Plan for Today

- Talk about computer arithmetic
- Begin Cache discussion

A Little History

- Von Neumann and Goldstine - 1947
  - "Can't expect to solve even big (n>15) linear systems without carrying many decimal digits [d>8], otherwise the computed answer would be completely inaccurate." – WGOO
- Turing - 1949
  - "Carrying d digits is equivalent to changing the input data in the d-th place and then solving Ax = b. So if A is only known to d digits, the answer is as accurate as the data deserves."
  - Backward Error Analysis
  - Rediscovered in 1961 by Wilkinson and publicized
  - Starting in the 1960s: many papers doing backward error analysis of various algorithms
  - Many years where each machine did FP arithmetic slightly differently
    - Both rounding and exception handling differed
    - Hard to write portable and reliable software
    - Motivated search for industry-wide standard, beginning late 1970s
  - ACM Turing Award 1989 to W. Kahan for design of the IEEE Floating Point Standards 754 (binary) and 854 (decimal)
  - Nearly universally implemented in general purpose machines

Defining Floating Point Arithmetic

- Representable numbers:
  - Scientific notation: \( a \cdot b^{e} \)
  - Sign bit +/-
  - Radix \( r \) (usually 2 or 10, sometimes 16)
  - Significand \( d.d\ldots d \)
  - Exponent \( \exp \)
- Operations:
  - Arithmetic: +, -, *, /...
  - Comparison (<, =, >)
  - Conversion between different formats
    - Short to long FP numbers, FP to integer
  - Exception handling
    - What to do for \( 0/0, 2\times\text{largest number}, \text{etc.} \)
  - Binary/decimal conversion
    - \( \text{for} 0/0, \text{whereas real number} \)
- Language/library support for these operations

IEEE Floating Point Arithmetic

- Normalized Nonzero Representable Numbers:
  - \( +1 \cdot d.d\ldots d \cdot r^{e} \)
  - Macheps = Machine epsilon = \( 2^{-\text{#significand bits}} \)
  - Relative error in each operation
  - OV = Overflow threshold = largest number
  - UN = Underflow threshold = smallest number
- Format  | #bits  | #significant bits | macheps  | Exponent bits | Exponent range
----|---|---|---|---|---
-Single  | 32  | 23+1  | 2^{15} (10^{-15})  | 8  | 2^{127} - 2^{1023} (10^{-38})
-Double  | 64  | 52+1  | 2^{11} (10^{-16})  | 11 | 2^{1022} - 2^{1023} (10^{-308})
-Extended | >=80 | >=64 | <=2 | >=15 | 2^{16382} - 2^{16383} (10^{-4932})

IEEE Floating Point Arithmetic Standard 754 - "Denorms"

- Denormalized Numbers:
  - Nonzero significant, minimum exponent
  - Fits in gap between UN and 0
- Underflow Exception
  - Occurs when exact nonzero result is less than underflow threshold d UN
- Ex: UN/2
- Returns a denorm, or zero
- Why bother?
  - Necessary so that following code never divides by zero
    \[ \text{if} (a > 0) \text{ then } x = a/b \text{ or } 0 \]
### IEEE Floating Point Arithmetic

#### Standard 754 – Infinity

- **Infinity**: Sign bit, zero significand, maximum exponent
- **Overflow Exception**: Occurs when exact finite result too large to represent accurately
- Ex: 2°OV
- Return = ± infinity
- **Sign of zero important!**
- Also return ± infinity for 3+infinity, 2*infinity, infinity*infinity
- Result is exact, not an exception!

#### NAN (Not A Number)

- **NAN**: Sign bit, nonzero significand, maximum exponent
- **Invalid Exception**: Occurs when exact result not a well-defined real number
- 0/0
- sqrt(-1)
- infinity-infinity, infinity/infinity, 0*infinity
- NAN = 3
- NAN > 3?

- **Two kinds of NANs**
  - Quiet - propagates without raising an exception
  - Signaling - generate an exception when touched
    - Good for detecting uninitialized data

### Error Analysis

- **Basic error formula**
  \[ f(x + a o p b) = (a o p b)(1 + d) \]
  where
  - \( o p \) one of +,-,*,/\n  - \(|d| \leq \text{macheps}\)
  - Assuming no overflow, underflow, or divide by zero

#### Example: adding 4 numbers

\[
\begin{align*}
  f(x_1 + x_2 + x_3 + x_4) &= \left( (x_1 + x_2)(1 + d_1) + x_3(1 + d_2) + x_4(1 + d_3) \right) \\
  &= x_1(1 + d_1)(1 + d_2)(1 + d_3) + \\
  &\quad x_2(1 + d_1)(1 + d_2)(1 + d_3) + \\
  &\quad 2x_1(x_2 + x_3) + x_4(1 + d_4) \\
  &= x_1^*(1 + e_1) + x_2^*(1 + e_2) + x_3^*(1 + e_3) + x_4^*(1 + e_4)
\end{align*}
\]

- get exact sum of slightly changed summands \( x_i^*(1 + e_i) \)
- Backward Error Analysis - algorithm called numerically stable if it gives the exact result for slightly changed inputs
- Numerical Stability is an algorithm design goal

### Backward error

- **Approximate solution is exact solution to modified problem.**
- **How large a modification to original problem is required to give result actually obtained?**
- **How much data error in initial input would be required to explain all the error in computed results?**
- **Approximate solution is good if it is exact solution to "nearby" problem.**

### Sensitivity and Conditioning

- **Problem is insensitive or well conditioned if relative change in input causes commensurate relative change in solution.**
- **Problem is sensitive or ill-conditioned, if relative change in solution can be much larger than that in input data.**

\[
\text{Cond} = \frac{\text{Relative change in solution}}{\text{Relative change in input data}} = \frac{\|f(x) - f(x')\|/\|f(x)\|}{\|x - x'\|/\|x\|}
\]

- Problem is sensitive, or ill-conditioned, if \( \text{Cond} \gg 1 \).
- When function \( f \) is evaluated for approximate input \( x' = x + h \) instead of true input value of \( x \),
- Absolute error = \( f(x + h) - f(x) \approx h f'(x) \)
- Relative error = \( [f(x + h) - f(x)] / f(x) \approx h f'(x) / f(x) \)

### Sensitivity: 2 Examples

- **cos(p/2) and 2-d System of Equations**
  - Consider problem of computing cosine function for argument near \( \pi/2 \)
  - Let \( x = \pi/2 \) and let \( h \) be small perturbation to \( x \), then
  - Absolute error = \( \cos(x + h) - \cos(x) \) = \( -h \sin(x) \) = \( -h \)
  - Relative error = \( h \tan(x) \approx 8 \)
  - So small change in \( x \) near \( \pi/2 \) causes large relative change in \( \cos(x) \) regardless of method used.
  - \( \cos(1.57079) = 0.63267949 \times 10^{-5} \)
  - \( \cos(1.57078) = 1.64267949 \times 10^{-5} \)
  - Relative change in output is a quarter million times greater than relative change in input.
Sensitivity: 2 Examples

cos(p/2) and 2-d System of Equations

- Consider problem of computing cosine function for arguments near p/2.
- Let x = p/2 and let h be small perturbation to x. Then:

  \[ \text{absolute error} = \cos(x+h) - \cos(x) = -h \sin(x) = -h, \]
  \[ \text{relative error} = -h \tan(x) \approx -h. \]

- So small change in x near p/2 causes large relative change in \( \cos(x) \) regardless of method used.

\( \cos(1.57079) = 0.63267949 \times 10^{-5} \)
\( \cos(1.57078) = 1.64267949 \times 10^{-5} \)

Relative change in output is a quarter million times greater than relative change in input.

Example: Polynomial Evaluation Using Horner’s Rule

- Horner’s rule to evaluate \( p = \sum_{k=0}^{n} c_k \cdot x^k \)
  \( p = c_n \), for \( k=n-1 \) down to 0, \( p = x^k p + c_k \)
- Numerically Stable
- Apply to \( (x-2)^9 = x^9 - 18x^8 + \ldots - 512 \)
  \(-2^9 + x^8(2^8 - x^*(2^7 + \ldots))\)
- Evaluated around 2

Example: Polynomial Evaluation (continued)

\( (x-2)^9 = x^9 - 18x^8 + \ldots - 512 \)

We can compute error bounds using

\( f(a \oplus b) = (a \oplus b) \oplus (1+d) \)

Exception Handling

- What happens when the “exact value” is not a real number, or too small or too large to represent accurately?

  - 5 Exceptions:
    - Overflow - exact result > OV, too large to represent
    - Underflow - exact result nonzero and < UN, too small to represent
    - Divide-by-zero - nonzero/0
    - Invalid - O/O, sqrt(-1), ...
    - Inexact - you made a rounding error (very common)

- Possible responses
  - Stop with error message (unfriendly, not default)
  - Keep computing (default, but how?)

Summary of Values Representable in IEEE FP

- + - Zero
- Normalized nonzero numbers
- Denormalized numbers
- + - Infinity
- NaNs
  - Signaling and quiet
  - Many systems have only quiet
Hazards of Parallel and Heterogeneous Computing

- What new bugs arise in parallel floating point programs?
  - Ex 1: Nonrepeatability
    - Makes debugging hard!
  - Ex 2: Different exception handling
    - Can cause programs to hang
  - Ex 3: Different rounding (even on IEEE FP machines)
    - Can cause hanging, or wrong results with no warning
- See www.netlib.org/lapack/lawns/lawn112.ps

Lecture 5: Memory Hierarchy and Cache

Cache: A safe place for hiding and storing things.
Webster’s New World Dictionary (1976)

Tools for Performance Evaluation

- Timing and performance evaluation has been an art
  - Resolution of the clock
  - Issues about cache effects
  - Different systems
- Situation about to change
  - Today’s processors have counters

Performance Counters

- Almost all high performance processors include hardware performance counters.
- On most platforms the APIs, if they exist, are not appropriate for a common user, functional or well documented.
- Existing performance counter APIs
  - Intel Pentium
  - SGI MIPS R10000
  - IBM Power series
  - DEC Alpha pfm pseudo-device interface
  - Via Windows 95, NT and Linux on these systems

Performance Data (cont.)

- Cycle count
- Floating point instruction count
- Integer instruction count
- Instruction count
- Load/store count
- Branch taken / not taken count
- Branch mispredictions
- Pipeline stalls due to memory subsystem
- Pipeline stalls due to resource conflicts
- I/D cache misses for different levels
- Cache invalidations
- TLB misses
- TLB invalidations

PAPI Usage

- Application is instrumented with PAPI
- Will be layered over the best existing vendor-specific APIs for these platforms
- call PAPIf_flops( real_time, proc_time, flpins, mflops, check )
- PAPI_flops( &real_time, &proc_time, &flpins, &mflops):
- Show example http://www.cs.utk.edu/~terpstra/using_papi/
Cache and Its Importance in Performance

- **Motivation:**
  - Time to run code = clock cycles running code + clock cycles waiting for memory
  - For many years, CPU's have sped up an average of 50% per year over memory chip speed ups.
  - Hence, memory access is the bottleneck to computing fast.
- **Definition of a cache:**
  - Dictionary: a safe place to hide or store things.
  - Computer: a level in a memory hierarchy.

What is a cache?
- Small, fast storage used to improve average access time to slow memory
- Exploits spacial and temporal locality
- In computer architecture, almost everything is a cache!
  - Registers: "a cache" on variables - software managed
  - First-level cache a cache on second-level cache
  - Second-level cache a cache on memory
  - Memory a cache on disk (virtual memory)
  - TLB a cache on page table
  - Branch-prediction a cache on prediction information?

Who Cares About the Memory Hierarchy?

Processor-DRAM Memory Gap (latency)

Matrix-multiply, optimized several ways

Cache Sporting Terms
- **Cache Hit**: The CPU requests data that is already in the cache. We want to maximize this. The hit rate is the percentage of cache hits.
- **Cache Miss**: The CPU requests data that is not in cache. We want to minimize this. The miss rate is how long it takes to get data, which can be variable and is highly architecture dependent.
- Two level caches are common. The L1 cache is on the CPU chip and the L2 cache is separate. The L1 misses are handled faster than the L2 misses in most designs.
- Upstream caches are closer to the CPU than downstream caches. A typical Alpha CPU has L1-L3 caches. Some MIPS CPUs do, too.

Cache Benefits
- **Data cache was designed with two key concepts in mind**
  - **Spatial Locality**
    - When an element is referenced its neighbors will be referenced too
    - Cache lines are fetched together
    - Work on consecutive data elements in the same cache line
  - **Temporal Locality**
    - When an element is referenced, it might be referenced again soon
    - Arrange code so that data in cache is reused often
Cache-Related Terms

Least Recently Used (LRU): Cache replacement strategy for set associative caches. The cache block that is least recently used is replaced with a new block.

Random Replace: Cache replacement strategy for set associative caches. A cache block is randomly replaced.

Levels of the Memory Hierarchy

<table>
<thead>
<tr>
<th>Capacity</th>
<th>Access Time</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Registers</td>
<td>100 bytes</td>
<td>1 ns</td>
</tr>
<tr>
<td>Cache</td>
<td>N bytes</td>
<td>100 ns</td>
</tr>
<tr>
<td>Main Memory</td>
<td>N bytes</td>
<td>10 ms</td>
</tr>
<tr>
<td>Disk</td>
<td>G bytes, 10 ms</td>
<td>10,000 ns</td>
</tr>
<tr>
<td>Tape</td>
<td>infinite</td>
<td>100 s</td>
</tr>
</tbody>
</table>

Reality

Modern processors use a variety of techniques for performance:
- **Caches**: small amount of fast memory where values are “cached” in hope of reusing recently used or nearby data
- **Parallelism**: superscalar processors have multiple “functional units” that can run in parallel
- **Pipelining**: a form of parallelism, like an assembly line in a factory

Why is this your problem?
In theory, compilers understand all of this and can optimize your program; in practice they don’t.

Traditional Four Questions for Memory Hierarchy Designers

1. Where can a block be placed in the upper level? (Block placement)
- Fully Associative, Set Associative, Direct Mapped
2. How is a block found if it is in the upper level? (Block identification)
- Tag/Block
3. Which block should be replaced on a miss? (Block replacement)
- Random, LRU
4. What happens on a write? (Write strategy)
- Write Back or Write Through (with Write Buffer)
Cache-Related Terms
- **ICACHE**: Instruction cache
- **DCACHE (L1)**: Data cache closest to registers
- **SCACHE (L2)**: Secondary data cache
  - Data from SCACHE has to go through DCACHE to registers
  - SCACHE is larger than DCACHE
  - Not all processors have SCACHE

Unified versus Split Caches
- This refers to having a single or separate caches for data and machine instructions.
- Split is obviously superior. It reduces thrashing, which we will come to shortly.

Unified vs Split Caches
- **Unified vs Separate I&D**
  - Example:
    - 16KB I&D: Inst miss rate=0.64%, Data miss rate=6.47%
    - 32KB unified: Aggregate miss rate=1.99%
  - Which is better (ignore L2 cache)?
    - Assume 33% data ops ⇒ 75% accesses from instructions (1.0/1.33)
    - hit time=1, miss time=50
    - Note that data hit has 1 stall for unified cache (only one port?)

Where to misses come from?
- **Classifying Misses: 3 Cs**
  - **Compulsory**—The first access to a block is not in the cache, so the block must be brought into the cache. Also called cold start misses or first reference misses. (Misses in even an Infinite Cache)
  - **Capacity**—If the cache cannot contain all the blocks needed during execution of a program, capacity misses will occur due to blocks being discarded and later retrieved. (Misses in Fully Associative Size X Cache)
  - **Conflict**—If block-placement strategy is set associative or direct mapped, conflict misses (in addition to compulsory & capacity misses) will occur because a block can be discarded and later retrieved if too many blocks map to its set. Also called collision misses or interference misses. (Misses in N-way Associative, Size X Cache)

Simplest Cache: Direct Mapped
- **Memory Address** Memory
- 4 Byte Direct Mapped Cache
- Cache Index
- Location 0 can be occupied by data from:
  - Memory location 0, 4, 8, ... etc.
  - In general: any memory location whose 2 LSBs of the address are 0s
- Address[1:0] ⇒ cache index
- Which one should we place in the cache?
- How can we tell which one is in the cache?

Cache Mapping Strategies
- There are two common sets of methods in use for determining which cache lines are used to hold copies of memory.
- **Direct**: Cache address = memory address MODULO cache size.

- Set associative: There are N cache banks and memory is assigned to just one of the banks. There are three algorithmic choices for which line to replace:
  - **Random**: Choose any line using an analog random number generator. This is cheap and simple to make.
  - **LRU** (least recently used): Preserves temporal locality, but is expensive. This is not much better than random according to (biased) studies.
  - **FIFO** (first in, first out): Random is far superior.
Cache Basics

- Cache hit: a memory access that is found in the cache -- cheap
- Cache miss: a memory access that is not in the cache -- expensive, because we need to get the data from elsewhere
- Consider a tiny cache (for illustration only)

<table>
<thead>
<tr>
<th>Address</th>
<th>tag</th>
<th>line</th>
<th>offset</th>
</tr>
</thead>
<tbody>
<tr>
<td>0100</td>
<td>00</td>
<td>00</td>
<td>00</td>
</tr>
<tr>
<td>0100</td>
<td>00</td>
<td>00</td>
<td>00</td>
</tr>
<tr>
<td>0110</td>
<td>00</td>
<td>00</td>
<td>00</td>
</tr>
<tr>
<td>0110</td>
<td>00</td>
<td>00</td>
<td>00</td>
</tr>
</tbody>
</table>

- Cache line length: number of bytes loaded together in one entry
- Direct mapped: only one address (line) in a given range in cache
- Associative: 2 or more lines with different addresses exist

Direct-Mapped Cache

- Direct mapped cache: A block from main memory can go in exactly one place in the cache. This is called direct mapped because there is direct mapping from any block address in memory to a single location in the cache.

Set Associative Cache

- Set associative cache: The middle range of designs between direct mapped cache and fully associative cache is called set-associative. In a n-way set-associative cache a block from main memory can go into N (N > 1) locations in the cache.

Here assume cache has 8 blocks, while memory has 32

<table>
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<th>Fully associative</th>
<th>Direct mapped</th>
<th>Set associative</th>
</tr>
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<td>01234567</td>
<td>12 can go anywhere</td>
<td>12 can go only into block 4 (12 mod 8)</td>
<td>12 can go anywhere in Set 0 (12 mod 4)</td>
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## Diagrams

### Serial:
- CPU → 1st Cache → Main Memory

### Parallel:
- Shared Memory
- Network
- Cache 1 → Cache 2 → ... → Cache p
- CPU 1 → CPU 2 → ... → CPU p

## Tuning for Caches
1. Preserve locality.
2. Reduce cache thrashing.
3. Loop blocking when out of cache.
4. Software pipelining.

## Registers
- Registers are the source and destination of most CPU data operations.
- They hold one element each.
- They are made of static RAM (SRAM), which is very expensive.
- The access time is usually 1-1.5 CPU clock cycles.
- Registers are at the top of the memory subsystem.

## Memory Banking
- This started in the 1960's with both 2 and 4 way interleaved memory banks. Each bank can produce one unit of memory per bank cycle. Multiple reads and writes are possible in parallel.
- Memory chips must internally recover from an access before it is reaccessed.
- The bank cycle time is currently 4-8 times the CPU clock time and getting worse every year.
- Very fast memory (e.g., SRAM) is unaffordable in large quantities.
- This is not perfect. Consider a 4 way interleaved memory and a stride 4 algorithm. This is equivalent to non-interleaved memory systems.

## The Principle of Locality
- **The Principle of Locality:** Program access a relatively small portion of the address space at any instant of time.
- **Two Different Types of Locality:**
  - **Temporal Locality** (Locality in Time): If an item is referenced, it will tend to be referenced again soon (e.g., loops, reuse)
  - **Spatial Locality** (Locality in Space): If an item is referenced, items whose addresses are close by tend to be referenced soon (e.g., straightline code, array access)
- Last 15 years, HW relied on locality for speed.

## Principals of Locality
- **Temporal:** an item referenced now will be again soon.
- **Spatial:** an item referenced now causes neighbors to be referenced soon.
- **Lines, not words** are moved between memory levels. Both principals are satisfied. There is an optimal line size based on the properties of the data bus and the memory subsystem designs.
- Cache lines are typically 32-128 bytes with 1024 being the longest currently.
What happens on a write?

- **Write through**—The information is written to both the block in the cache and to the block in the lower-level memory.
- **Write back**—The information is written only to the block in the cache. The modified cache block is written to main memory only when it is replaced in cache.
- **Pros and Cons of each?**
  - WT: read misses cannot result in writes
  - WB: no repeated writes to same location
- **WT always combined with write buffers so that don’t wait for lower level memory**

Cache Thrashing

- Thrashing occurs when frequently used cache lines replace each other. There are three primary causes for thrashing:
  - Instructions and data can conflict, particularly in unified caches.
  - Too many variables or too large of arrays are accessed that do not fit into cache.
  - Indirect addressing, e.g., sparse matrices.
- Machine architects can add sets to the associativity. Users can buy another vendor’s machine. However, neither solution is realistic.

Cache Coherence for Multiprocessors

- All data must be coherent between memory levels. Multiple processors with separate caches must inform the other processors quickly about data modifications (by the cache line). Only hardware is fast enough to do this.
- **Standard protocols on multiprocessors:**
  - Snoopy: all processors monitor the memory bus.
  - Directory based: Cache lines maintain an extra 2 bits per processor to maintain clean/dirty status bits.

Processor Stall

- Processor stall is the condition where a cache miss occurs and the processor waits on the data.
- A better design allows any instruction in the instruction queue to execute that is ready. You see this in the design of some RISC CPUs, e.g., the RS6000 line.
- Memory subsystems with hardware data prefetch allow scheduling of data movement to cache.
- Software pipelining can be done when loops are unrolled. In this case, the data movement overlaps with computing, usually with reuse of the data.
- Out of order execution, software pipelining, and prefetch.

Indirect Addressing

```
d = 0
  do i = 1,n
    j = ind(i)
    d = d + sqrt( x(j)*x(j) + y(j)*y(j) + z(j)*z(j) )
  end do

  d = d + sqrt( r(1,j)*r(1,j) + r(2,j)*r(2,j) + r(3,j)*r(3,j) )
```

- Change loop statement to
- Note that r(1,j) & r(3,j) are in contiguous memory and probably are in the same cache line (d is probably in a register and is irrelevant). The original form uses 3 cache lines at every instance of the loop and can cause cache thrashing.

Cache Thrashing by Memory Allocation

```
parameter ( m = 1024*1024 )

real a(m), b(m)
```

- For a 4 Mb direct mapped cache, a(i) and b(i) are always mapped to the same cache line. This is trivially avoided using padding.

```
real a(m), extra(32), b(m)
```

- Extra i is at least 128 bytes in length, which is longer than a cache line on all but one memory subsystem that is available today.
Cache Blocking

- We want blocks to fit into cache. On parallel computers we have \( p \times c \) cache so that data may fit into cache on \( p \) processors, but not one. This leads to superlinear speed up! Consider matrix-matrix multiply.

\[
do k = 1,n \\
\quad do j = 1,n \\
\quad\quad do i = 1,n \\
\quad\quad\quad c(i,j) = c(i,j) + a(i,k) \cdot b(k,j) \\
\quad\quad end do \\
\quad end do \\
end do
\]

An alternate form is...

Summary: The Cache Design Space

- Several interacting dimensions
  - cache size
  - block size
  - associativity
  - replacement policy
  - write-through vs write-back
  - write allocation
- The optimal choice is a compromise
  - depends on access characteristics
    - workload
    - use (i-cache, D-cache, TLB)
  - depends on technology / cost
- Simplicity often wins

Lessons

- The 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
- Since we want to write fast programs, we must take the architecture into account, even on uniprocessors
- Since the actual performance is so complicated, we need simple models to help us design efficient algorithms
- We will illustrate with a common technique for improving cache performance, called blocking

Optimizing Matrix Addition for Caches

- Dimension \( A(n,n), B(n,n), C(n,n) \)
- \( A, B, C \) stored by column (as in Fortran)
- Algorithm 1:
  - for \( i=1:n \), for \( j=1:n \), \( A(i,j) = B(i,j) + C(i,j) \)
- Algorithm 2:
  - for \( j=1:n \), for \( i=1:n \), \( A(i,j) = B(i,j) + C(i,j) \)
- What is "memory access pattern" for Alg 1 and 2?
- Which is faster?
- What if \( A, B, C \) stored by row (as in C)?

Homework Assignment

- Implement, in Fortran or C, the six different ways to perform matrix multiplication by interchanging the loops. (Use 64-bit arithmetic.) Make each implementation a subroutine, like:
  - subroutine ijk ( a, m, n, lda, b, k, ldb, c, ldc )
  - subroutine ikj ( a, m, n, lda, b, k, ldb, c, ldc )
- ...
Loop Fusion Example

/* Before */
for (i = 0; i < N; i = i+1)
for (j = 0; j < N; j = j+1)
    a[i][j] = 1/b[i][j] * c[i][j];
for (i = 0; i < N; i = i+1)
for (j = 0; j < N; j = j+1)
    d[i][j] = a[i][j] + c[i][j];

/* After */
for (i = 0; i < N; i = i+1)
    for (j = 0; j < N; j = j+1)
        { a[i][j] = 1/b[i][j] * c[i][j];
          d[i][j] = a[i][j] + c[i][j];
        }

2 misses per access to a & c vs. one miss per access; improve spatial locality

Optimizing Matrix Multiply for Caches

- Several techniques for making this faster on modern processors
  - heavily studied
- Some optimizations done automatically by compiler, but can do much better
  - In general, you should use optimized libraries (often supplied by vendor) for this and other very common linear algebra operations
  - BLAS = Basic Linear Algebra Subroutines
- Other algorithms you may want are not going to be supplied by vendor, so need to know these techniques

Warm up: Matrix-vector multiplication 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 y = y + A*x

(read x(1:n) into fast memory)
(read y(1:n) into fast memory)
for i = 1:n
    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 = 3*n + n^2
- f = number of arithmetic operations = 2*n^2
- q = f/m ≈ 2
- Matrix-vector multiplication limited by slow memory speed

Multiply

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)

Matrix Multiply

C=C+A*B(unblocked, or untiled)

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)
(write C(i,j) back to slow memory)
Matrix Multiply (unblocked, or untiled)

Number of slow memory references on unblocked matrix multiply

\[ m = n^3 \] read each column of \( B \) \( n \) times
+ \( n^2 \) read each column of \( A \) once for each \( i \)
+ \( 2n^2 \) read and write each element of \( C \) once

\[ = n^3 + 3n^2 \]

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

\[ \approx 2 \] for large \( n \), no improvement over matrix-vector mult

\[ + \ast \]

\[ C(i,j) \leftarrow C(i,j) \ast A(i,:) \ast B(:,j) \]

More on BLAS (Basic Linear Algebra Subroutines)

- **Industry standard interface (evolving)**
  - Vendors, others supply optimized implementations
- **History**
  - BLAS1 (1970s):
    - vector operations: dot product, saxpy (\( y = a \ast x + y \)), etc
    - \( m=2n, f=2n, q \sim 1 \) or less
  - BLAS2 (mid 1980s):
    - matrix-vector operations: matrix vector multiply, etc
    - \( m=n^2, f=2n^2, q \sim 2 \), less overhead
    - somewhat faster than BLAS1
  - BLAS3 (late 1980s):
    - matrix-matrix operations: matrix matrix multiply, etc
    - \( m \gg n^2, f \gg n^3 \), so \( q \) can possibly be as large as \( n \), so BLAS 3 is potentially much faster than BLAS2
- **Good algorithms used BLAS3 when possible (LAPACK)**

Optimizing in practice

- **Tiling for registers**
  - loop unrolling, use of named "register" variables
- **Tiling for multiple levels of cache**
- **Exploiting fine-grained parallelism within the processor**
  - super scalar
  - pipeline
- **Complicated compiler interactions**
- **Hard to do by hand (but you’ll try)**
- **Automatic optimization an active research area**
  - PHIPAC: www.icsi.berkeley.edu/~bilmes/phipac
  - www.cs.berkeley.edu/~iyer/asci_slides.ps
  - ATLAS: www.netlib.org/atlas/index.html

BLAS for Performance

- Development of blocked algorithms important for performance
- Level 3 BLAS
- Level 2 BLAS
- Level 1 BLAS
- (n x n matrix multiply) vs BLAS 2 (n x n matrix vector multiply) vs BLAS 1 (saxPY of \( n \) vectors)

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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 $2 \times 2$ matrix multiply, normally 8 multiplies

$$
\begin{align*}
M &= \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \\
&= \begin{bmatrix} p_1 + p_2 - p_4 + p_6 \\ p_4 + p_5 \\ p_6 + p_7 \\ p_2 - p_3 + p_5 - p_7 \end{bmatrix}
\end{align*}
$$

Extends to divide and conquer

Strassen (continued)

- $T(n) = O(n^\log_2 7) = O(n^{2.81})$
- Available in several libraries
- Up to several time faster if $n$ large enough (100s)
- Needs more memory than standard algorithm
- Can be less accurate because of roundoff error
- Current world’s record is $O(n^{2.376})$

Summary

- Performance programming on uniprocessors requires
  - understanding of memory system
  - levels, costs, sizes
- Blocking (tiling) is a basic approach that can be applied to
  many matrix algorithms
- Applies to unprocessors and parallel processors
  - The technique works for any architecture, but choosing the
  blocksize $b$ and other details depends on the architecture
- Similar techniques are possible on other data structures
- You will get to try this in Assignment 2 (see the class
  homepage)

Summary: Memory Hierarchy

- Virtual memory was controversial at the time:
  - can SW automatically manage 64KB across many
    programs?
  - 1000X DRAM growth removed the controversy
- Today VM allows many processes to share single
  memory without having to swap all processes to disk;
  today VM protection is more important than
  memory hierarchy
- Today CPU time is a function of (ops, cache
  misses) vs. just f(ops):
  What does this mean to Compilers, Data
  structures, Algorithms?

Performance = Effective Use of Memory Hierarchy

- Can only do arithmetic on
data at the top of the
hierarchy
- Higher level BLAS lets us
do this

<table>
<thead>
<tr>
<th>Level</th>
<th>BLAS</th>
<th>Memory</th>
<th>Flops</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level 1</td>
<td>$\gamma = \alpha$</td>
<td>$n$</td>
<td>$2n$</td>
</tr>
<tr>
<td>Level 2</td>
<td>$\gamma = \gamma \times \alpha$</td>
<td>$n^2$</td>
<td>$2n^2$</td>
</tr>
<tr>
<td>Level 3</td>
<td>$\gamma = \gamma \times \alpha$</td>
<td>$n^3$</td>
<td>$n^2 \times n^2$</td>
</tr>
</tbody>
</table>

Homework Assignment

- Implement, in Fortran or C, the six different ways
  to perform matrix multiplication by interchanging
  the loops. (Use 64-bit arithmetic.) Make each
  implementation a subroutine, like:

  subroutine ijk (a, m, n, lda, b, k, ldb, c, ldc)

  subroutine ikj (a, m, n, lda, b, k, ldb, c, ldc)

  ...

BLAS Memory Flops/ Memory

- Level 1: $\gamma = \alpha$
- Level 2: $\gamma = \gamma \times \alpha$
- Level 3: $\gamma = \gamma \times \alpha$

Development of blocked algorithms important for
performance
Thanks

These slides came in part from courses taught by the following people:

- Kathy Yelick, UC, Berkeley
- Dave Patterson, UC, Berkeley
- Randy Katz, UC, Berkeley
- Craig Douglas, U of Kentucky

Computer Architecture A Quantitative Approach, Chapter 8, Hennessy and Patterson, Morgan Kaufman Pub.

---

Schematic View of a Typical Memory Hierarchy: IBM 590

- Main memory: arbitrary size
  Access time: 27/32 cycles

- Cache: 32,768 doublewords
  Access time: 3 cycles

- Data packets: 1 doubleword
  Access time: 0 cycles

Design your program for optimal spatial and temporal data locality!

---

Effect of Stride and Array Size on Access Time

![Graph showing effect of stride on access time](image)

Optimal Data Locality: Data Structures

```fortran
  dimension r(n), f(n)
  a(2)(n), f(2)(n)

  do 100 i=1,n
    do 100 j=1,i-1
      dist=(r(i)-r(j))^2 +
      f(i)-f(j)^2 +...
      if (dist.le.cutoff) then
        calculate interaction
      endif
      100       continue
  end
```

Instruction Level Parallelism: Floating Point

- IBM RS/6000 Power2 (130 MHz)
  - 2 FP units, each capable of:
    1 fused multiply-add (1;2) or
    1 add (1;1) or
    1 multiply (1;2)
  - 1 quad load/store (1;1)
  - Leading to (up to)
    4 FP Ops per CP

- DEC Alpha EV5 (350 MHz)
  - 1 FP unit, capable of:
    1 floating point add pipeline (1;4)
    1 floating point mult. pipeline (1;4)
  - Leading to (up to)
    2 FP Ops per CP

- SGI R10000 (200 MHz)
  - 1 FP unit capable of:
    1 floating point add pipeline (1;2)
    1 floating point mult. pipeline (1;2)
  - Leading to (up to)
    1 FP Ops per CP

Code Restructuring for On-Chip Parallelism: Original Code

```fortran
  program length
  parameter (n=2**14)
  dimension a(n)

  subroutine length1(n,aa,tt)
    implicit real*8 (a-h,o-z)
    dimension a(n)
    tt=0.d0
    do 100, j=1,n
      tt=tt+a(j)*a(j)
    100   continue
    return
  end
```

---

---
Modified Code for On-Chip Parallelism

```
Subroutine length4 (n,a,tt)
  Implicit real*8 (a-h,o-z)
  Dimension a(n)

  t1=0.d0
  t2=0.d0
  t3=0.d0
  t4=0.d0
  Do 100, j=1,n-3,4
    c first floating point instruction unit, all even cycles
    t1=t1+a(j+0)*a(j+0)
    c first floating point instruction unit, all odd cycles
    t2=t2+a(j+1)*a(j+1)
    c second floating point instruction unit, all even cycles
    t3=t3+a(j+2)*a(j+2)
    c second floating point instruction unit, all odd cycles
    t4=t4+a(j+3)*a(j+3)
  100 Continue
  tt=t1+t2+t3+t4
  Return
End
```

Software Pipelining

```
Subroutine mult(n1,nd1,n2,nd2,y,a,x)
  Implicit real*8 (a-h,o-z)
  Dimension a(nd1,nd2),y(nd2),x(nd1)

  Do 10, i=1,n1-3,4
    t1=0.d0
    t2=0.d0
    t3=0.d0
    t4=0.d0
    Do 20, j=1,n2-3,4
      t1=t1+a(j+0,i+0)*x(j+0)+a(j+1,i+0)*x(j+1)+a(j+2,i+0)*x(j+2)+a(j+3,i+0)*x(j+3)
      t2=t2+a(j+0,i+1)*x(j+0)+a(j+1,i+1)*x(j+1)+a(j+2,i+1)*x(j+2)+a(j+3,i+0)*x(j+3)
      t3=t3+a(j+0,i+2)*x(j+0)+a(j+1,i+2)*x(j+1)+a(j+2,i+2)*x(j+2)+a(j+3,i+2)*x(j+3)
      t4=t4+a(j+0,i+3)*x(j+0)+a(j+1,i+3)*x(j+1)+a(j+2,i+3)*x(j+2)+a(j+3,i+3)*x(j+3)
    20 Continue
    y(i+0)=t1
    y(i+1)=t2
    y(i+2)=t3
    y(i+3)=t4
  10 Continue
End
```

Improving Ratio of Floating Point Operations to Memory Accesses

```
Subroutine mult(n1,nd1,n2,nd2,y,a,x)
  Implicit real*8 (a-h,o-z)
  Dimension a(nd1,nd2),y(nd2),x(nd1)

  Do 10, i=1,n1-3,4
    t=0.d0
    Do 20, j=1,n2-3,4
      t=t+ax(j,i)*x(j)
    20 Continue
    y(i)=t
  10 Continue
End
```

Summary of Optimization Techniques (II)

- Achieving high-performance requires code restructuring. Minimization of memory traffic is the single most important goal.
- Compilers are getting better: good at software pipelining. But they are not there yet: can do loop transformations only in simple cases, usually fail to produce optimal blocking, heuristics for unrolling may not match your code well, etc.
- The optimization process is machine-specific and requires detailed architectural knowledge.
Amdahl’s Law

Amdahl’s Law places a strict limit on the speedup that can be realized by using multiple processors. Two equivalent expressions for Amdahl’s Law are given below:

\[ t_N = \left( \frac{f_p}{N} + f_s \right) t_1 \]  
Effect of multiple processors on run time

\[ S = \frac{1}{f_s + \frac{f_p}{N}} \]  
Effect of multiple processors on speedup

Where:

\[ f_s = \text{serial fraction of code} \]
\[ f_p = \text{parallel fraction of code} = 1 - f_s \]
\[ N = \text{number of processors} \]

Illustration of Amdahl’s Law

It takes only a small fraction of serial content in a code to degrade the parallel performance. It is essential to determine the scaling behavior of your code before doing production runs using large numbers of processors.

Amdahl’s Law vs. Reality

Amdahl’s Law provides a theoretical upper limit on parallel speedup assuming that there are no costs for communications. In reality, communications (and I/O) will result in a further degradation of performance.

More on Amdahl’s Law

• Amdahl’s Law can be generalized to any two processes of with different speeds

  Ex.: Apply to \( f_{\text{processor}} \) and \( f_{\text{memory}} \):

  The growing processor-memory performance gap will undermine our efforts at achieving maximum possible speedup!

Gustafson’s Law

• Thus, Amdahl’s Law predicts that there is a maximum scalability for an application, determined by its parallel fraction, and this limit is generally not large.

• There is a way around this: increase the problem size

  ➢ bigger problems mean bigger grids or more particles: bigger arrays
  ➢ number of serial operations generally remains constant; number of parallel operations increases: parallel fraction increases

Parallel Performance Metrics: Speedup

Speedup is only one characteristic of a program - it is not synonymous with performance. In this comparison of two machines the code achieves comparable speedups but one of the machines is faster.
Fixed-Problem Size Scaling

- a.k.a. Fixed-load, Fixed-Problem Size, Strong Scaling, Problem-Constrained, constant-problem size (CPS), variable subgrid
- Amdahl Limit: $S_A(n) = \frac{T(1)}{T(n)} = \frac{1}{f/n + (1 - f)}$
- This bounds the speedup based only on the fraction of the code that cannot use parallelism ($1 - f$); it ignores all other factors
- $S_A \to \frac{1}{1 - f}$ as $n \to \infty$

Fixed-Problem Size Scaling (Cont’d)

- Efficiency ($\eta$) = $\frac{T(1)}{T(n) \cdot n}$
- Memory requirements decrease with $n$
- Surface-to-volume ratio increases with $n$
- Superlinear speedup possible from cache effects
- Motivation: what is the largest # of procs I can use effectively and what is the fastest time that I can solve a given problem?
- Problems:
  - Sequential runs often not possible (large problems)
  - Speedup (and efficiency) is misleading if processors are slow

Fixed-Problem Size Scaling: Examples


Scaled Speedup Experiments

- Motivation: Want to use a larger machine to solve a larger global problem in the same amount of time.
- Memory and surface-to-volume effects remain constant.

- Be wary of benchmarks that scale problems to unreasonably-large sizes
  - scale the problem to fill the machine when a smaller size will do;
  - simplify the science in order to add computation
    - “World’s largest MD simulation - 10 gazillion particles!”
  - run grid sizes for only a few cycles because the full run won’t finish during this lifetime or because the resolution makes no sense compared with resolution of input data
- Suggested alternate approach (Gustafson): Constant time benchmarks
  - run code for a fixed time and measure work done
Example of a Scaled Speedup

<table>
<thead>
<tr>
<th>Processors</th>
<th>NChains</th>
<th>Time</th>
<th>Natoms</th>
<th>Time per Atom</th>
<th>Time per Proc</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32</td>
<td>38.4</td>
<td>2368</td>
<td>1.62E-02</td>
<td>1.62E-02</td>
<td>1.000</td>
</tr>
<tr>
<td>2</td>
<td>64</td>
<td>38.4</td>
<td>4736</td>
<td>8.11E-03</td>
<td>1.62E-02</td>
<td>0.997</td>
</tr>
<tr>
<td>4</td>
<td>128</td>
<td>38.5</td>
<td>9472</td>
<td>4.06E-03</td>
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<td>0.997</td>
</tr>
<tr>
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<td>0.857</td>
</tr>
</tbody>
</table>

TBON on ASCI Red

![Performance Optimization](image)