Part 2, course 2: Cache Oblivious Algorithms

CR05: Data Aware Algorithms

September 17, 2010
Outline

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
Outline

Cache Oblivious Algorithms and Data Structures

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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 value of cache parameters
  $\rightarrow$ optimal for any level of the cache hierarchy!

Cache-Oblivious model:
- Ideal-cache model
- No explicit operations on blocks as in external memory algos.
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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:

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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}
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- If \( N > 1 \), compute:
  \[
  C_{1,1} = \text{RecMatMult}(A_{1,1}, B_{1,1}) + \text{RecMatMult}(A_{1,2}, B_{2,1})
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  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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- 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 for the analysis: 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)
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- No cost on merge, all I/O cost on leaves
- Height of the recursive call tree: \(h = \log_2(N/(\sqrt{M}/3))\)
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- Same performance as blocked algorithm!
- What if we choose \(3N^2 = B\) as base case?
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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:
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<table>
<thead>
<tr>
<th></th>
<th>x: 000</th>
<th>x: 001</th>
<th>x: 010</th>
<th>x: 011</th>
<th>x: 100</th>
<th>x: 101</th>
<th>x: 110</th>
<th>x: 111</th>
</tr>
</thead>
<tbody>
<tr>
<td>y: 000</td>
<td>000000</td>
<td>000001</td>
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<td>000101</td>
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<td>y: 010</td>
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<td>010001</td>
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<td>y: 100</td>
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<tr>
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Recursive Matrix Layout

NB: previous analysis need \textit{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
Proposed algorithm to transpose an $n \times n$ matrix $A$ into $B$:

MatrixTranspose($A$):
for $i=1, \ldots, n$ do
  for $j=1, \ldots, n$ do
    $B_{i,j} \leftarrow A_{j,i}$
return $B$

Both matrices $A$ and $B$ are stored in row-major layout (each row one after the other).

1. Compute the I/O complexity of this algorithm in the external memory model, with cache size $M$ and block size $B$.

2. Design a cache-oblivious divide-and-conquer algorithm for this problem (when $n$ is a power of two), and analyse its I/O complexity. Is it asymptotically optimal?
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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 $\sim \sqrt{N} \rightarrow$ recursive layout
  - $\sim \sqrt{N}$ subtrees of size $\sim \sqrt{N} \rightarrow$ recursive layout
  - If height $h$ is not a power of 2, set subtree height to $2^{\lceil \log_2 h \rceil} = \lceil \lceil h \rceil \rceil$
  - one subtree stored contiguously in memory (any order among subtrees)
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 element of left and right buffers to output

- 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:**

\[
\frac{1}{2} - \frac{1}{4}d/h \leq \rho \leq \frac{3}{4} + \frac{1}{4}d/h
\]

$d$: depth of the node, $h$: height of the tree

→ up in the tree: less slack on density
Packed Memory Array: Details

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 leafs
     Some additional scans
  3. For big changes in $N$: rebuild everything

(Same for deletions)

Amortized cost of insertion: $O(1 + \log^2 N/B)$
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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
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
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

What about the 3D problem?
Distribution sweeping for geometric problem

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What about the 3D problem?
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
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Cache-oblivious version: ?
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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: $O(SORT(N))$
Outline

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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 $N$