CSE 548: Analysis of Algorithms

Lectures 27 & 28 (Analyzing I/O and Cache Performance)

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Iterative Matrix-Multiply Variants

double Z[n][n], X[n][n], Y[n][n];



Performance of Iterative Matrix-Multiply Variants

Processor: 2.7 GHz Intel Xeon E5-2680 (used only one core)

Caches & RAM: private 32KB L1, private 256KB L2, shared 20MB L3, 32 GB RAM

Optimizations: none (icc 13.0 with -O0)























Memory: Fast, Large & Cheap!

For efficient computation we need

- fast processors
- fast and large (but not so expensive) memory

But memory <u>cannot be cheap, large and fast</u> at the same time, because of

- finite signal speed
- lack of space to put enough connecting wires

A reasonable compromise is to use a *memory hierarchy*.

The Memory Hierarchy



A memory hierarchy is

- almost as fast as its fastest level
- almost as large as its largest level
- inexpensive

The Memory Hierarchy



To perform well on a memory hierarchy algorithms must have <u>high locality</u> in their memory access patterns.

Locality of Reference

Spatial Locality: When a block of data is brought into the cache it should contain as much useful data as possible.

Temporal Locality: Once a data point is in the cache as much useful work as possible should be done on it before evicting it from the cache.

CPU-bound vs. Memory-bound Algorithms

The Op-Space Ratio: Ratio of the number of operations performed by an algorithm to the amount of space (input + output) it uses.

Intuitively, this gives an upper bound on the average number of operations performed for every memory location accessed.

CPU-bound Algorithm:

- high op-space ratio
- more time spent in computing than transferring data
- a faster CPU results in a faster running time

Memory-bound Algorithm:

- low op-space ratio
- more time spent in transferring data than computing
- a faster memory system leads to a faster running time

The Two-level I/O Model

The *two-level I/O model* [Aggarwal & Vitter, CACM'88] consists of:

- an internal memory of size M
- an arbitrarily large *external memory* partitioned into blocks
 of size *B*.

I/O complexity of an algorithm



= number of blocks transferred between these two levels

Basic I/O complexities: $scan(N) = \Theta\left(\frac{N}{B}\right)$ and $sort(N) = \Theta\left(\frac{N}{B}\log_{\frac{M}{B}}\frac{N}{B}\right)$

Algorithms often crucially depend on the knowledge of M and B

 \Rightarrow algorithms do not adapt well when *M* or *B* changes

<u>The Ideal-Cache Model</u>

The *ideal-cache model* [Frigo et al., FOCS'99] is an extension of the I/O model with the following constraint:

algorithms are not allowed to use knowledge of *M* and *B*.

Consequences of this extension

- algorithms can simultaneously adapt to all levels of a multilevel memory hierarchy
- algorithms become more flexible and portable

Algorithms for this model are known as *cache-oblivious algorithms*.



- Optimal offline cache replacement policy
- □ Exactly two levels of memory
- Automatic replacement & full associativity

- Optimal offline cache replacement policy
 - LRU & FIFO allow for a constant factor approximation of optimal [Sleator & Tarjan, JACM'85]
 - Exactly two levels of memory
 - Automatic replacement & full associativity

- Optimal offline cache replacement policy
- Exactly two levels of memory
 - can be effectively removed by making several reasonable assumptions about the memory hierarchy [Frigo et al., FOCS'99]
- Automatic replacement & full associativity

- Optimal offline cache replacement policy
- Exactly two levels of memory
- □ Automatic replacement & full associativity
 - in practice, cache replacement is automatic
 (by OS or hardware)
 - fully associative LRU caches can be simulated in software
 with only a constant factor loss in expected performance
 [Frigo et al., FOCS'99]

The model makes the following assumptions:

- Optimal offline cache replacement policy
- Exactly two levels of memory
- □ Automatic replacement & full associativity

Often makes the following assumption, too:

 $\square M = \Omega(B^2), \text{ i.e., the cache is } tall$

The model makes the following assumptions:

- Optimal offline cache replacement policy
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- □ Automatic replacement & full associativity

Often makes the following assumption, too:

 $\square M = \Omega(B^2), \text{ i.e., the cache is } tall$

most practical caches are tall

The Ideal-Cache Model: I/O Bounds

Cache-oblivious vs. cache-aware bounds:

□ Basic I/O bounds (same as the cache-aware bounds):

$$- \quad scan(N) = \Theta\left(\frac{N}{B}\right)$$

$$- \quad sort(N) = \Theta\left(\frac{N}{B}\log_{\frac{M}{B}}\frac{N}{B}\right)$$

- Most cache-oblivious results match the I/O bounds of their cache-aware counterparts
- There are few exceptions; e.g., no cache-oblivious solution to the *permutation* problem can match cache-aware I/O bounds [Brodal & Fagerberg, STOC'03]

Some Known Cache Aware / Oblivious Results

Problem	Cache-Aware Results	Cache-Oblivious Results		
Array Scanning (<i>scan</i> (<i>N</i>))	$O\left(\frac{N}{B}\right)$	$O\left(\frac{N}{B}\right)$		
Sorting (sort(N))	$O\left(\frac{N}{B}\log_{\frac{M}{B}}\frac{N}{B}\right)$	$O\left(\frac{N}{B}\log_{\frac{M}{B}}\frac{N}{B}\right)$		
Selection	O(scan(N))	O(scan(N))		
B-Trees [Am] (Insert, Delete)	$O\left(\log_B \frac{N}{B}\right)$	$O\left(\log_{B}\frac{N}{B}\right)$		
Priority Queue [Am] (Insert, Weak Delete, Delete-Min)	$O\left(rac{1}{B}\log_{rac{M}{B}}rac{N}{B} ight)$	$O\left(\frac{1}{B}\log_{\frac{M}{B}}\frac{N}{B}\right)$		
Matrix Multiplication	$O\left(\frac{N^3}{B\sqrt{M}}\right)$	$O\left(\frac{N^3}{B\sqrt{M}}\right)$		
Sequence Alignment	$O\left(\frac{N^2}{BM}\right)$	$O\left(\frac{N^2}{BM}\right)$		
Single Source Shortest Paths	$O\left(\left(V + \frac{E}{B}\right) \cdot \log_2 \frac{V}{B}\right)$	$O\left(\left(V + \frac{E}{B}\right) \cdot \log_2 \frac{V}{B}\right)$		
Minimum Spanning Forest	$O\left(\min\left(sort\left(E\right)\log_{2}\log_{2}V, V+sort\left(E\right)\right)\right)$	$O\left(\min\left(sort(E)\log_2\log_2\frac{VB}{E}, V+sort(E)\right)\right)$		

<u>Table 1</u>: **N** = #elements, **V** = #vertices, **E** = #edges, Am = Amortized.

Matrix Multiplication

Iterative Matrix Multiplication

Iterative Matrix Multiplication





Each iteration of the <u>for loop in line 3</u> incurs O(n) cache misses. I/O-complexity of *Iter-MM*, $Q(n) = O(n^3)$

Iterative Matrix Multiplication





Each iteration of the <u>for loop in line 3</u> incurs $O\left(1+\frac{n}{B}\right)$ cache misses. I/O-complexity of *Iter-MM*, $Q(n) = O\left(n^2\left(1+\frac{n}{B}\right)\right) = O\left(\frac{n^3}{B}+n^2\right)$

Block Matrix Multiplication



Block Matrix Multiplication



Choose $m = \sqrt{M/3}$, so that X_{ik} , Y_{kj} and Z_{ij} just fit into the cache. Then line 4 incurs $\Theta\left(m\left(1+\frac{m}{B}\right)\right)$ cache misses.

I/O-complexity of *Block-MM* [assuming a *tall cache*, i.e., $M = \Omega(B^2)$]

$$= \Theta\left(\left(\frac{n}{m}\right)^3 \left(m + \frac{m^2}{B}\right)\right) = \Theta\left(\frac{n^3}{m^2} + \frac{n^3}{Bm}\right) = \Theta\left(\frac{n^3}{M} + \frac{n^3}{B\sqrt{M}}\right) = \Theta\left(\frac{n^3}{B\sqrt{M}}\right)$$

(Optimal: Hong & Kung, STOC'81)

Block Matrix Multiplication



I/0

Optimal: Hong & Kung, STOC'81)

Multiple Levels of Cache



Multiple Levels of Cache



Multiple Levels of Cache



Recursive Matrix Multiplication



Recursive Matrix Multiplication



Rec-MM(Z, X, Y)

1. *if* $Z \equiv 1 \times 1$ matrix *then* $Z \leftarrow Z + X \cdot Y$

2. else

3. Rec-MM(Z_{11}, X_{11}, Y_{11}), Rec-MM(Z_{11}, X_{12}, Y_{21})

4. Rec-MM(Z_{12}, X_{12}, Y_{12}), Rec-MM(Z_{12}, X_{12}, Y_{22})

- 5. $Rec-MM(Z_{21}, X_{21}, Y_{11}), Rec-MM(Z_{21}, X_{22}, Y_{21})$
- 6. Rec-MM (Z_{22}, X_{21}, Y_{12}), Rec-MM (Z_{22}, X_{22}, Y_{22})

Recursive Matrix Multiplication



I/O-complexity (for
$$n > M$$
), $Q(n) = \begin{cases} 0\left(n + \frac{n^2}{B}\right), & \text{if } n^2 \le \alpha M \\ 8Q\left(\frac{n}{2}\right) + O(1), & \text{otherwise} \end{cases}$

$$= O\left(\frac{n^3}{M} + \frac{n^3}{B\sqrt{M}}\right) = O\left(\frac{n^3}{B\sqrt{M}}\right), when M = \Omega(B^2)$$

I/O-complexity (for all n) = $O\left(\frac{n^3}{B\sqrt{M}} + \frac{n^2}{B} + 1\right)$ (why?)





	<i>Z</i> ₁₁₁₁	<i>Z</i> ₁₁₁₂	<i>Z</i> ₁₂₁₁	<i>Z</i> ₁₂₁₂				
	<i>Z</i> ₁₁₂₁	Z ₁₁₂₂	<i>Z</i> ₁₂₂₁	<i>Z</i> ₁₂₂₂				
	Z ₂₁₁₁	Z ₂₁₁₂	Z ₂₂₁₁	Z ₂₂₁₂				
	Z ₂₁₂₁	Z ₂₁₂₂	Z ₂₂₂₁	Z ₂₂₂₂				
$Z_{1111} Z_{1112} Z_{1121} Z_{1122}$	$Z_{1211} Z_{1212}$	$Z_{1221} Z_{1222}$	$Z_{2111} Z_{2112}$	$Z_{2121} Z_{2122}$	$Z_{2211} Z_{2212} Z_{2221} Z_{2221} Z_{2222}$			
Z ₁₁	Z	12	Z	21	Z ₂₂			
Z								



Source: wikipedia

Rec-MM(
$$Z, X, Y$$
)
1. if $Z \equiv 1 \times 1$ matrix then $Z \leftarrow Z + X \cdot Y$
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I/O-complexity (for
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I/O-complexity (for all n) = $O\left(\frac{n^3}{B\sqrt{M}} + \frac{n^2}{B} + 1\right)$

	x: 000	1 001	2 010	3 011	4 100	5 101	6 110	7 111
y: 0 000	000000	000001	000100	000101	010000	010001	010100	010101
1 001	000010	000011	000110	000111	010010	010011	010110	010111
2 010	001000	001001	001100	001101	011000	011001	011100	011101
3 011	001010	001011	001110	001111	011010	011011	011110	011111
4 100	100000	100001	100100	100101	110000	110001	110100	110101
5 101	100010	100011	100110	100111	110010	110011	110110	110111
6 110	101000	101001	101100	101101	111000	111001	111100	111101
7 111	101010	101011	101110	101111	111010	111011	111110	111111

Source: wikipedia

Searching (Static B-Trees)

A Static Search Tree



- □ A perfectly balanced binary search tree
- Static: no insertions or deletions
- $\square \text{ Height of the tree, } h = \Theta(\log_2 n)$

A Static Search Tree



- A perfectly balanced binary search tree
- Static: no insertions or deletions
- **T** Height of the tree, $h = \Theta(\log_2 n)$
 - A search path visits O(h) nodes, and incurs $O(h) = O(\log_2 n)$ I/Os

I/O-Efficient Static B-Trees



- □ Each node stores *B* keys, and has degree *B* + 1
- $\Box \quad \text{Height of the tree, } h = \Theta(\log_B n)$

I/O-Efficient Static B-Trees



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- $\Box \quad \text{Height of the tree, } h = \Theta(\log_B n)$

A search path visits O(h) nodes, and incurs $O(h) = O(\log_B n)$ I/Os

Cache-Oblivious Static B-Trees?





If the tree contains n nodes,



If the tree contains n nodes,



If the tree contains n nodes,



If the tree contains n nodes,



If the tree contains n nodes,

I/O-Complexity of a Search



I/O-Complexity of a Search



Sorting (Mergesort)

Merge Sort



Merging k Sorted Sequences

- $k \ge 2$ sorted sequences S_1, S_2, \dots, S_k stored in external memory
- $|S_i| = n_i \text{ for } 1 \le i \le k$
- $n = n_1 + n_2 + \dots + n_k$ is the length of the merged sequence S
- S (initially empty) will be stored in external memory
- Cache must be large enough to store
 - one block from each S_i
 - one block from *S*

Thus $M \ge (k+1)B$

Merging k Sorted Sequences

- Let \mathcal{B}_i be the cache block associated with S_i , and let \mathcal{B} be the block associated with S (initially all empty)
- Whenever a \mathcal{B}_i is empty fill it up with the next block from S_i
- Keep transferring the next smallest element among all \mathcal{B}_i s to \mathcal{B}
- Whenever $\mathcal B$ becomes full, empty it by appending it to S
- In the *Ideal Cache Model* the block emptying and replacements
 will happen automatically \Rightarrow cache-oblivious merging

I/O Complexity

- Reading S_i : #block transfers $\leq 2 + \frac{n_i}{R}$
- Writing S: #block transfers $\leq 1 + \frac{n}{B}$

- Total #block transfers $\leq 1 + \frac{n}{B} + \sum_{1 \leq i \leq k} \left(2 + \frac{n_i}{B}\right) = O\left(k + \frac{n}{B}\right)$

Cache-Oblivious 2-Way Merge Sort

Merge-Sort (A, p, r){ sort the elements in A[$p \dots r$] }1. if p < r then2. $q \leftarrow \lfloor (p + r) / 2 \rfloor$ 3. Merge-Sort (A, p, q)4. Merge-Sort (A, q + 1, r)5. Merge (A, p, q, r)

I/O Complexity:
$$Q(n) = \begin{cases} O\left(1 + \frac{n}{B}\right), & \text{if } n \le M, \\ 2Q\left(\frac{n}{2}\right) + O\left(1 + \frac{n}{B}\right), & \text{otherwise.} \end{cases}$$
$$= O\left(\frac{n}{B}\log\frac{n}{M}\right)$$

How to improve this bound?

Cache-Oblivious k-Way Merge Sort

I/O Complexity:
$$Q(n) = \begin{cases} O\left(1 + \frac{n}{B}\right), & \text{if } n \le M, \\ k \cdot Q\left(\frac{n}{k}\right) + O\left(k + \frac{n}{B}\right), & \text{otherwise.} \end{cases}$$
$$= O\left(k \cdot \frac{n}{M} + \frac{n}{B}\log_k \frac{n}{M}\right)$$

How large can k be?

Recall that for k-way merging, we must ensure

$$M \ge (k+1)B \Rightarrow k \le \frac{M}{B} - 1$$

$$\frac{\text{Cache-Aware}\left(\frac{M}{B}-1\right)-\text{Way Merge Sort}}{I/O \text{ Complexity: } Q(n)} = \begin{cases} O\left(1+\frac{n}{B}\right), & \text{if } n \leq M, \\ k \cdot Q\left(\frac{n}{k}\right)+O\left(k+\frac{n}{B}\right), & \text{otherwise.} \end{cases}$$
$$= O\left(k \cdot \frac{n}{M} + \frac{n}{B}\log_k \frac{n}{M}\right)$$

Using
$$k = \frac{M}{B} - 1$$
, we get:
 $Q(n) = O\left(\left(\frac{M}{B} - 1\right)\frac{n}{M} + \frac{n}{B}\log_{\frac{M}{B}}\left(\frac{n}{M}\right)\right) = O\left(\frac{n}{B}\log_{\frac{M}{B}}\left(\frac{n}{M}\right)\right)$

Sorting (Funnelsort)



<u>Memory layout of a *k*-merger</u>:

$$R$$
 L_1
 B_1
 L_2
 B_2
 $L_{\sqrt{k}}$
 $B_{\sqrt{k}}$

k-Merger (k-Funnel)



Space usage of a k-merger:
$$S(k) = \begin{cases} \Theta(1), & \text{if } k \leq 2, \\ (\sqrt{k}+1)S(\sqrt{k}) + \Theta(k^2), & \text{otherwise} \end{cases}$$
$$= \Theta(k^2)$$

A k-merger occupies $\Theta(k^2)$ contiguous locations.



Each invocation of a k-merger

– produces a sorted sequence of length k^3

- incurs
$$O\left(1+k+\frac{k^3}{B}+\frac{k^3}{B}\log_M\left(\frac{k}{B}\right)\right)$$
 cache misses provided $M=\Omega(B^2)$



Cache-complexity:

$$Q'(k) = \begin{cases} O\left(1+k+\frac{k^3}{B}\right), & \text{if } k < \alpha \sqrt{M}, \\ \left(2k^{\frac{3}{2}}+2\sqrt{k}\right)Q'(\sqrt{k}) + \Theta(k^2), & \text{otherwise.} \end{cases}$$
$$= O\left(\frac{k^3}{B}\log_M\left(\frac{k}{B}\right)\right), & \text{provided } M = \Omega(B^2) \end{cases}$$



$$k < \alpha \sqrt{M}$$
: $Q'(k) = O\left(1 + k + \frac{k^3}{B}\right)$

- Let r_i be #items extracted the *i*-th input queue. Then $\sum_{i=1}^{k} r_i = O(k^3)$.
- Since $k < \alpha \sqrt{M}$ and $M = \Omega(B^2)$, at least $\frac{M}{B} = \Omega(k)$ cache blocks are available for the input buffers.
- Hence, #cache-misses for accessing the input queues (assuming circular buffers) = $\sum_{i=1}^{k} O\left(1 + \frac{r_i}{B}\right) = O\left(k + \frac{k^3}{B}\right)$



$$k < \alpha \sqrt{M}$$
: $Q'(k) = O\left(1 + k + \frac{k^3}{B}\right)$

- #cache-misses for accessing the input queues = $O\left(k + \frac{k^3}{B}\right)$
- #cache-misses for writing the output queue = $O\left(1 + \frac{k^3}{B}\right)$
- #cache-misses for touching the internal data structures = $O\left(1 + \frac{k^2}{B}\right)$
- Hence, total #cache-misses = $O\left(1 + k + \frac{k^3}{B}\right)$



$$k \ge \alpha \sqrt{M}: Q'^{(k)} = \left(2k^{\frac{3}{2}} + 2\sqrt{k}\right)Q'\left(\sqrt{k}\right) + \Theta(k^2)$$

Each call to R outputs k^{3/2}/₂ items. So, #times merger R is called = k³/_{k²/₂} = k^{3/2}/_{k²/₂}
Each call to an L_i puts k^{3/2}/₂ items into B_i. Since k³ items are output, and the buffer space is $\sqrt{k} \times 2k^{3/2} = 2k^2$, #times the L_i's are called $\leq k^{3/2} + 2\sqrt{k}$

- Before each call to R, the merger must check each L_i for emptiness, and thus incurring $O(\sqrt{k})$ cache-misses. So, #such cache-misses = $k^{\frac{3}{2}} \times O(\sqrt{k}) = O(k^2)$

Funnelsort

- Split the input sequence A of length n into $n^{\frac{1}{3}}$ contiguous subsequences $A_1, A_2, \dots, A_{n^{\frac{1}{3}}}$ of length $n^{\frac{2}{3}}$ each
- Recursively sort each subsequence
- Merge the $n^{\frac{1}{3}}$ sorted subsequences using a $n^{\frac{1}{3}}$ -merger

Cache-complexity:

$$Q(n) = \begin{cases} O\left(1 + \frac{n}{B}\right), & \text{if } n \le M, \\ \frac{1}{n^3}Q\left(n^{\frac{2}{3}}\right) + Q'\left(n^{\frac{1}{3}}\right), & \text{otherwise.} \end{cases}$$

$$= \begin{cases} O\left(1+\frac{n}{B}\right), & \text{if } n \leq M, \\ n^{\frac{1}{3}}Q\left(n^{\frac{2}{3}}\right) + O\left(\frac{n}{B}\log_{M}\left(\frac{n}{B}\right)\right), & \text{otherwise.} \end{cases}$$

 $= O\left(1 + \frac{n}{B}\log_M n\right)$