Applied Algorithms Lec 4: Cache Misses and External Memory

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Williams College

- Office hours 2:30-4 and 5-6:30 today
- No office hours tomorrow; Wed 2-4 in TCL 312 instead
- Slack vs email (everything important will be on email)
- Some reading today! Optional/potentially useful for reference. We don't cover the topic in exactly the same way
 - For ex: we'll have K = 1; no distribution sort; no *B*-trees

Admin: Talks coming up

- Tomorrow 7PM: Landing a tech internship (featuring your fellow Williams students)
- Thursday 5PM: "How'd you get there?" talk about jobs in sustainable tech (need preregister)
- Friday 2:30: Colloquium is by Andrew McGregor, who works in randomized streaming algorithms (topic in Part 2 of course)
 - More details later. But almost certainly one of the most relevant talks to this course this year

Admin: Assignment 1

- Assignment 1 due Wednesday 10pm
- Emailed out small Assignment 1 updates
- Extra test run at 7pm Wed
- Add -1m to make debug
- Tips for fast sorting added to website

Any Assignment 1 Questions?

- Avoid branches (ifs, etc.)
- If you do create a branch, ask yourself how easy it is to predict!
- Compiler can remove a lot of branch mispredictions
- Only way to be sure is to experiment

Profilers examples: gprof

- Compile with -pg option; then run normally; then run gprof on the executable
- Gives information about what calls what and how much time is in each
- Not perfect, but gives us some information, especially for simpler programs
 - Can see if one function is called a LOT
 - Can see if one function is only ever called by one other function
 - (Can be issues with optimizations, especially -03)
- I may ask you to use this, but be aware of its limitations

Profilers examples: cachegrind

- Compile with debugging info on -g AND optimizations on
 - What does this entail immediately?
- Then valgrind --tool=cachegrind [your program]
- Use --branch-sim=yes for branch prediction statistics.
 - Very oversimplified unfortunately
- Outputs number of cache misses for instructions, then data, then combined
- *Simulates* a simple cache (based on your machine) with separate L1 caches for instructions and data, and unified L2 and (if on machine) L3 caches
- Does L1 misses vs last level (L3) misses

• Data is stored in different places on the computer

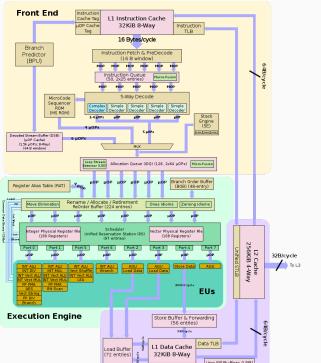
• Cost to access it frequently dominates running time

A Typical Memory Hierarchy

• Everything is a cache for something else...

| | Access time | Capacity | Managed By |
|---------------------------------|-------------|----------|-------------------|
| On the Registers | l cycle | І КВ | Software/Compiler |
| Level I Cache | 2-4 cycles | 32 KB | Hardware |
| Level 2 Cache | 10 cycles | 256 KB | Hardware |
| On chip | 40 cycles | I0 MB | Hardware |
| Other Main Memory | 200 cycles | 10 GB | Software/OS |
| chips Flash Drive | 10-100us | 100 GB | Software/OS |
| Mechanical Hard Disk devices | 10ms | I TB | Software/OS |

- Stores data in the optimal(ish) place
- Moves data around in cache lines of ≈ 64 bytes
- Example: cachemisses.c
- Modern caches are very complicated
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- Stores data in the optimal(ish) place
- Moves data around in cache lines of 64 bytes
- Modern caches are **very** complicated
- Basically: close is good; recent is good; jumping around is bad.
- Your compiler has limited capability to improve cache efficiency!

Optimization Conclusions

- Different places where we can incur costs:
 - Operations
 - Branches and moving around instructions
 - Cache misses
- Determining costs is a matter of experimentation on modern machines!
 - Rarely perfect!
- Theme throughout class: design different experiments to test different aspects of code performance.

- Today: cache misses. (Best place to gain performance algorithmically)
- Thursday: Assignment 2 algorithm, discussion about optimizing loops and functions
 - Inlining, loop unrolling, more about compiler options
- Monday: more external memory, Assignment 1 code review, any other loose ends

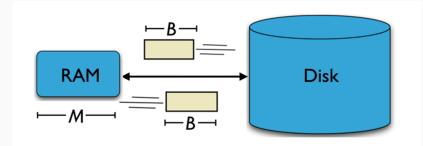
External Memory Model

- Takeaway from today's examples: cache performance is often *more important* than number of operations
- But algorithmic analysis measures number of operations
- Can we algorithmically examine the cache performance of a program?
- Yes: external memory model

- Simple, but able to capture major performance considerations
- Parameters for the model? How can we make it universal across computers that may have very different cache parameters?
- Do we want asymptotics? Worst case?

- Cache of size M
- Cache line of size B
- Computation is free: *only* count number of "cache misses." Can perform arbitrary computation on items in cache.
- We will say something like "O(n/B) cache misses" rather than "O(n) operations" to emphasize the model.

External Memory Model Basics



Transferring B consecutive items to/from the disk costs 1. Can only store M things in cache.

• Can only hold *M* items in cache!



- So when we bring *B* in, need to write *B* items back to disk. (We can bring them in later if we need them again)
- Assume that the computer does this optimally.
 - Reasonable; it's really good at it. Very cool algorithms behind this!

- "Cache" of size *M*; "disk" of unlimited size
- With the cost of one "cache miss" can bring in *B* consecutive items
 - (Sometimes called "memory access" or "I/Os" but I will try not to use those terms.)

• These *B* items are called a "block" or a "cache line".

- What is the cost of our algorithm in the external memory model if the items are stored in order?
- Answer: O(n/B)
- What is the cost of our algorithm in the external memory model if the items have stride *B* + 1?
- Answer: O(n)
- The external memory model predicts the real-world slowdown of this process.

• How many cache misses in the external memory model?

• Answer: O(n/B)

- What is the recurrence for binary search in terms of number of operations?
- What is the recurrence for binary search in terms of the number of cache misses?
- Each recursive call takes 1 cache miss.
- Base case: can perform *all* operations on *B* items with only 1 cache miss
- Total: $O(\log_2(n/B))$ cache misses.

- Simple model that captures one level of the memory hierarchy
- Idea: usually one level has by far the largest cost.
 - Small programs may be dominated by L1 cache misses
 - Larger programs it may be by L3 cache misses
- External memory model zooms in on one crucial level of the memory hierarchy (with particular *B*, *M*); gives asymptotics for how well we do on that level.

Question about External Memory Model Basics?

almost impossible to convince programmers to stick to that subset. The C compiler which I use can generate warning messages concerning portability, but it is no effort at all to write a non-portable program which generates no compiler warnings. programmers are the same people who were playing with toy computers as adolescents? We said at the time that using BASIC as a first language would create bad habits which would be very difficult to eradicate. Now we're seeing the evidence of that.

C is a medium-level language combining the power of assembly language with the readability of assembly language.

Joke to break up the material



Matrix Multiplication in External Memory

Matrix Multiplication Reminder

- Given two $n \times n$ matrices A, B
- Want to compute their product C:

•
$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

Example:

$$\begin{bmatrix} 1 & 2 \\ 8 & -1 \end{bmatrix} \times \begin{bmatrix} 2 & 3 \\ -2 & 7 \end{bmatrix} = \begin{bmatrix} -2 & 17 \\ 18 & 17 \end{bmatrix}$$

for i = 1 to n:
 for j = 1 to n:
 for k = 1 to n:
 C[i][j] += A[i][k] +
 B[k][j]

- Recall: $c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$
- How many I/Os does this take?
- Assume matrices are stored in row-major order.
 - First: assume $M < n^2$
 - What if $M > n^2$?
 - Answer: O(n³) I/Os. Every inner loop operation requires an I/O for B.

• One idea: transpose *B*.

• Another idea: swap the loops!

```
for i = 1 to n:
    for k = 1 to n:
    for j = 1 to n:
        C[i][j] += A[i][k] + B[k][j]
```

• This gives us $O(n^3/B)$ I/Os. Is this actually worth doing?

Yep!

I am given two functions for finding the product of two matrices:

I ran and profiled two executables using gprof, each with identical code except for this function. The second of these is significantly (about 5 times) faster for matrices of size 2048 x 2048. Any ideas as to why?



We haven't used the cache yet

- No *M*s in any running times
- Why? All algorithms so far have read the data once and then thrown it away.
- Goal: bring items into cache so that we can perform *many* computations on them before writing them back.
- Note: can't do this with linear scan. O(n/B) is optimal.

- Standard technique for improving cache performance of algorithms.
- Idea: break problems into subproblems of size O(M)
 - Can solve any such problem in O(M/B) I/Os
 - Efficiently combine them for a cache-efficient solution

- Split A, B, and C into blocks of size M/3
 - $\sqrt{M/3} \times \sqrt{M/3}$ -sized blocks
 - Really want blocks with size $T = \lfloor \sqrt{M/3} \rfloor$. Assume that T divides *n* for now.

• Multiply blocks one at a time

Classic result: if we treat the blocks as single elements of the matrices, and multiply (and add) them as normal, we obtain the same result as we would have in normal matrix multiplication.

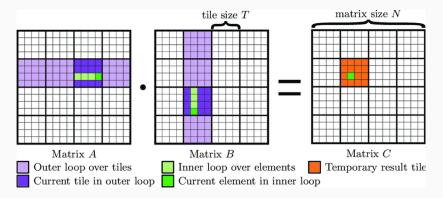
- This idea is used in recursive matrix multiplication
- And Strassen's algorithm for matrix multiplication

Example: Recall how to multiply $2x^2$ matrices:

 $\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \cdot \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11} \cdot B_{11} + A_{12} \cdot B_{21} & A_{11} \cdot B_{12} + A_{12} \cdot B_{22} \\ A_{21} \cdot B_{11} + A_{22} \cdot B_{21} & A_{21} \cdot B_{12} + A_{22} \cdot B_{22} \end{bmatrix}$ $\begin{bmatrix} 17 & 15 & 20 & 4 \\ 15 & 3 & 20 & 8 \\ 1 & 10 & 15 & 2 \\ 3 & 19 & 3 & 14 \end{bmatrix} \cdot \begin{bmatrix} 4 & 12 & 9 & 1 \\ 4 & 6 & 11 & 2 \\ 13 & 18 & 8 & 20 \\ 3 & 11 & 18 & 9 \end{bmatrix} =$ $\begin{bmatrix} 17 & 15\\ 15 & 3 \end{bmatrix} \cdot \begin{bmatrix} 4 & 12\\ 4 & 6 \end{bmatrix} + \begin{bmatrix} 20 & 4\\ 20 & 8 \end{bmatrix} \cdot \begin{bmatrix} 13 & 8\\ 3 & 11 \end{bmatrix} \begin{bmatrix} 17 & 15\\ 15 & 3 \end{bmatrix} \cdot \begin{bmatrix} 9 & 1\\ 11 & 2 \end{bmatrix} + \begin{bmatrix} 20 & 4\\ 20 & 8 \end{bmatrix} \cdot \begin{bmatrix} 8 & 20\\ 18 & 9 \end{bmatrix}$ $\begin{bmatrix} 1 & 10\\ 3 & 19 \end{bmatrix} \cdot \begin{bmatrix} 4 & 12\\ 4 & 6 \end{bmatrix} + \begin{bmatrix} 15 & 2\\ 3 & 14 \end{bmatrix} \cdot \begin{bmatrix} 13 & 8\\ 3 & 11 \end{bmatrix} \begin{bmatrix} 1 & 10\\ 3 & 19 \end{bmatrix} \cdot \begin{bmatrix} 9 & 1\\ 11 & 2 \end{bmatrix} + \begin{bmatrix} 15 & 2\\ 3 & 14 \end{bmatrix} \cdot \begin{bmatrix} 8 & 20\\ 18 & 9 \end{bmatrix}$

Blocked Matrix Multiplication

- Decompose matrix into blocks of length T (recall that $T^2 \leq M/3$)
- Do a normal $n/T \times n/T$ matrix multiplication



```
MatrixMultiply(A, B, C, n, T):
  for i = 1 to n/T:
    for j = 1 to n/T:
     for k = 1 to n/T:
       A' = TxT matrix with upper left corner A[Ti][Tk]
       B' = TxT matrix with upper left corner B[Tk][Tj]
       C' = TxT matrix with upper left corner C[Ti][Tj]
       BlockMultiply(A', B', C', T)
BlockMultiply(A, B, C, n):
  for i = 1 to n:
     for j = 1 to n:
        for k = 1 to n:
          C[i][j] += A[i][k] + B[k][j]
```

Let's analyze the cost of this algorithm in the EM model

Analysis

- Creating A', B', C' and passing them to BlockMultiply all can be done in $O(T^2/B + T)$ cache misses. If $B = O(M^2)$ then we can simplify this to O(M/B). (Called the "tall cache assumption.")
- BlockMultiply only accesses elements of A', B', C'. Since all three matrices are in cache, it requires zero additional cache misses
- Therefore, our total running time is the number of loop iterations times the cost of a loop. This is $O((n/T)^3 \cdot (T^2/B)) = O((n/\sqrt{M})^3 \cdot (M/B)) = O(n^3/B\sqrt{M}).$

Implementation questions!

- What do we do if *n* is not divisible by *T*?
 - Easy answer: pad it out! Doesn't change asymptotics.
 - Can carefully make it work without padding as well
- How do we figure out *M*? We don't have a two-level cache and we're ignoring that space is used for other programs, other variables, etc.
 - Experiment! Try different values of *M* and see what's fastest on a particular machine.
- Is blocking actually worthwhile?
 - Yes; it is used all the time to speed up programs with poor cache performance.
 - (Not a panacea; some programs (like linear scan, binary search) can't be blocked.)

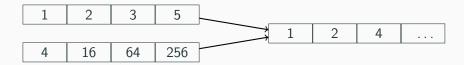
Sorting in External Memory

What about algorithms we know?

- How long does Mergesort take in external memory?
- Merge is O(n/B); base case is when n = B, so total is $n/B \log_2 n/B$.
- How about quicksort?
- Essentially same; partition is O(n/B); total is $n/B \log_2 n/B$.
- Heapsort is $n \log_2 n/B$ unless we're careful...
- Can we do better?

- Blocking? A little unclear. (We'll come back to this.)
- Does anyone know the sorting lower bound? Where does $n \log n$ come from?
- Answer: each time you compare two numbers, can only have two outcomes.
- Each time we bring a cache line into cache, how many more things can we compare it to?

- Divide array into two equal parts
- Recursively sort both parts
- Merge them in O(n) time (and O(n/B) cache misses)

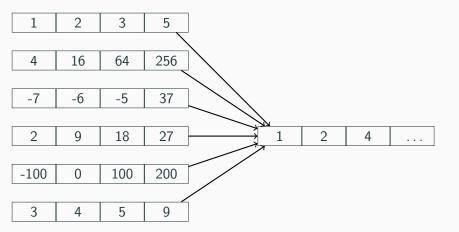


• Divide array into M/B equal parts

• Recursively sort all M/B parts

Merge all *M*/*B* arrays in *O*(*n*) time (and *O*(*n*/*B*) cache misses)

Diagram of M/B-way merge sort



- Keep *B* slots for each array in cache. (*M*/*B* arrays so this fits!)
- When all *B* slots are empty for the array, take *B* more items from the array in cache.
- Example on board

- Divide array into *M*/*B* parts; combine in *O*(*N*/*B*) cache misses.
- Recursion:

$$T(N) = T(N/(M/B)) + O(N/B)T(B) = O(1)$$

- Solves to $O(\frac{n}{B} \log_{M/B} n/B)$ cache misses
- Optimal!

• Can be useful if your data is VERY large

• Distribution sort: similar idea, but with Quicksort instead of Mergesort

• Another method is most popular in practice: Timsort

• Developed to be the sorting method for python

• Now also used in Java, Rust

• Keeps cache in mind, but focuses more on taking advantage of easy patterns in data

Blocking revisited: run generation

- Basic idea: sort all *M*-sized subarrays. That would give us sorted subarrays of length *M* to start out with
- This is wasteful, as we empty out cache between each subarray
- Timsort starts with "run generation": a greedy version of this that uses the same cache for as long as possible. Always outputs sorted runs of length at least *M*; can be MUCH longer

• First, run generation

• Then, super optimized (2-way) merge sort

• Insertion sort on any very small arrays that are encountered (size < 64)

• M/B way merge sort is most efficient

• Timsort is very popular in practice; uses a simpler blocking approach to stay cache-friendly.