E eliminated one cache to speed up misses
  - IBM uses a level of cache as a “victim cache” which is cheaper
- There are other levels of the memory hierarchy
  - Register, pages (TLB, virtual memory), …
  - And it isn’t always a hierarchy

Experimental Study of Memory (Membench)

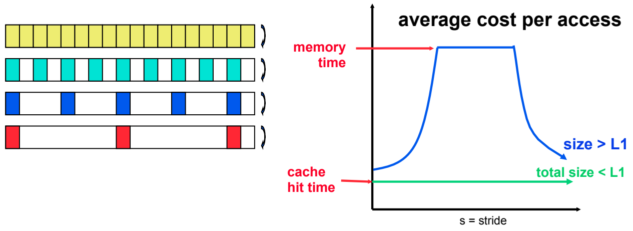
- Microbenchmark for memory system performance



```
•     for array A of length L from 4KB to 8MB by 2x
         for stride s from 4 Bytes (1 word) to L/2 by 2x
              time the following loop
              (repeat many times and average)
                    for i from 0 to L-1 by s
                         load A[i] from memory (4 Bytes)
```

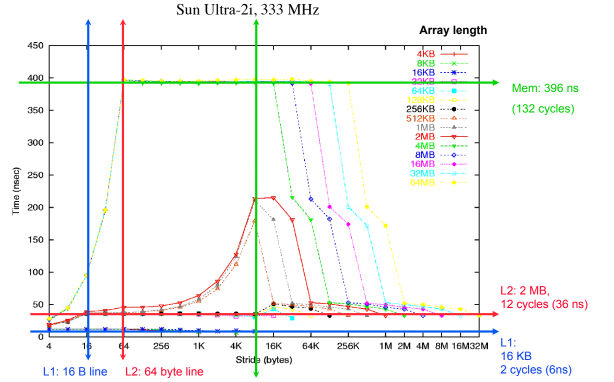
1 experiment

Membench: What to Expect



- Consider the average cost per load
  - Plot one line for each array length, time vs. stride
  - Small stride is best: if cache line holds 4 words, at most ¼ miss
  - If array is smaller than a given cache, all those accesses will hit (after the first run, which is negligible for large enough runs)
  - Picture assumes only one level of cache
  - Values have gotten more difficult to measure on modern procs

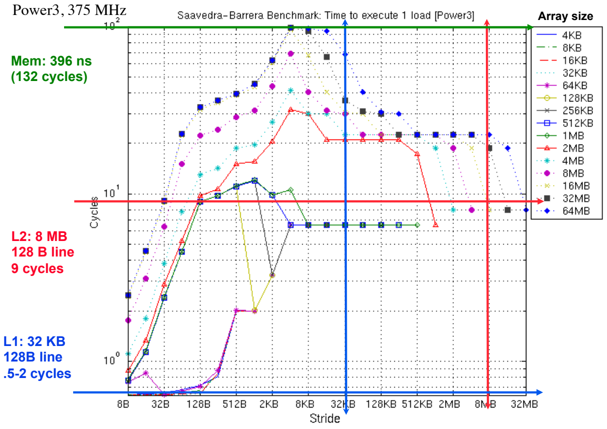
Memory Hierarchy on a Sun Ultra-2i



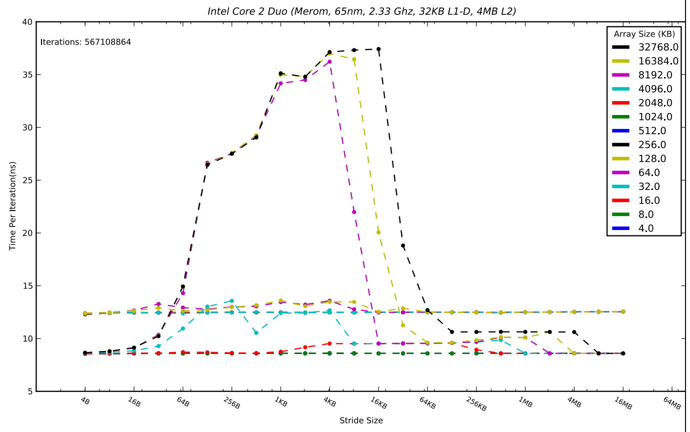
8 K pages,
32 TLB entries

See `www.cs.berkeley.edu/~yelick/arvindk/t3d-isca95.ps` for details

Memory Hierarchy on a Power3 (Seaborg)



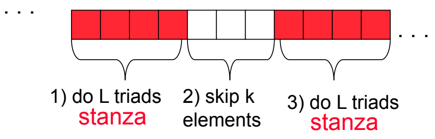
Memory Hierarchy on an Intel Core 2 Duo



Stanza Triad

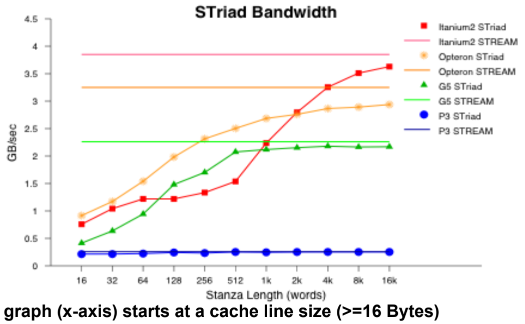
- Even smaller benchmark for prefetching
- Derived from STREAM Triad
- Stanza (L) is the length of a unit stride run

```
while i < arraylength
  for each L element stanza
    A[i] = scalar * X[i] + Y[i]
  skip k elements
```



Source: Kamil et al, MSP05

Stanza Triad Results



- This graph (x-axis) starts at a cache line size (>=16 Bytes)
- If cache locality was the only thing that mattered, we would expect
  - Flat lines equal to measured memory peak bandwidth (STREAM) as on Pentium3
- Prefetching gets the next cache line (pipelining) while using the current one
  - This does not "kick in" immediately, so performance depends on L
  - http://crd-legacy.lbl.gov/~oliker/papers/msp_2005.pdf

Lessons

- Actual performance of a simple program can be a complicated function of the architecture
  - Slight changes in the architecture or program change the performance significantly
  - To write fast programs, need to consider architecture
    - True on sequential or parallel processor
  - We would like simple models to help us design efficient algorithms
- We will illustrate with a common technique for improving cache performance, called blocking or tiling
  - Idea: used divide-and-conquer to define a problem that fits in register/L1-cache/L2-cache

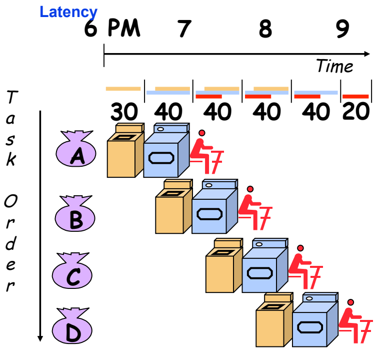
Outline

- Idealized and actual costs in modern processors
- Memory hierarchies
  - Use of microbenchmarks to characterized performance
- Parallelism within single processors
  - Hidden from software (sort of)
  - Pipelining
  - SIMD units
- Case study: Matrix Multiplication
  - Use of performance models to understand performance
  - Attainable lower bounds on communication

What is Pipelining?

Dave Patterson's Laundry example: 4 people doing laundry

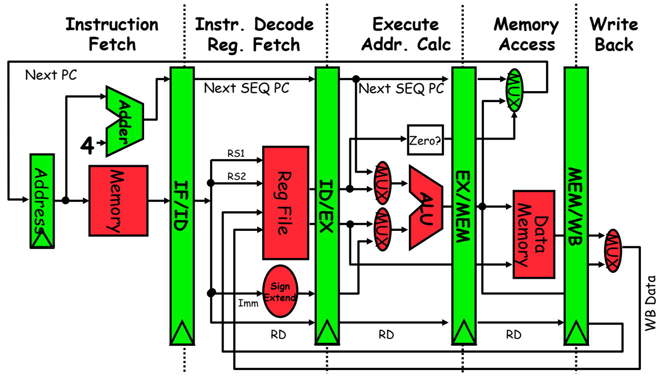
wash (30 min) + dry (40 min) + fold (20 min) = 90 min



- In this example:
  - Sequential execution takes 4 * 90min = 6 hours
  - Pipelined execution takes 30+4*40+20 = 3.5 hours
- Bandwidth = loads/hour
- BW = 4/6 l/h w/o pipelining
- BW = 4/3.5 l/h w pipelining
- BW <= 1.5 l/h w pipelining, more total loads
- Pipelining helps bandwidth but not latency (90 min)
- Bandwidth limited by slowest pipeline stage
- Potential speedup = Number of pipe stages

Example: 5 Steps of MIPS Datapath

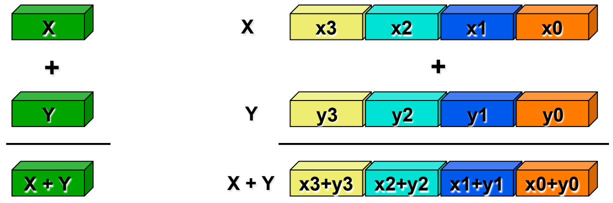
Figure 3.4, Page 134 , CA:AQA 2e by Patterson and Hennessy



- **Pipelining is also used within arithmetic units**
  - a fp multiply may have latency 10 cycles, but throughput of 1/cycle

SIMD: Single Instruction, Multiple Data

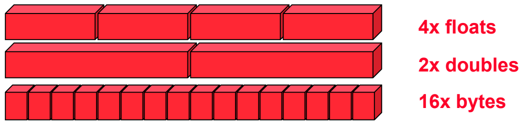
- Scalar processing
  - traditional mode
  - one operation produces one result
- SIMD processing
  - with SSE / SSE2
  - SSE = streaming SIMD extensions
  - one operation produces multiple results



Slide Source: Alex Klimovitski & Dean Macri, Intel Corporation

SSE / SSE2 SIMD on Intel

- SSE2 data types: anything that fits into 16 bytes, e.g.,



- Instructions perform add, multiply etc. on all the data in this 16-byte register in parallel
- Challenges:
  - Need to be contiguous in memory and aligned
  - Some instructions to move data around from one part of register to another
- Similar on GPUs, vector processors (but many more simultaneous operations)

What does this mean to you?

- In addition to SIMD extensions, the processor may have other special instructions
  - Fused Multiply-Add (FMA) instructions:

    x = y + c * z

    is so common some processor execute the multiply/add as a single instruction, at the same rate (bandwidth) as + or * alone
- In theory, the compiler understands all of this
  - When compiling, it will rearrange instructions to get a good “schedule” that maximizes pipelining, uses FMAs and SIMD
  - It works with the mix of instructions inside an inner loop or other block of code
- But in practice the compiler may need your help
  - Choose a different compiler, optimization flags, etc.
  - Rearrange your code to make things more obvious
  - Using special functions (“intrinsics”) or write in assembly ☹

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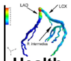
- Parallelism within single processors
- Case study: Matrix Multiplication
  - Use of performance models to understand performance
  - Attainable lower bounds on communication
  - Simple cache model
  - Warm-up: Matrix-vector multiplication
  - Naïve vs optimized Matrix-Matrix Multiply
    - Minimizing data movement
    - Beating O(n^3) operations
    - Practical optimizations (*continued next time*)

Why Matrix Multiplication?

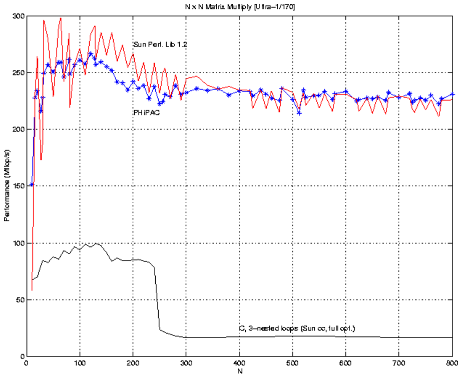
- An important kernel in many problems
  - Appears in many linear algebra algorithms
    - Bottleneck for dense linear algebra, including Top500
  - One of the 7 dwarfs / 13 motifs of parallel computing
  - Closely related to other algorithms, e.g., transitive closure on a graph using Floyd-Warshall
- Optimization ideas can be used in other problems
- The best case for optimization payoffs
- The most-studied algorithm in high performance computing

What do commercial and CSE applications have in common?

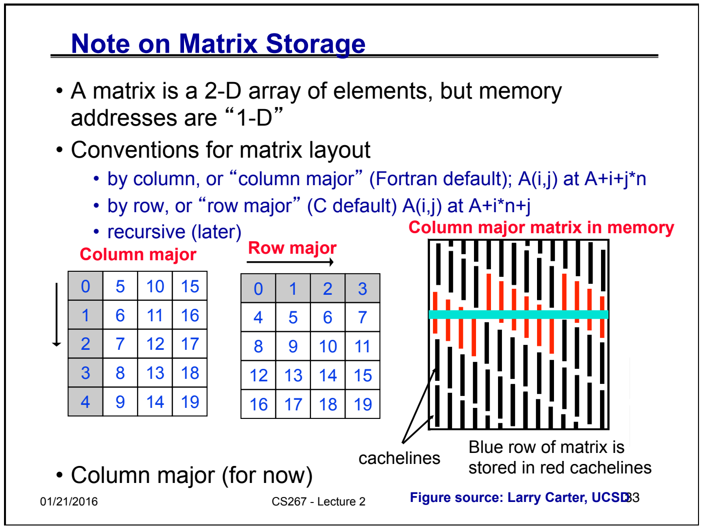
Motif/Dwarf: Common Computational Methods
(Red Hot → Blue Cool)

	Embed	SPEC	DB	Games	ML	HPC	 Health	Image	Speech	Music	Browser
1 Finite State Mach.	🟥	🟥	🟥	🟨	🟨	🟦	🟦	🟦	🟦	🟦	🟥
2 Combinational	🟥	🟦	🟩	🟦	🟩	🟦	🟦	🟦	🟦	🟦	🟥
3 Graph Traversal	🟥	🟨	🟨	🟨	🟥	🟦	🟥	🟦	🟥	🟩	🟩
4 Structured Grid	🟥	🟥	🟦	🟨	🟦	🟥	🟦	🟥	🟦	🟦	🟦
5 Dense Matrix	🟥	🟥	🟨	🟥	🟥	🟥	🟦	🟥	🟥	🟥	🟦
6 Sparse Matrix	🟨	🟨	🟦	🟥	🟥	🟥	🟥	🟦	🟦	🟥	🟦
7 Spectral (FFT)	🟨	🟦	🟦	🟨	🟨	🟥	🟦	🟩	🟥	🟥	🟥
8 Dynamic Prog	🟨	🟦	🟥	🟦	🟥	🟦	🟦	🟦	🟨	🟦	🟥
9 N-Body	🟦	🟨	🟦	🟨	🟦	🟥	🟩	🟦	🟦	🟦	🟦
10 MapReduce	🟦	🟩	🟥	🟦	🟥	🟥	🟥	🟥	🟨	🟥	🟨
11 Backtrack/ B&B	🟦	🟦	🟨	🟦	🟥	🟦	🟦	🟦	🟦	🟨	🟦
12 Graphical Models	🟦	🟦	🟨	🟦	🟥	🟦	🟦	🟦	🟦	🟥	🟦
13 Unstructured Grid	🟦	🟦	🟦	🟨	🟨	🟥	🟥	🟦	🟦	🟥	🟦

Matrix-multiply, optimized several ways



Speed of n-by-n matrix multiply on Sun Ultra-1/170, peak = 330 MFlops



Note on Matrix Storage

- A matrix is a 2-D array of elements, but memory addresses are “1-D”
- Conventions for matrix layout
  - by column, or “column major” (Fortran default); A(i,j) at A+i+j*n
  - by row, or “row major” (C default) A(i,j) at A+i*n+j
  - recursive (later)

Column major

0	5	10	15
1	6	11	16
2	7	12	17
3	8	13	18
4	9	14	19

Row major

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15
16	17	18	19

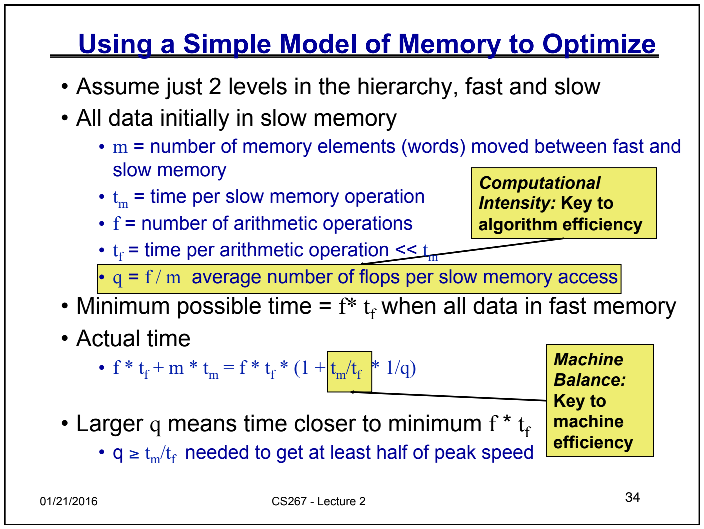
Column major matrix in memory

cachelines

Blue row of matrix is stored in red cachelines

- Column major (for now)

Figure source: Larry Carter, UCSD

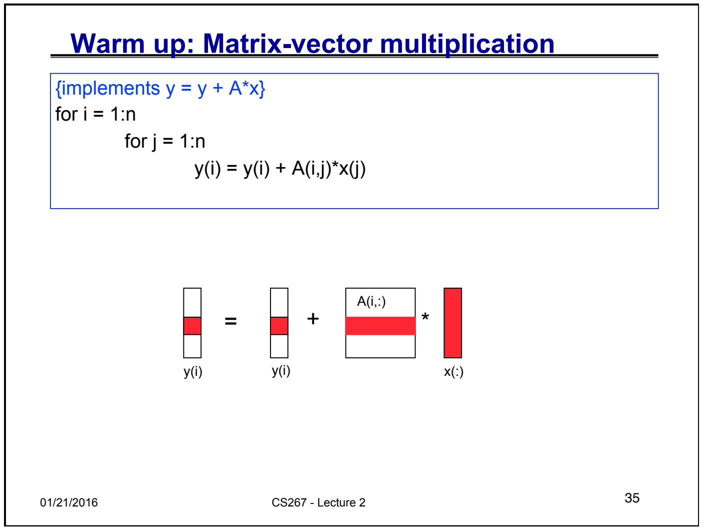


Using a Simple Model of Memory to Optimize

- Assume just 2 levels in the hierarchy, fast and slow
- All data initially in slow memory
  - m = number of memory elements (words) moved between fast and slow memory
  - t_m = time per slow memory operation
  - f = number of arithmetic operations
  - t_f = time per arithmetic operation << t_m
  - q = f / m average number of flops per slow memory access
- Minimum possible time = f* t_f when all data in fast memory
- Actual time
  - $f * t_f + m * t_m = f * t_f * (1 + t_m/t_f * 1/q)$
- Larger q means time closer to minimum f * t_f
  - q ≥ t_m/t_f needed to get at least half of peak speed

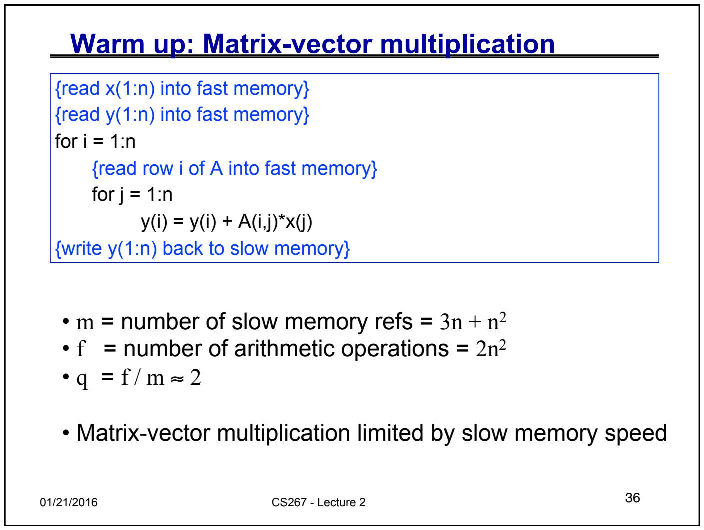
Computational Intensity: **Key to algorithm efficiency**

Machine Balance: **Key to machine efficiency**



Warm up: Matrix-vector multiplication

```
{implements y = y + A*x}
for i = 1:n
        for j = 1:n
                y(i) = y(i) + A(i,j)*x(j)
```



Warm up: Matrix-vector multiplication

```
{read x(1:n) into fast memory}
{read y(1:n) into fast memory}
for i = 1:n
     {read row i of A into fast memory}
     for j = 1:n
          y(i) = y(i) + A(i,j)*x(j)
{write y(1:n) back to slow memory}
```

- m = number of slow memory refs = $3n + n^2$
- f = number of arithmetic operations = $2n^2$
- q = f / m ≈ 2

- Matrix-vector multiplication limited by slow memory speed

Modeling Matrix-Vector Multiplication

- Compute time for nxn = 1000x1000 matrix
- Time
  - $f * t_f + m * t_m = f * t_f * (1 + t_m/t_f * 1/q)$
  - $= 2*n^2 * t_f * (1 + t_m/t_f * 1/2)$
- For t_f and t_m, using data from R. Vuduc's PhD (pp 351-3)
  - http://bebop.cs.berkeley.edu/pubs/vuduc2003-dissertation.pdf
  - For t_m use minimum-memory-latency / words-per-cache-line

	Clock	Peak	Mem Lat (Min,Max)		Linesize	t_m/t_f
	MHz	Mflop/s	cycles		Bytes	
Ultra 2i	333	667	38	66	16	24.8
Ultra 3	900	1800	28	200	32	14.0
Pentium 3	500	500	25	60	32	6.3
Pentium3M	800	800	40	60	32	10.0
Power3	375	1500	35	139	128	8.8
Power4	1300	5200	60	10000	128	15.0
Itanium1	800	3200	36	85	32	36.0
Itanium2	900	3600	11	60	64	5.5

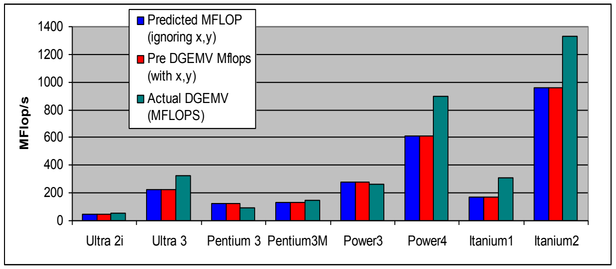
machine balance (q must be at least this for ½ peak speed)

Simplifying Assumptions

- What simplifying assumptions did we make in this analysis?
  - Ignored parallelism in processor between memory and arithmetic within the processor
    - Sometimes drop arithmetic term in this type of analysis
  - Assumed fast memory was large enough to hold three vectors
    - Reasonable if we are talking about any level of cache
    - Not if we are talking about registers (~32 words)
  - Assumed the cost of a fast memory access is 0
    - Reasonable if we are talking about registers
    - Not necessarily if we are talking about cache (1-2 cycles for L1)
  - Memory latency is constant
- Could simplify even further by ignoring memory operations in X and Y vectors
  - Mflop rate/element = $2 / (2* t_f + t_m)$

Validating the Model

- How well does the model predict actual performance?
  - Actual DGEMV: Most highly optimized code for the platform
- Model sufficient to compare across machines
- But under-predicting on most recent ones due to latency estimate

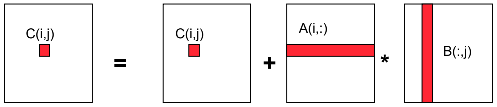


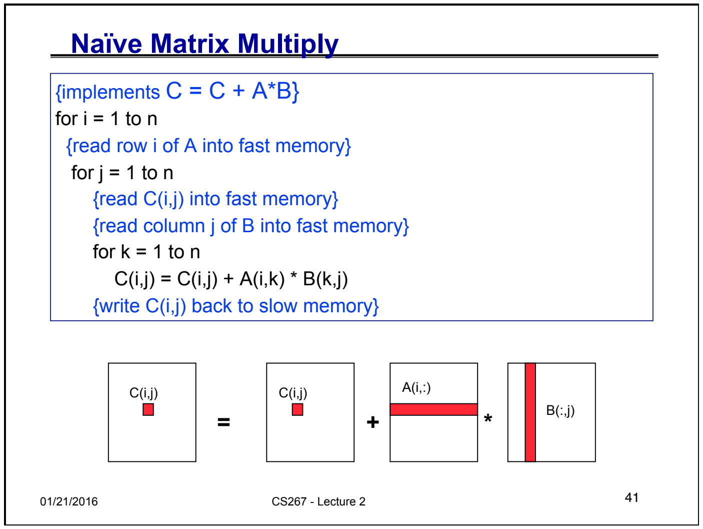
Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
    for j = 1 to n
        for k = 1 to n
            C(i,j) = C(i,j) + A(i,k) * B(k,j)
```

Algorithm has $2*n^3 = O(n^3)$ Flops and operates on $3*n^2$ words of memory

q potentially as large as $2*n^3 / 3*n^2 = O(n)$





Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
 {read row i of A into fast memory}
  for j = 1 to n
     {read C(i,j) into fast memory}
     {read column j of B into fast memory}
     for k = 1 to n
         C(i,j) = C(i,j) + A(i,k) * B(k,j)
     {write C(i,j) back to slow memory}
```

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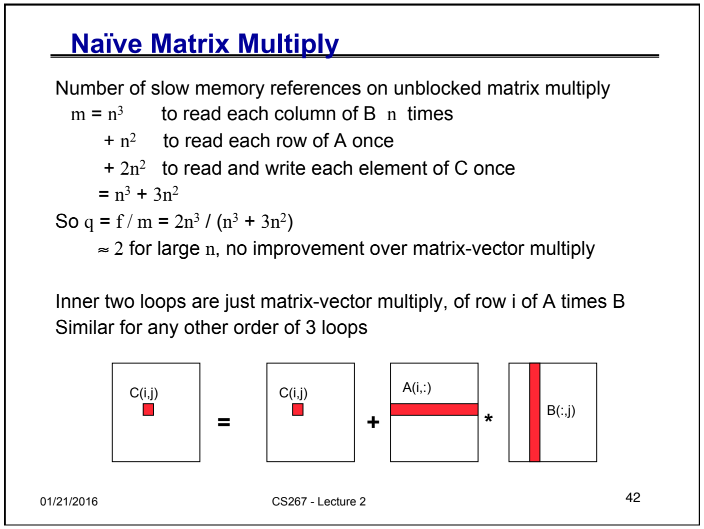

Naïve Matrix Multiply

Number of slow memory references on unblocked matrix multiply

$m = n^3$ to read each column of B n times

$+ n^2$ to read each row of A once

$+ 2n^2$ to read and write each element of C once

$= n^3 + 3n^2$

So $q = f / m = 2n^3 / (n^3 + 3n^2)$

≈ 2 for large n, no improvement over matrix-vector multiply

Inner two loops are just matrix-vector multiply, of row i of A times B

Similar for any other order of 3 loops

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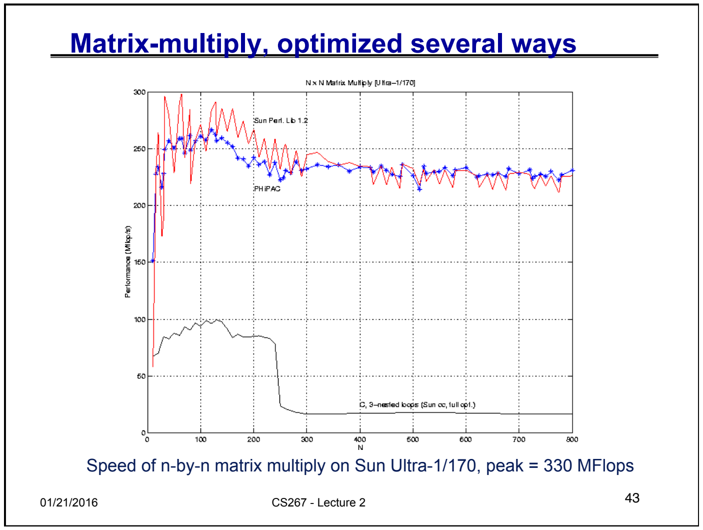

Matrix-multiply, optimized several ways

Speed of n-by-n matrix multiply on Sun Ultra-1/170, peak = 330 MFlops

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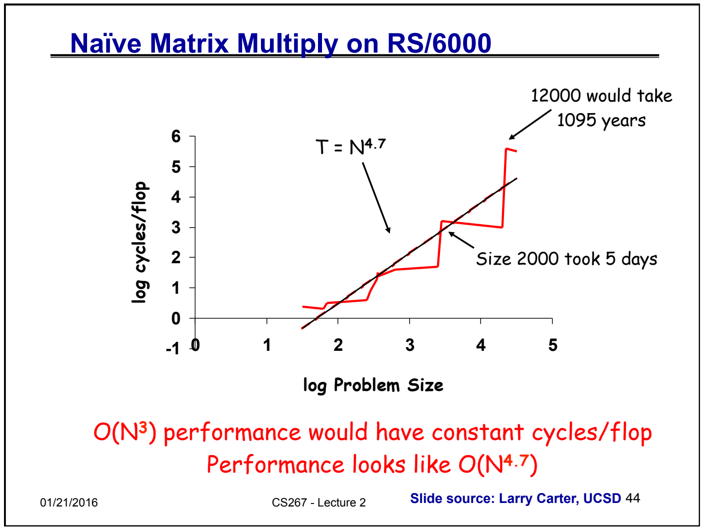

Naïve Matrix Multiply on RS/6000

O(N³) performance would have constant cycles/flop

Performance looks like O(N⁴·⁷)

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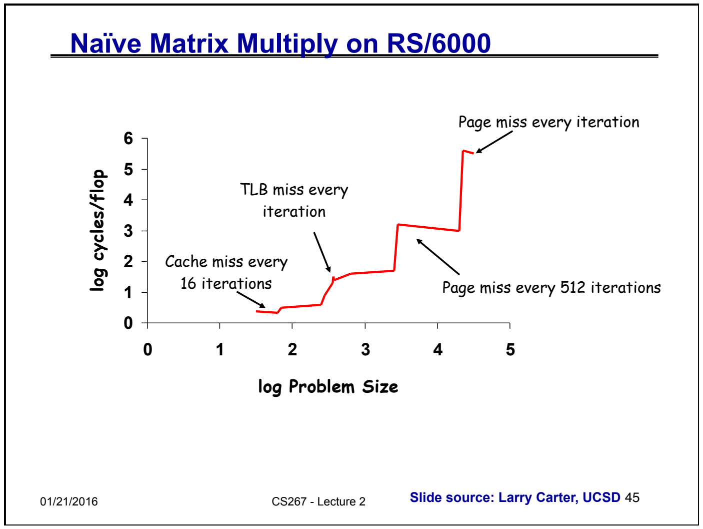
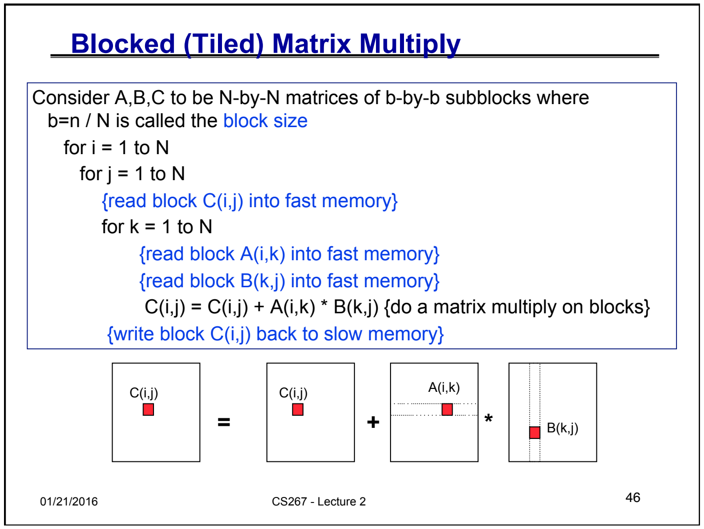


Naïve Matrix Multiply on RS/6000

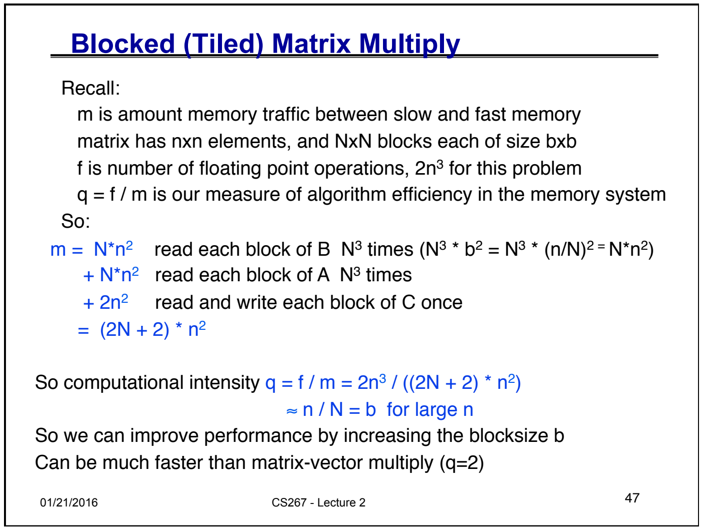
Slide source: Larry Carter, UCSD



Blocked (Tiled) Matrix Multiply

```
Consider A,B,C to be N-by-N matrices of b-by-b subblocks where
  b=n / N is called the block size
    for i = 1 to N
      for j = 1 to N
         {read block C(i,j) into fast memory}
         for k = 1 to N
              {read block A(i,k) into fast memory}
              {read block B(k,j) into fast memory}
               C(i,j) = C(i,j) + A(i,k) * B(k,j) {do a matrix multiply on blocks}
          {write block C(i,j) back to slow memory}
```

C(i,j)
=
C(i,j)
+
A(i,k)
*
B(k,j)



Blocked (Tiled) Matrix Multiply

Recall:

m is amount memory traffic between slow and fast memory

matrix has nxn elements, and NxN blocks each of size bxb

f is number of floating point operations, $2n^3$ for this problem

q = f / m is our measure of algorithm efficiency in the memory system

So:

$m = N^*n^2$ read each block of B N^3 times ($N^3 * b^2 = N^3 * (n/N)^2 = N^*n^2$)

$+ N^*n^2$ read each block of A N^3 times

$+ 2n^2$ read and write each block of C once

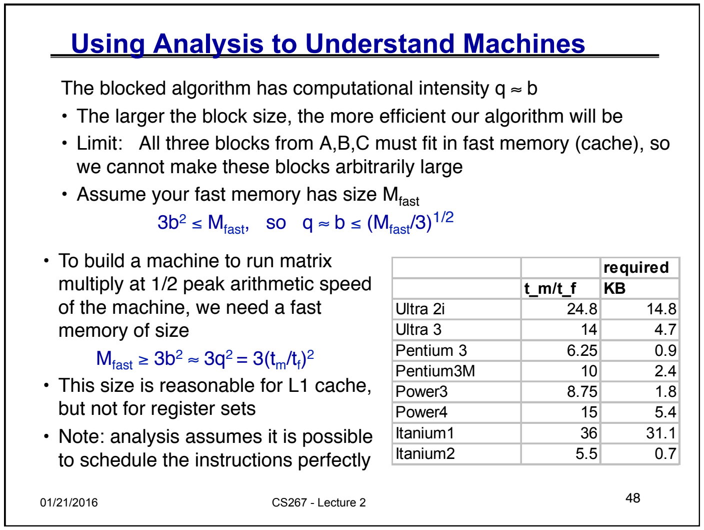
$= (2N + 2) * n^2$

So computational intensity $q = f / m = 2n^3 / ((2N + 2) * n^2)$

$\approx n / N = b$ for large n

So we can improve performance by increasing the blocksize b

Can be much faster than matrix-vector multiply (q=2)



Using Analysis to Understand Machines

The blocked algorithm has computational intensity $q \approx b$

- The larger the block size, the more efficient our algorithm will be
- Limit: All three blocks from A,B,C must fit in fast memory (cache), so we cannot make these blocks arbitrarily large
- Assume your fast memory has size M_{fast}

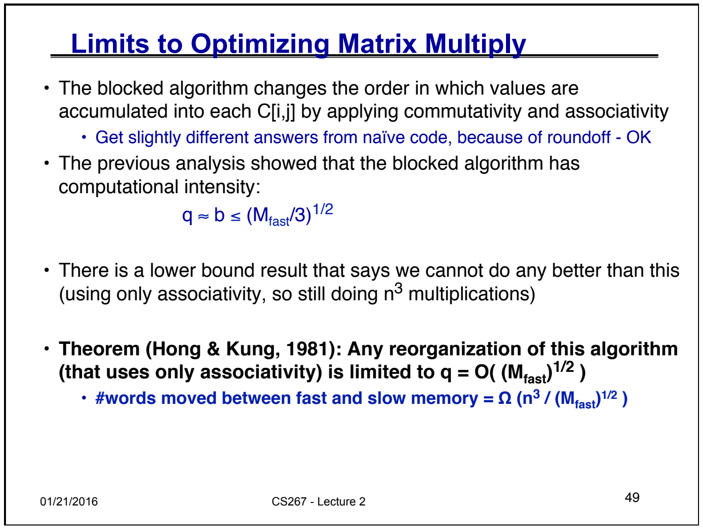
$$3b^2 \le M_{fast}, \quad \text{so} \quad q \approx b \le (M_{fast}/3)^{1/2}$$

- To build a machine to run matrix multiply at 1/2 peak arithmetic speed of the machine, we need a fast memory of size

$$M_{fast} \ge 3b^2 \approx 3q^2 = 3(t_m/t_f)^2$$

- This size is reasonable for L1 cache, but not for register sets
- Note: analysis assumes it is possible to schedule the instructions perfectly

		required
	t_m/t_f	KB
Ultra 2i	24.8	14.8
Ultra 3	14	4.7
Pentium 3	6.25	0.9
Pentium3M	10	2.4
Power3	8.75	1.8
Power4	15	5.4
Itanium1	36	31.1
Itanium2	5.5	0.7

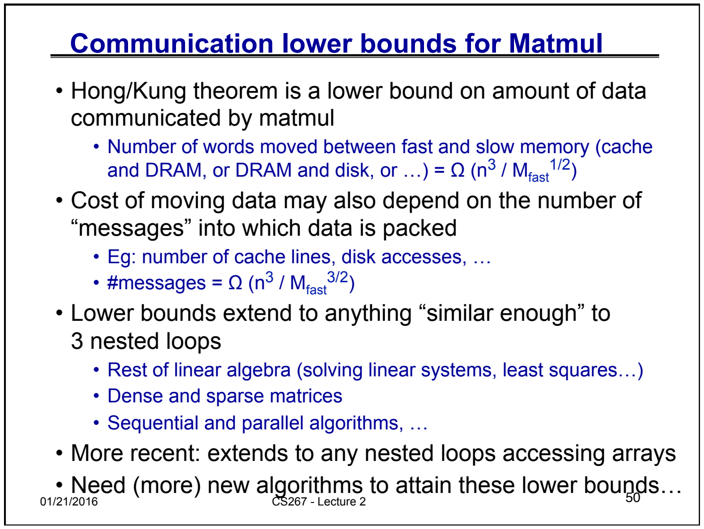


Limits to Optimizing Matrix Multiply

- The blocked algorithm changes the order in which values are accumulated into each C[i,j] by applying commutativity and associativity
  - Get slightly different answers from naïve code, because of roundoff - OK
- The previous analysis showed that the blocked algorithm has computational intensity:

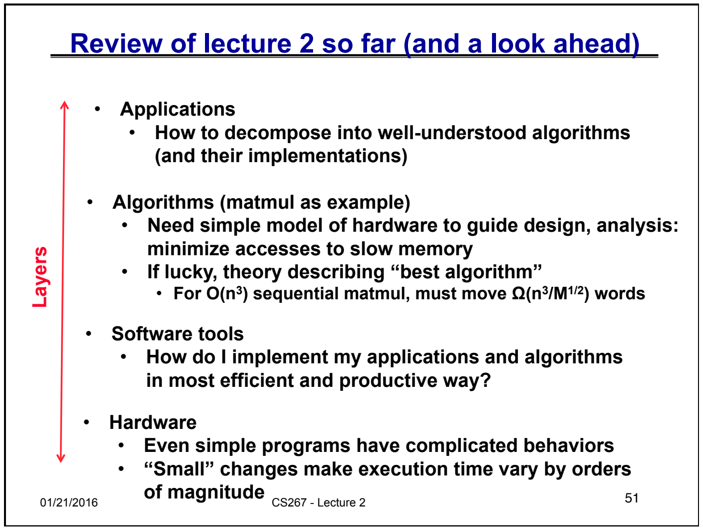
  $q \approx b \leq (M_{fast}/3)^{1/2}$

- There is a lower bound result that says we cannot do any better than this (using only associativity, so still doing n^3 multiplications)
- **Theorem (Hong & Kung, 1981): Any reorganization of this algorithm (that uses only associativity) is limited to $q = O((M_{fast})^{1/2})$**
  - **#words moved between fast and slow memory = Ω (n^3 / $(M_{fast})^{1/2}$)**



Communication lower bounds for Matmul

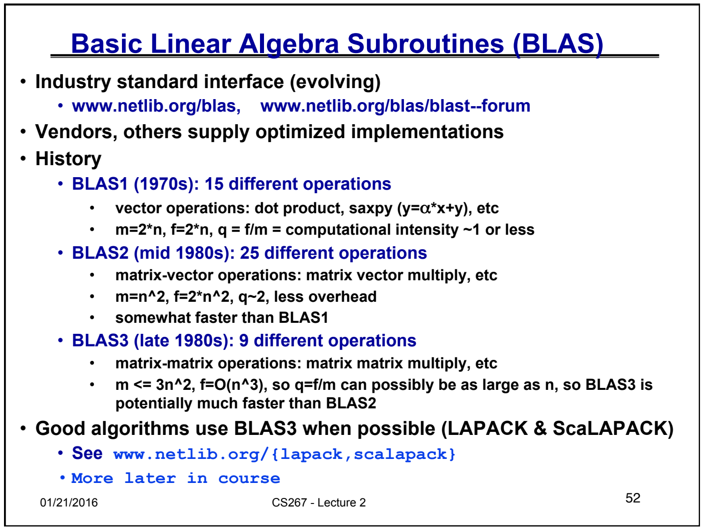
- Hong/Kung theorem is a lower bound on amount of data communicated by matmul
  - Number of words moved between fast and slow memory (cache and DRAM, or DRAM and disk, or …) = Ω (n^3 / $M_{fast}{}^{1/2}$)
- Cost of moving data may also depend on the number of “messages” into which data is packed
  - Eg: number of cache lines, disk accesses, …
  - #messages = Ω (n^3 / $M_{fast}{}^{3/2}$)
- Lower bounds extend to anything “similar enough” to 3 nested loops
  - Rest of linear algebra (solving linear systems, least squares…)
  - Dense and sparse matrices
  - Sequential and parallel algorithms, …
- More recent: extends to any nested loops accessing arrays
- Need (more) new algorithms to attain these lower bounds…



Review of lecture 2 so far (and a look ahead)

Layers

- **Applications**
  - **How to decompose into well-understood algorithms (and their implementations)**
- **Algorithms (matmul as example)**
  - **Need simple model of hardware to guide design, analysis: minimize accesses to slow memory**
  - **If lucky, theory describing “best algorithm”**
    - **For O(n^3) sequential matmul, must move $\Omega(n^3/M^{1/2})$ words**
- **Software tools**
  - **How do I implement my applications and algorithms in most efficient and productive way?**
- **Hardware**
  - **Even simple programs have complicated behaviors**
  - **“Small” changes make execution time vary by orders of magnitude**

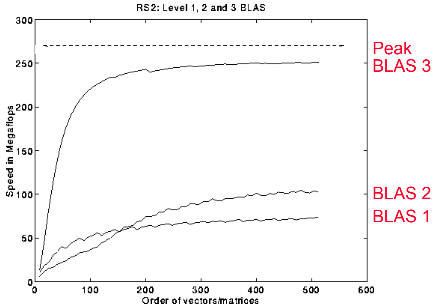


Basic Linear Algebra Subroutines (BLAS)

- **Industry standard interface (evolving)**
  - **www.netlib.org/blas, www.netlib.org/blas/blast--forum**
- **Vendors, others supply optimized implementations**
- **History**
  - **BLAS1 (1970s): 15 different operations**
    - **vector operations: dot product, saxpy (y=α*x+y), etc**
    - **m=2*n, f=2*n, q = f/m = computational intensity ~1 or less**
  - **BLAS2 (mid 1980s): 25 different operations**
    - **matrix-vector operations: matrix vector multiply, etc**
    - **m=n^2, f=2*n^2, q~2, less overhead**
    - **somewhat faster than BLAS1**
  - **BLAS3 (late 1980s): 9 different operations**
    - **matrix-matrix operations: matrix matrix multiply, etc**
    - **m <= 3n^2, f=O(n^3), so q=f/m can possibly be as large as n, so BLAS3 is potentially much faster than BLAS2**
- **Good algorithms use BLAS3 when possible (LAPACK & ScaLAPACK)**
  - **See `www.netlib.org/{lapack,scalapack}`**
  - **`More later in course`**

BLAS speeds on an IBM RS6000/590

Peak speed = 266 Mflops

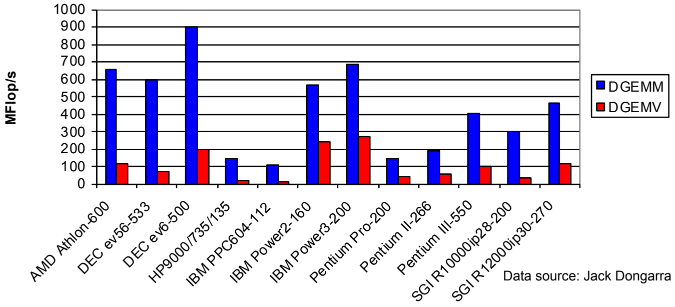


BLAS 3 (n-by-n matrix matrix multiply) vs
BLAS 2 (n-by-n matrix vector multiply) vs
BLAS 1 (saxpy of n vectors)

Dense Linear Algebra: BLAS2 vs. BLAS3

- BLAS2 and BLAS3 have very different computational intensity, and therefore different performance

BLAS3 (MatrixMatrix) vs. BLAS2 (MatrixVector)



Data source: Jack Dongarra

What if there are more than 2 levels of memory?

- Need to minimize communication between all levels
  - Between L1 and L2 cache, cache and DRAM, DRAM and disk…
- The tiled algorithm requires finding a good block size
  - Machine dependent
  - Need to "block" b x b matrix multiply in inner most loop
    - 1 level of memory ⇒ 3 nested loops (naïve algorithm)
    - 2 levels of memory ⇒ 6 nested loops
    - 3 levels of memory ⇒ 9 nested loops …
- Cache Oblivious Algorithms offer an alternative
  - Treat nxn matrix multiply as a set of smaller problems
  - Eventually, these will fit in cache
  - Will minimize # words moved between every level of memory hierarchy – at least asymptotically
  - "Oblivious" to number and sizes of levels

Recursive Matrix Multiplication (RMM) (1/2)

- $C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = A \cdot B = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \cdot \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$

$$= \begin{pmatrix} A_{11} \cdot B_{11} + A_{12} \cdot B_{21} & A_{11} \cdot B_{12} + A_{12} \cdot B_{22} \\ A_{21} \cdot B_{11} + A_{22} \cdot B_{21} & A_{21} \cdot B_{12} + A_{22} \cdot B_{22} \end{pmatrix}$$

- True when each A_{ij} etc 1x1 or n/2 x n/2
- For simplicity: square matrices with $n = 2^m$
  - Extends to general rectangular case

```
func C = RMM (A, B, n)
   if n = 1, C = A * B, else
     { $C_{11}$ = RMM ($A_{11}$ , $B_{11}$ , n/2) + RMM ($A_{12}$ , $B_{21}$ , n/2)
       $C_{12}$ = RMM ($A_{11}$ , $B_{12}$ , n/2) + RMM ($A_{12}$ , $B_{22}$ , n/2)
       $C_{21}$ = RMM ($A_{21}$ , $B_{11}$ , n/2) + RMM ($A_{22}$ , $B_{21}$ , n/2)
       $C_{22}$ = RMM ($A_{21}$ , $B_{12}$ , n/2) + RMM ($A_{22}$ , $B_{22}$ , n/2) }
   return
```

Recursive Matrix Multiplication (2/2)

```
func C = RMM (A, B, n)
   if n=1, C = A * B, else
     { $C_{11}$ = RMM ($A_{11}$ , $B_{11}$ , n/2) + RMM ($A_{12}$ , $B_{21}$ , n/2)
       $C_{12}$ = RMM ($A_{11}$ , $B_{12}$ , n/2) + RMM ($A_{12}$ , $B_{22}$ , n/2)
       $C_{21}$ = RMM ($A_{21}$ , $B_{11}$ , n/2) + RMM ($A_{22}$ , $B_{21}$ , n/2)
       $C_{22}$ = RMM ($A_{21}$ , $B_{12}$ , n/2) + RMM ($A_{22}$ , $B_{22}$ , n/2)  }
   return
```

A(n) = # arithmetic operations in RMM(. , . , n)
= 8 · A(n/2) + 4(n/2)^2 if n > 1, else 1
= 2n^3 … same operations as usual, in different order

W(n) = # words moved between fast, slow memory by RMM(. , . , n)
= 8 · W(n/2) + 4· 3(n/2)^2 if 3n^2 > M_{fast} , else 3n^2
= O(n^3 / (M_{fast})$^{1/2}$ + n^2) … same as blocked matmul

Don't need to know M_{fast} for this to work!

Recursion: Cache Oblivious Algorithms

- The tiled algorithm requires finding a good block size
- Cache Oblivious Algorithms offer an alternative
  - Treat nxn matrix multiply set of smaller problems
  - Eventually, these will fit in cache
- Cases for A (nxm) * B (mxp)
- Case1: n>= max{m,p}: split A horizontally:
- Case 2: m>= max{n,p}: split A vertically and B horizontally
- Case 3: p>= max{m,n}: split B vertically

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} B = \begin{pmatrix} A_1 B \\ A_2 B \end{pmatrix}$$

Case 1

$$(A_1, A_2)\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = (A_1 B_1 + A_2 B_2)$$

Case 2

$$A(B_1, B_2) = (A\ B_1, A\ B_2)$$

Case 3

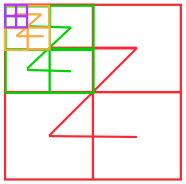
- Attains lower bound in O() sense

Experience with Cache-Oblivious Algorithms

- In practice, need to cut off recursion well before 1x1 blocks
  - Call "micro-kernel" on small blocks
- Implementing high-performance Cache-Oblivious code not easy
  - Careful attention to micro-kernel is needed
- Using fully recursive approach with highly optimized recursive micro-kernel, Pingali et al report that they never got more than 2/3 of peak. (unpublished, presented at LACSI'06)
- Issues with Cache Oblivious (recursive) approach
  - Recursive Micro-Kernels yield less performance than iterative ones using same scheduling techniques
  - Pre-fetching is needed to compete with best code: not well-understood in the context of Cache-Oblivious codes
- More recent work on CARMA (UCB) uses recursion for parallelism, but aware of available memory, very fast (later)
  - Up to **6.6x** faster than Intel MKL for some matrix shapes, **17%** for square

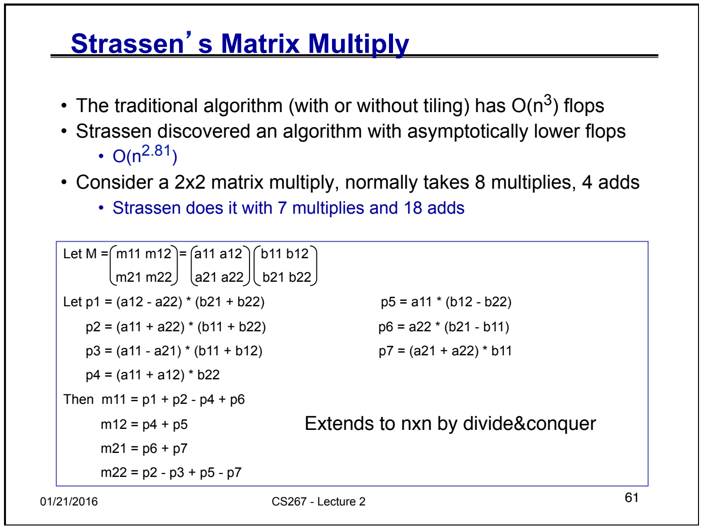
Recursive Data Layouts

- A related idea is to use a recursive structure for the matrix
  - Improve locality with machine-independent data structure
  - Can minimize latency with multiple levels of memory hierarchy
- There are several possible recursive decompositions depending on the order of the sub-blocks
- This figure shows Z-Morton Ordering ("space filling curve")
- See papers on "cache oblivious algorithms" and "recursive layouts"
  - Gustavson, Kagstrom, et al, SIAM Review, 2004



Advantages:
- the recursive layout works well for any cache size

Disadvantages:
- The index calculations to find A[i,j] are expensive
- Implementations switch to column-major for small sizes



Strassen's Matrix Multiply

- The traditional algorithm (with or without tiling) has $O(n^3)$ flops
- Strassen discovered an algorithm with asymptotically lower flops
  - $O(n^{2.81})$
- Consider a 2x2 matrix multiply, normally takes 8 multiplies, 4 adds
  - Strassen does it with 7 multiplies and 18 adds

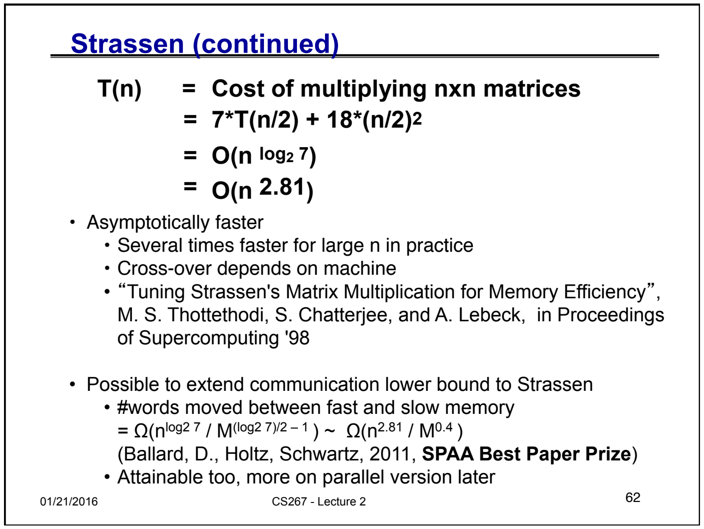
Let $M = \begin{pmatrix} m11 & m12 \\ m21 & m22 \end{pmatrix} = \begin{pmatrix} a11 & a12 \\ a21 & a22 \end{pmatrix} \begin{pmatrix} b11 & b12 \\ b21 & b22 \end{pmatrix}$

Let p1 = (a12 - a22) * (b21 + b22)
p2 = (a11 + a22) * (b11 + b22)
p3 = (a11 - a21) * (b11 + b12)
p4 = (a11 + a12) * b22

p5 = a11 * (b12 - b22)
p6 = a22 * (b21 - b11)
p7 = (a21 + a22) * b11

Then m11 = p1 + p2 - p4 + p6
m12 = p4 + p5
m21 = p6 + p7
m22 = p2 - p3 + p5 - p7

Extends to nxn by divide&conquer

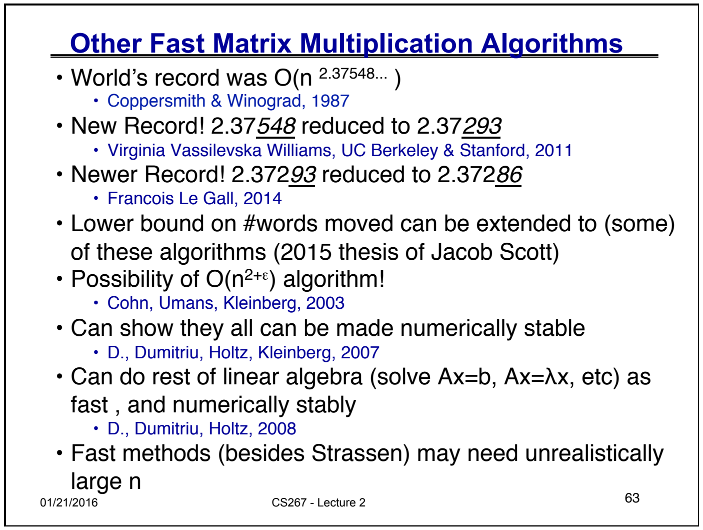


Strassen (continued)

T(n) = Cost of multiplying nxn matrices
= 7*T(n/2) + 18*(n/2)²

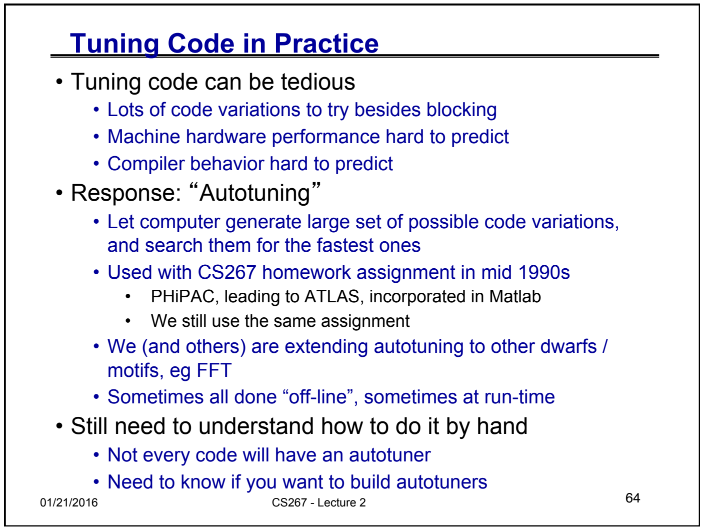
$$\begin{aligned} T(n) &= \text{Cost of multiplying nxn matrices} \\ &= 7*T(n/2) + 18*(n/2)^2 \\ &= O(n^{\log_2 7}) \\ &= O(n^{2.81}) \end{aligned}$$

- Asymptotically faster
  - Several times faster for large n in practice
  - Cross-over depends on machine
  - "Tuning Strassen's Matrix Multiplication for Memory Efficiency", M. S. Thottethodi, S. Chatterjee, and A. Lebeck, in Proceedings of Supercomputing '98
- Possible to extend communication lower bound to Strassen
  - #words moved between fast and slow memory $= \Omega(n^{\log2\ 7} / M^{(\log2\ 7)/2 - 1}) \sim \Omega(n^{2.81} / M^{0.4})$ (Ballard, D., Holtz, Schwartz, 2011, **SPAA Best Paper Prize**)
  - Attainable too, more on parallel version later



Other Fast Matrix Multiplication Algorithms

- World's record was $O(n^{2.37548...})$
  - Coppersmith & Winograd, 1987
- New Record! 2.37*548* reduced to 2.37*293*
  - Virginia Vassilevska Williams, UC Berkeley & Stanford, 2011
- Newer Record! 2.372*93* reduced to 2.372*86*
  - Francois Le Gall, 2014
- Lower bound on #words moved can be extended to (some) of these algorithms (2015 thesis of Jacob Scott)
- Possibility of $O(n^{2+\varepsilon})$ algorithm!
  - Cohn, Umans, Kleinberg, 2003
- Can show they all can be made numerically stable
  - D., Dumitriu, Holtz, Kleinberg, 2007
- Can do rest of linear algebra (solve Ax=b, $Ax=\lambda x$, etc) as fast , and numerically stably
  - D., Dumitriu, Holtz, 2008
- Fast methods (besides Strassen) may need unrealistically large n



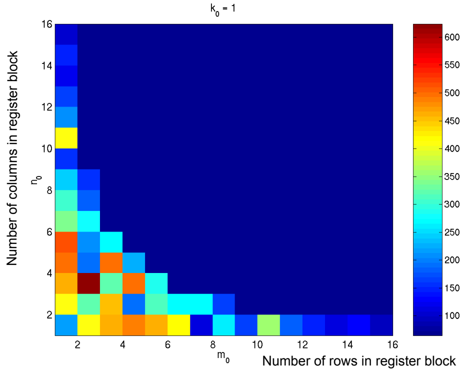
Tuning Code in Practice

- Tuning code can be tedious
  - Lots of code variations to try besides blocking
  - Machine hardware performance hard to predict
  - Compiler behavior hard to predict
- Response: "Autotuning"
  - Let computer generate large set of possible code variations, and search them for the fastest ones
  - Used with CS267 homework assignment in mid 1990s
    - PHiPAC, leading to ATLAS, incorporated in Matlab
    - We still use the same assignment
  - We (and others) are extending autotuning to other dwarfs / motifs, eg FFT
  - Sometimes all done "off-line", sometimes at run-time
- Still need to understand how to do it by hand
  - Not every code will have an autotuner
  - Need to know if you want to build autotuners

Search Over Block Sizes

- Performance models are useful for high level algorithms
  - Helps in developing a blocked algorithm
  - Models have not proven very useful for block size selection
    - too complicated to be useful
      - See work by Sid Chatterjee for detailed model
    - too simple to be accurate
      - Multiple multidimensional arrays, virtual memory, etc.
  - Speed depends on matrix dimensions, details of code, compiler, processor

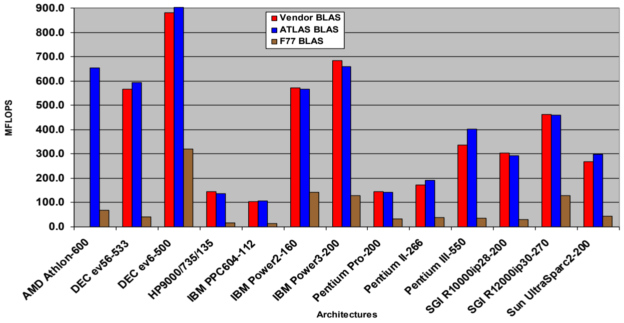
What the Search Space Looks Like



A 2-D slice of a 3-D register-tile search space. The dark blue region was pruned. (Platform: Sun Ultra-IIi, 333 MHz, 667 Mflop/s peak, Sun cc v5.0 compiler)

ATLAS (DGEMM n = 500)

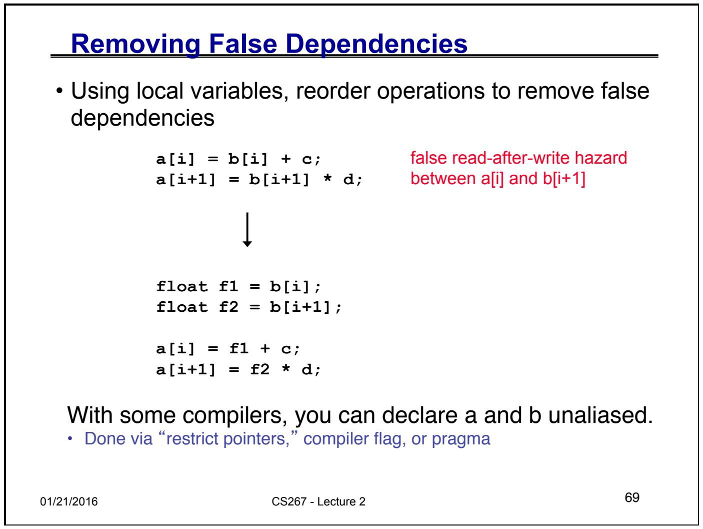
Source: Jack Dongarra



- ATLAS is faster than all other portable BLAS implementations and it is comparable with machine-specific libraries provided by the vendor.

Optimizing in Practice

- Tiling for registers
  - loop unrolling, use of named “register” variables
- Tiling for multiple levels of cache and TLB
- Exploiting fine-grained parallelism in processor
  - superscalar; pipelining
- Complicated compiler interactions (flags)
- Hard to do by hand (but you’ll try)
- Automatic optimization an active research area
  - ASPIRE: `aspire.eecs.berkeley.edu`
  - BeBOP: `bebop.cs.berkeley.edu`
    - Weekly group meeting Mondays 1pm
  - PHiPAC: `www.icsi.berkeley.edu/~bilmes/phipac`
    in particular `tr-98-035.ps.gz`
  - ATLAS: `www.netlib.org/atlas`



Removing False Dependencies

- Using local variables, reorder operations to remove false dependencies

```
a[i] = b[i] + c;
a[i+1] = b[i+1] * d;
```

false read-after-write hazard between a[i] and b[i+1]

↓

```
float f1 = b[i];
float f2 = b[i+1];

a[i] = f1 + c;
a[i+1] = f2 * d;
```

With some compilers, you can declare a and b unaliased.

- Done via "restrict pointers," compiler flag, or pragma

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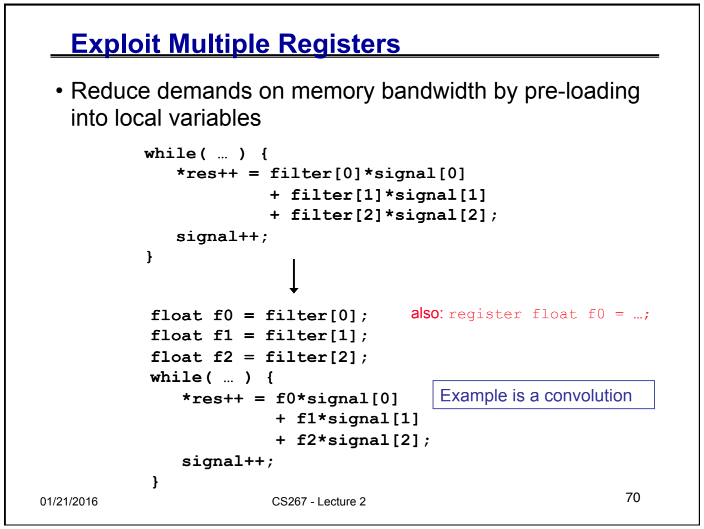

Exploit Multiple Registers

- Reduce demands on memory bandwidth by pre-loading into local variables

```
while( … ) {
   *res++ = filter[0]*signal[0]
            + filter[1]*signal[1]
            + filter[2]*signal[2];
   signal++;
}
```

↓

```
float f0 = filter[0];
float f1 = filter[1];
float f2 = filter[2];
while( … ) {
   *res++ = f0*signal[0]
            + f1*signal[1]
            + f2*signal[2];
   signal++;
}
```

also: `register float f0 = …;`

Example is a convolution

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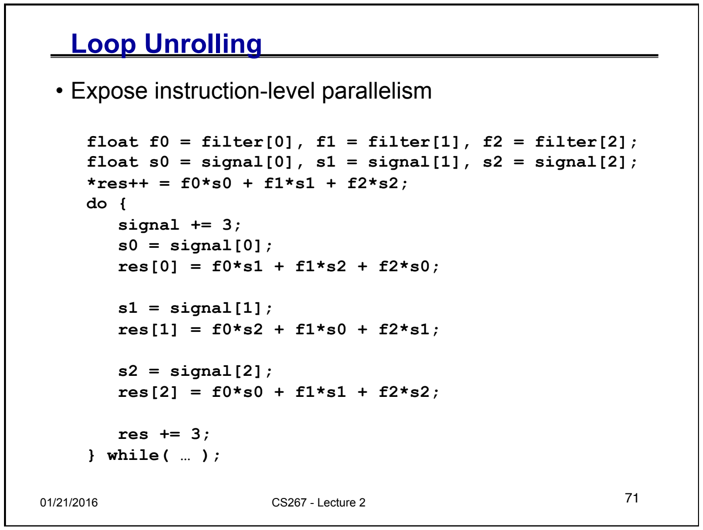

Loop Unrolling

- Expose instruction-level parallelism

```
float f0 = filter[0], f1 = filter[1], f2 = filter[2];
float s0 = signal[0], s1 = signal[1], s2 = signal[2];
*res++ = f0*s0 + f1*s1 + f2*s2;
do {
   signal += 3;
   s0 = signal[0];
   res[0] = f0*s1 + f1*s2 + f2*s0;

   s1 = signal[1];
   res[1] = f0*s2 + f1*s0 + f2*s1;

   s2 = signal[2];
   res[2] = f0*s0 + f1*s1 + f2*s2;

   res += 3;
} while( … );
```

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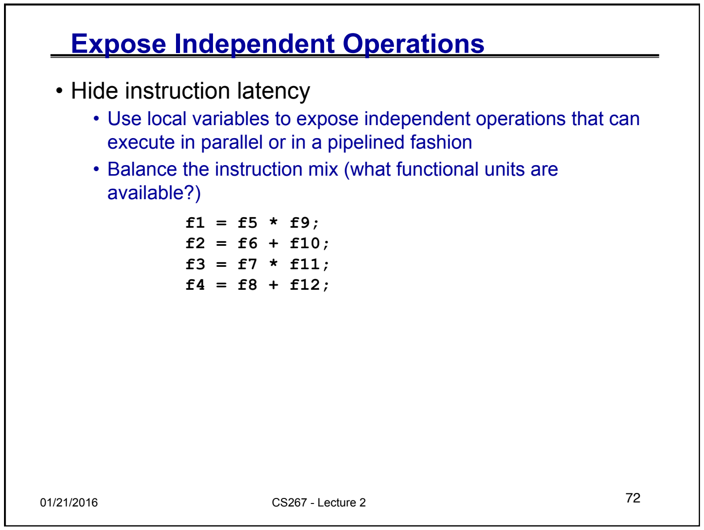

Expose Independent Operations

- Hide instruction latency
  - Use local variables to expose independent operations that can execute in parallel or in a pipelined fashion
  - Balance the instruction mix (what functional units are available?)

```
f1 = f5 * f9;
f2 = f6 + f10;
f3 = f7 * f11;
f4 = f8 + f12;
```

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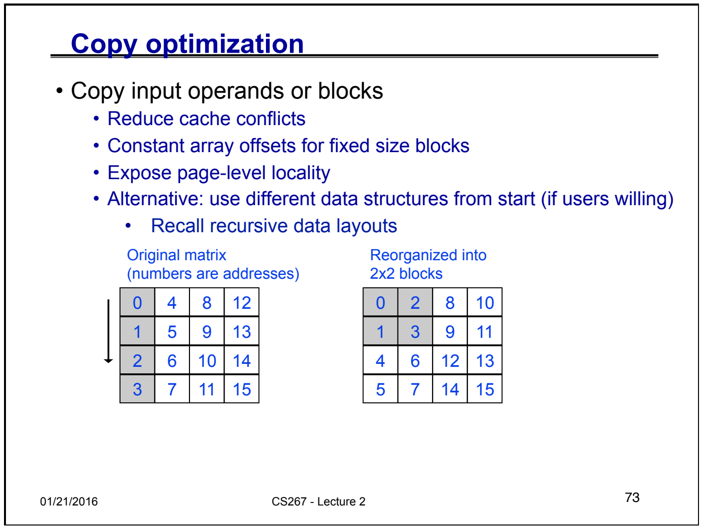


Copy optimization

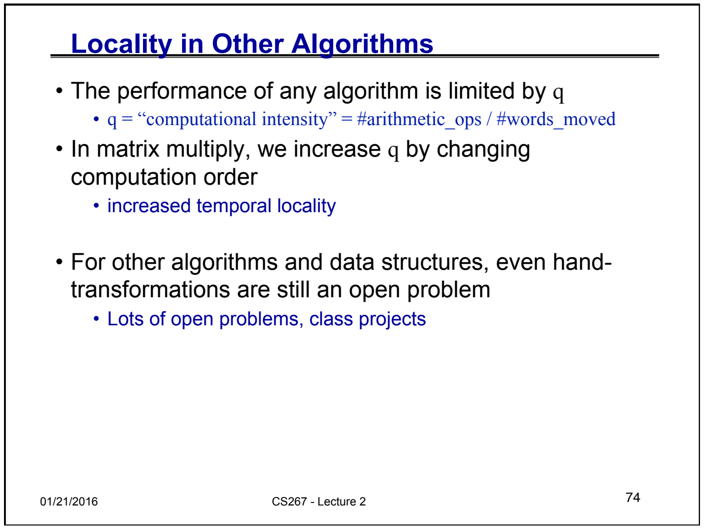
- Copy input operands or blocks
  - Reduce cache conflicts
  - Constant array offsets for fixed size blocks
  - Expose page-level locality
  - Alternative: use different data structures from start (if users willing)
    - Recall recursive data layouts

Original matrix (numbers are addresses)

0	4	8	12
1	5	9	13
2	6	10	14
3	7	11	15

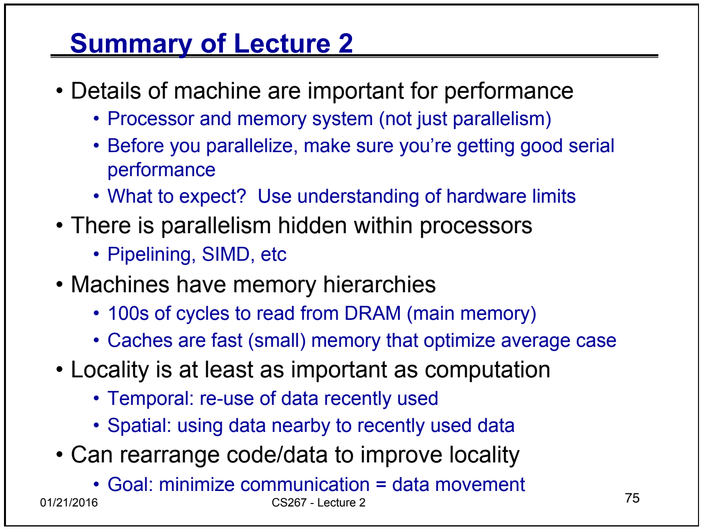
Reorganized into 2x2 blocks

0	2	8	10
1	3	9	11
4	6	12	13
5	7	14	15



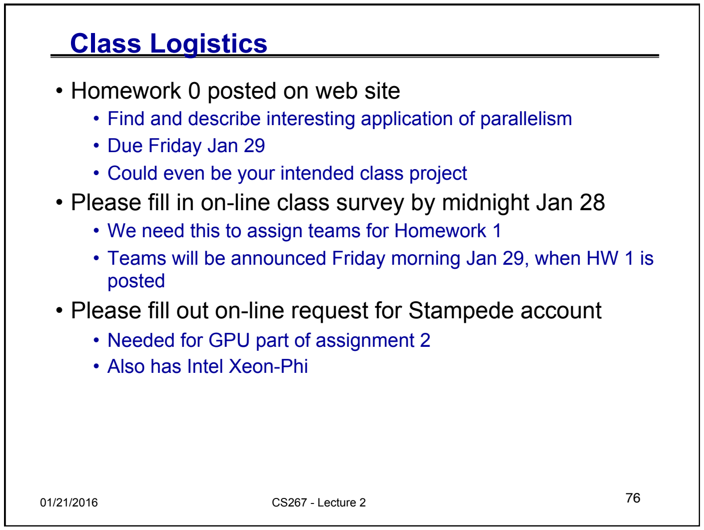
Locality in Other Algorithms

- The performance of any algorithm is limited by q
  - q = “computational intensity” = #arithmetic_ops / #words_moved
- In matrix multiply, we increase q by changing computation order
  - increased temporal locality
- For other algorithms and data structures, even hand-transformations are still an open problem
  - Lots of open problems, class projects



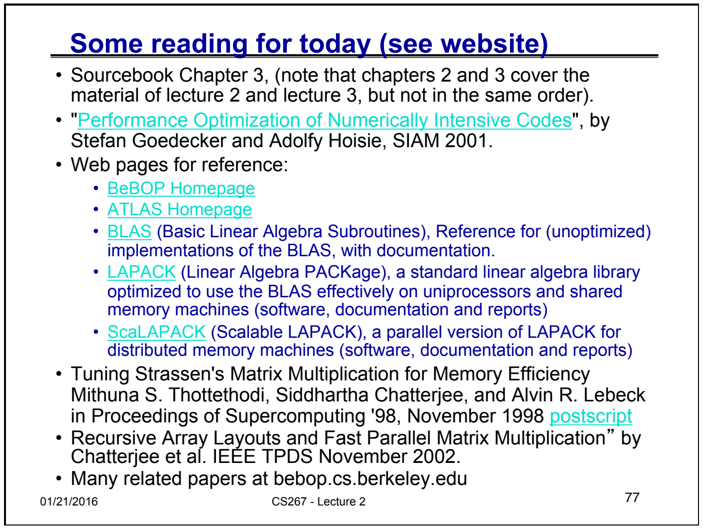
Summary of Lecture 2

- Details of machine are important for performance
  - Processor and memory system (not just parallelism)
  - Before you parallelize, make sure you’re getting good serial performance
  - What to expect? Use understanding of hardware limits
- There is parallelism hidden within processors
  - Pipelining, SIMD, etc
- Machines have memory hierarchies
  - 100s of cycles to read from DRAM (main memory)
  - Caches are fast (small) memory that optimize average case
- Locality is at least as important as computation
  - Temporal: re-use of data recently used
  - Spatial: using data nearby to recently used data
- Can rearrange code/data to improve locality
  - Goal: minimize communication = data movement



Class Logistics

- Homework 0 posted on web site
  - Find and describe interesting application of parallelism
  - Due Friday Jan 29
  - Could even be your intended class project
- Please fill in on-line class survey by midnight Jan 28
  - We need this to assign teams for Homework 1
  - Teams will be announced Friday morning Jan 29, when HW 1 is posted
- Please fill out on-line request for Stampede account
  - Needed for GPU part of assignment 2
  - Also has Intel Xeon-Phi



Some reading for today (see website)

- Sourcebook Chapter 3, (note that chapters 2 and 3 cover the material of lecture 2 and lecture 3, but not in the same order).
- "Performance Optimization of Numerically Intensive Codes", by Stefan Goedecker and Adolfy Hoisie, SIAM 2001.
- Web pages for reference:
  - BeBOP Homepage
  - ATLAS Homepage
  - BLAS (Basic Linear Algebra Subroutines), Reference for (unoptimized) implementations of the BLAS, with documentation.
  - LAPACK (Linear Algebra PACKage), a standard linear algebra library optimized to use the BLAS effectively on uniprocessors and shared memory machines (software, documentation and reports)
  - ScaLAPACK (Scalable LAPACK), a parallel version of LAPACK for distributed memory machines (software, documentation and reports)
- Tuning Strassen's Matrix Multiplication for Memory Efficiency Mithuna S. Thottethodi, Siddhartha Chatterjee, and Alvin R. Lebeck in Proceedings of Supercomputing '98, November 1998 postscript
- Recursive Array Layouts and Fast Parallel Matrix Multiplication” by Chatterjee et al. IEEE TPDS November 2002.
- Many related papers at bebop.cs.berkeley.edu