Part 2, course 2: Cache Oblivious Algorithms

CR10: Data Aware Algorithms

October 2, 2019
Agenda

Previous course (Sep. 25):
  ▶ Ideal Cache Model and External Memory Algorithms

Today:
  ▶ Cache Oblivious Algorithms and Data Structures

Next week (Oct. 9):
  ▶ Parallel External Memory Algorithms
  ▶ Parallel Cache Oblivious Algorithms: Multithreaded Computations

The week after (Oct. 16):
  ▶ Test (∼1.5h)
    (on pebble games, external memory and cache oblivious algorithms)
  ▶ Presentation of the projects

NB: no course on Oct. 25.
Cache Oblivious Algorithms and Data Structures

Motivation
Divide and Conquer
Static Search Trees
Cache-Oblivious Sorting: Funnels
Dynamic Data-Structures
Distribution sweeping for geometric problem
Conclusion
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Motivation for Cache-Oblivious Algorithms

I/O-optimal algorithms in the external memory model:
Depend on the memory parameters $B$ and $M$: cache-aware

- Blocked-Matrix-Product: block size $b = \sqrt{M}/3$
- Merge-Sort: $K = M/B - 1$
- B-Trees: degree of a node in $O(B)$

Goal: design I/O-optimal algorithms that do not known $M$ and $B$

- Self-tuning
- Optimal for any cache parameters
  - optimal for any level of the cache hierarchy!

Ideal cache model:

- Ideal-cache model
- No explicit operations on blocks as in EM
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Main Tool: Divide and Conquer

Major tool:

- Split problem into smaller sizes
- At some point, size gets smaller than the cache size: no I/O needed for next recursive calls
- Analyse I/O for these “leaves” of the recursion tree and divide/merge operations

Example: Recursive matrix multiplication:

\[
A = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \quad B = \begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix} \quad C = \begin{pmatrix} C_{1,1} & C_{1,2} \\ C_{2,1} & C_{2,2} \end{pmatrix}
\]

- If \( N > 1 \), compute:
  
  \[
  \begin{align*}
  C_{1,1} &= \text{RecMatMult}(A_{1,1}, B_{1,1}) + \text{RecMatMult}(A_{1,2}, B_{2,1}) \\
  C_{1,2} &= \text{RecMatMult}(A_{1,1}, B_{1,2}) + \text{RecMatMult}(A_{1,2}, B_{2,2}) \\
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  \]

- Base case: multiply elements
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Recursive Matrix Multiply: Analysis

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Analysis:

- 8 recursive calls on matrices of size \( N/2 \times N/2 \)
- Number of I/O for size \( N \times N \): \( T(N) = 8T(N/2) \)
- Base case: when 3 blocks fit in the cache: \( 3N^2 \leq M \) no more I/O for smaller sizes, then \( T(N) = O(N^2/B) = O(M/B) \)
- No cost on merge, all I/O cost on leaves
- Height of the recursive call tree: \( h = \log_2(N/(\sqrt{M}/3)) \)
- Total I/O cost:

\[
T(N) = O(8^h M/B) = O(N^3/(B\sqrt{M}))
\]

- Same performance as blocked algorithm!
Recursive Matrix Multiply: Analysis

RecMatMultAdd(A_{1,1}, B_{1,1}, C_{1,1}); RecMatMultAdd(A_{1,2}, B_{2,1}, C_{1,1})
RecMatMultAdd(A_{1,1}, B_{1,2}, C_{1,2}); RecMatMultAdd(A_{1,2}, B_{2,2}, C_{1,2})
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Analysis:

- 8 recursive calls on matrices of size $N/2 \times N/2$
- Number of I/O for size $N \times N$: $T(N) = 8T(N/2)$
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Recursive Matrix Layout

NB: previous analysis need tall-cache assumption \((M \geq B^2)\)
If not, use recursive layout, e.g. bit-interleaved layout:
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<table>
<thead>
<tr>
<th>x: 0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>001</td>
<td>010</td>
<td>011</td>
<td>100</td>
<td>101</td>
<td>110</td>
<td>111</td>
</tr>
</tbody>
</table>

| y: 0  |
| 000  |
| 001  |
| 100  |
| 101  |
| 110  |
| 111  |

```
000000 000001 001000 001010 010000 010001 010100 010101
000010 000011 001100 001110 010100 010110 011010 011011
001000 001001 001100 001101 011000 011001 011010 011011
001010 001011 001110 001111 011100 011101 011110 011111
100000 100001 100100 100101 110000 110001 110100 110101
100010 100011 100110 100111 110100 110101 111010 111011
101000 101001 101100 101101 111000 111001 111100 111101
101010 101011 101110 101111 111100 111101 111110 111111
```
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NB: previous analysis need tall-cache assumption \((M \geq B^2)\)
If not, use recursive layout, e.g. bit-interleaved layout:

Also known as the Z-Morton layout

Other recursive layouts:
  ▶ U-Morton, X-Morton, G-Morton
  ▶ Hilbert layout

Address computations may become expensive 😞

Possible mix of classic tiles/recursive layout
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  Cache-Oblivious Sorting: Funnels
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  Distribution sweeping for geometric problem
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Static Search Trees

Problem with B-trees: degree depends on $B$ 😞

Binary search tree with recursive layout:

- Complete binary search tree with $N$ nodes
  (one node per element)
- Stored in memory using recursive “van Emde Boas” layout:
  - Split the tree at the middle height
  - Top subtree of size $\sim \sqrt{N}$ → recursive layout
  - $\sim \sqrt{N}$ subtrees of size $\sim \sqrt{N}$ → recursive layout
  - If height $h$ is not a power of 2, set subtree height to $2^{\lceil \log_2 h \rceil} = \lceil h \rceil$
Static Search Trees – Analysis

I/O complexity of search operation:

- For simplicity, assume $N$ is a power of two
- For some height $h$, a subtree fits in one block ($B \approx 2^h$)
- Reading such a subtree requires at most 2 blocks
- Root-to-leaf path of length $\log_2 N$
- I/O complexity: $O(\log_2 N / \log_2 B) = O(\log_B N)$
- Meets the lower bound 😊
- Only static data-structure 😞
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Cache-Oblivious Sorting: Funnels

- Binary Merge Sort: cache-oblivious 😊, not I/O optimal 😞
- K-way MergeSort: depends on $M$ and $B$ 😞, I/O optimal 😊

New data-structure: K-funnel

- Complete binary tree with $K$ leaves
- Stored using van Emde Boas layout
- Buffer of size $K^{3/2}$ between each subtree and the topmost part (total: $K^2$ in these buffers)
- Each recursive subtree is a $\sqrt{K}$-funnel

Total storage in a $K$ funnel: $\Theta(K^2)$
(storage $S(K) = K^2 + (1 + \sqrt{K})S(\sqrt{K})$)
Cache-Oblivious Sorting: Funnels

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Lazy Funnels

- Consider resulting tree where edges are buffers
- Output buffer of a K-funnel has size $K^3$

**Fill algorithm: while output buffer not full**

1. If left input buffer empty, call Fill on left child
2. If right input buffer empty, call Fill on right child
3. Perform one merge step:
   Move smallest of left and right buffers (front) to output (rear)

- Buffer exhaustion propagates upward
- I/O complexity of filling output buffer of size $K^3$:

$$O\left(\frac{K^3}{B} \log_M K^3 + K\right)$$
Funnel Sort

Funnel-Sort

1. Split input in $N^{1/3}$ segments of size $N^{2/3}$
2. Sort segments recursively
3. Use funnel with $K = N^{1/3}$ to produce output

I/O complexity: $O(SORT(N))$
Nb of comparisons: $O(N \log N)$

Analysis (big picture):
- Some $J$-funnel fits in cache, together with its input buffers
- When input buffer empty, $J$-funnel may be flushed to memory
- Bound the number of flushes and I/Os in the funnel
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PMA: Packed Memory Array

Goal: Store \( N \) ordered elements in array of size \( P = cN \)
Contradictory objectives:
- Pack nodes for fast scan of \( S \) elements \((O(1 + S/B))\)
- Leave enough room for fast insertion

PMA:
- Array divided into segments of size \( \log P \)
- Virtual complete binary tree whose leaves are these segments
- Density of a node:

\[
\rho = \frac{\text{number of elements in subtree}}{\text{capacity of the subtree}}
\]

- Constraints on density: \( 1/2 - 1/4d/h \leq \rho \leq 1/2 + 1/4d/h \)
  
  \( d \): depth of the node, \( h \): height of the tree
  
  \( \rightarrow \) up in the tree: less slack on density
Insertion algorithm:

- Find segment (leaf in the tree)
- If segment not full, insert (move other elements if needed)
- If segment full, before inserting the element:
  1. Climb in tree to find ancestor that respects density constraints
     Parallel left and right scan counting elements
  2. Rebalance subtree: redistribute all elements uniformly in existing leaves
     Some additional scans
  3. For big changes in $N$: rebuild everything

(Same for deletions)
Amortized cost of insertion: $O(1 + \log^2 N/B)$
Packed Memory Array: Details

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Cache-Oblivious B-Trees

- PMA to store elements
- Static Search Tree with $\Theta(N)$ leaves
  a node store the maximum of its two children
- Bi-directional pointers between tree leaves and PMA cells
- Search: using search tree
- Insertion: in the PMA, then propagate changes in the tree

Theorem (Cache-oblivious B-Trees).

This data-structure has the following I/O cost:

- Insertion and deletions in $O(\log_B N + (\log^2 N)/B)$ (amortized)
- Search in $O(\log_B N)$
- Scanning $K$ consecutive elements in $O(\lceil K/B \rceil)$

NB: Removing the $(\log^2 N)/B$ term leads to loosing fast scanning
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Distribution sweeping for geometric problem

Distribution sweeping:
- Sort geometric objects (e.g. w.r.t. one dimension)
- Split problem into strips
- Divide-and-conquer approach on strips
- Merge results via a sweep of strips in another dimension (cache-oblivious merge: 2-way)

Multidimensional Maxima Problem
Given a set of points in \( d \) dimensions, a point \( p = (p_1, p_2, \ldots, p_d) \) dominates another point \( q \) if \( p_i \geq q_i \) for all \( i \). Given \( N \) points, report the maximal points (points non dominated).

- 1D: Single maximum
- 2D: Simple sweep algorithm:
  1. Sort point by decreasing first coordinate
  2. Report point if its second coordinate is larger than the one of the last reported point
Distribution sweeping for geometric problem

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Divide-and-Conquer for 3D Maxima

- Sort points according to \( z \)
- Divide points in strips
- For each strip: report (output) maximal points sorted by decreasing \( x \)

Base case: strip with a single point (reported)
When merging strips \( A \) and \( B \) (with \( z_B > z_A \)):  
- all points in \( B \) have larger \( z \): all maximal points kept
- maximal points in \( A \) are maximal in \( A \cup B \) iff there are not dominated by some maximal point of \( B \)

Merging Algorithm:
- Scan maximal points of \( A \) and \( B \) by decreasing \( x \)
- Keep track of the largest \( y_B \) of nodes from \( B \)
- If next node comes from \( B \): keep it (output), update \( y_B \)
- If next node comes from \( A \) and has larger \( y \) than current \( y_B \): keep it (output), otherwise, delete it
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Summary of algorithm:

1. Sort by decreasing $z$
2. Recursively process strips
3. Merge sorted sequences by comparing to $y_B$, remove some nodes

Cache-oblivious version:

- Step 1: (Lazy) Funnel-Sort
- Step 3: (Lazy) Funnel-Sort with modified merger to remember $y_B$
  ($O(1)$ extra space on each node)

Complexity: $O(SORT(N))$
Divide-and-Conquer for 3D Maxima

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▶ Clean model, algorithms independent from architectural parameters $M$ and $B$
▶ Good news: match external memory bounds in most cases

▶ Best tool: divide-and-conquer
▶ Base case of the analysis differs from algorithm base case:
  ▶ Sometimes $N = \Theta(M)$ (mergesort, matrix mult., . . .)
  ▶ Sometimes $N\Theta(B)$ (static search tree, . . .)

▶ New algorithmic solutions to force data locality
▶ Can lead to real performance gains for large $N$