Performance Engineering of Software Systems

LECTURE 15 Cache-Oblivious Algorithms

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Heat Diffusion



2D heat equation

The **heat function** u(t,x,y) is the heat at time t of a point (x,y).



 α is the **thermal diffusivity**.

The heat equation was originally formulated by Jean Baptiste Joseph Fourier, *Théorie de la Propagation de la Chaleur dans les Solides*, 1807.

2D Heat-Diffusion Simulation



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1D Heat Equation

$$\frac{\partial \mathsf{u}}{\partial \mathsf{t}} = \alpha \frac{\partial^2 \mathsf{u}}{\partial \mathsf{x}^2}$$



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Finite-Difference Method

The famous Swiss mathematician Leonhard Euler (1707–1783) invented the finite-difference method around 1768.

We owe to Euler the notations f(x) for a function, e for the base of the natural logarithm, i for the square root of -1, π for the area of a unit circle, \sum for summation, and Δ for finite differences.



Finite-Difference Approximation

$$\frac{\partial}{\partial t} u(t,x) \approx \frac{u(t+\Delta t,x) - u(t,x)}{\Delta t},$$

$$\frac{\partial}{\partial x} u(t,x) \approx \frac{u(t,x) - u(t,x-\Delta x)}{\Delta x} \, , \label{eq:utility}$$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

1D heat equation

$$\begin{split} \frac{\partial^2}{\partial x^2} \mathsf{u}(\mathsf{t},\mathsf{x}) &\approx \frac{\frac{\partial}{\partial \mathsf{x}} \mathsf{u}(\mathsf{t},\mathsf{x} + \Delta \mathsf{x}) - \frac{\partial}{\partial \mathsf{x}} \mathsf{u}(\mathsf{t},\mathsf{x})}{\Delta \mathsf{x}} \\ &\approx \frac{\frac{\mathsf{u}(\mathsf{t},\mathsf{x} + \Delta \mathsf{x}) - \mathsf{u}(\mathsf{t},\mathsf{x})}{\Delta \mathsf{x}} - \frac{\mathsf{u}(\mathsf{t},\mathsf{x}) - \mathsf{u}(\mathsf{t},\mathsf{x} - \Delta \mathsf{x})}{\Delta \mathsf{x}}}{\Delta \mathsf{x}} \\ &\approx \frac{\frac{\mathsf{u}(\mathsf{t},\mathsf{x} + \Delta \mathsf{x}) - \mathsf{u}(\mathsf{t},\mathsf{x}) + \mathsf{u}(\mathsf{t},\mathsf{x} - \Delta \mathsf{x})}{\Delta \mathsf{x}}}{(\Delta \mathsf{x})^2} \,. \end{split}$$

Discretized Heat Equation

$$\frac{\mathsf{u}(\mathsf{t} + \Delta \mathsf{t}, \mathsf{x}) - \mathsf{u}(\mathsf{t}, \mathsf{x})}{\Delta \mathsf{t}} = \alpha \Big(\frac{\mathsf{u}(\mathsf{t}, \mathsf{x} + \Delta \mathsf{x}) - 2\mathsf{u}(\mathsf{t}, \mathsf{x}) + \mathsf{u}(\mathsf{t}, \mathsf{x} - \Delta \mathsf{x})}{(\Delta \mathsf{x})^2} \Big)$$

Now, put the one term involving $t + \Delta t$ on the left and the other terms involving just t on the right:

$$\mathbf{u}(\mathbf{t} + \Delta \mathbf{t}, \mathbf{x}) = \mathbf{u}(\mathbf{t}, \mathbf{x}) + \alpha \Delta \mathbf{t} \Big(\frac{\mathbf{u}(\mathbf{t}, \mathbf{x} + \Delta \mathbf{x}) - 2\mathbf{u}(\mathbf{t}, \mathbf{x}) + \mathbf{u}(\mathbf{t}, \mathbf{x} - \Delta \mathbf{x})}{(\Delta \mathbf{x})^2} \Big)$$

Assuming that $\Delta t = 1$ and $\Delta x = 1$, we obtain the following code for the **update rule**:

u[t+1][x] = u[t][x] + ALPHA * (u[t][x+1] - 2*u[t][x] + u[t][x-1]);

u[t+1][x] = u[t][x] + ALPHA * (u[t][x+1] - 2*u[t][x] + u[t][x-1]);



A stencil computation

u[t+1][x] = u[t][x] + ALPHA * (u[t][x+1] - 2*u[t][x] + u[t][x-1]);



A stencil computation

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A **stencil computation** updates each point in an array by a fixed pattern, called a **stencil**.



3-Point Stencil Code







3-Point Stencil Code







CACHE-OBLIVIOUS STENCIL COMPUTATIONS

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Recall: Ideal-Cache Model

Parameters

- Two-level hierarchy.
- Cache size of ${\mathcal M}$ bytes.
- Cache-line length (block size) of ${\mathcal B}$ bytes.
- Fully associative.
- Optimal omniscient replacement, or LRU.



Performance Measures
work T₁ (ordinary running time)
cache misses Q

Cache Behavior of Looping





Assume that $N > \mathcal{M}$ and that we use LRU replacement. Then $Q = \Theta(NT/\mathcal{B})$.

Cache-Oblivious 3-Point Stencil

Recursively traverse trapezoidal regions of space-time points (t,x) such that



Squat Trapezoid: Space Cut

If width $\ge 2 \cdot \text{height}$, cut the trapezoid with a line of slope -1 through the center (middle point of middle row). Traverse the trapezoid on the left first, and then the one on the right.



Squat Trapezoid: Space Cut

If width $\ge 2 \cdot \text{height}$, cut the trapezoid with a line of slope -1 through the center (middle point of middle row). Traverse the trapezoid on the left first, and then the one on the right.



Squat Trapezoid: Space Cut

If width ≥ 2 ·height, cut the trapezoid with a line of slope -1 through the center (middle point of middle row). Traverse the trapezoid on the left first, and then the one on the right.



Tall Trapezoid: Time Cut

If width $< 2 \cdot$ height, cut the trapezoid with a horizontal line through the center. Traverse the bottom trapezoid first, and then the top one.



Tall Trapezoid: Time Cut

If width $< 2 \cdot$ height, cut the trapezoid with a horizontal line through the center. Traverse the bottom trapezoid first, and then the top one.



Base Case

If height = 1, compute all space-time points in the trapezoid. Any order of computation is valid, since no point depends on another.



C Implementation

```
void trapezoid(int64 t t0, int64 t t1, //time start and end
               int64 t x0, int64 t dx0, //left pt of base & "slope"
               int64 t x1, int64 t dx1) {//rt pt of base & "slope"
 int64 t h = t1 - t0; //trapezoid height
 if (h == 1) { //base case
     for (int64 t x = x0; x < x1; x++)
        u[t1\%2][x] = kernel(\&u[t0\%2][x]); //same as in looping
 } else if (h > 1) {
   if (2^{*}(x1 - x0) + (dx1 - dx0)^{*} h \ge 4^{*}h) \{ //space cut \}
      int64 t xm = (2^{*}(x0 + x1) + (dx0 + dx1 + 2)^{*}h) / 4;
     trapezoid(t0, t1, x0, dx0, xm, -1); //left
     trapezoid(t0, t1, xm, -1, x1, dx1); //right
    } else { //time cut
      int64 t half h = h / 2;
     trapezoid(t0, t0 + half_h, x0, dx0, x1, dx1); //bottom
     trapezoid(t0 + half h, t1,
                x0 + dx0 * half h,
                dx0, x1 + dx1 * half h, dx1); //top
```

Work and Cache Analysis



- The bottom of a leaf trapezoid just fits in the cache, so $w = \Theta(\mathcal{M})$.
- A leaf trapezoid contains $\Theta(hw) = \Theta(w^2)$ points and $\Theta(w^2)$ work.
- Since $w \leq \mathcal{M}$, a leaf incurs $\Theta(w/\mathcal{B})$ cache misses.
- There are $\Theta(NT/hw) = \Theta(NT/w^2)$ leaves and internal nodes.
- The internal nodes contribute little to both work and cache misses.
- Work = $\Theta(NT/w^2) \cdot \Theta(w^2) = \Theta(NT)$.
- Cache misses = $\Theta(NT/w^2) \cdot \Theta(w/B) = \Theta(NT/Bw) = \Theta(NT/BM)$.

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Simulation: 3-Point Stencil



Looping v. Trapezoid on Heat



Impact on Performance

Q. How can the cache-oblivious trapezoidal decomposition have so many fewer cache misses, but the advantage gained over the looping version be so marginal?

A. Prefetching and a good memory architecture. The memory bandwidth for one core largely suffices.



PARALLELIZING THE CACHE-OBLIVIOUS STENCIL COMPUTATION

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Time Cuts Don't Parallelize

There's no way to parallelize a time cut. The bottom trapezoid must be traversed first, and then the top one.

Space Cuts Don't Parallelize, or Do They?

A space cut poses a similar problem. You must traverse the trapezoid on the left before you can traverse the one on the right.

Parallel Space Cuts

A parallel space cut produces two upright trapezoids (black) that can be executed in parallel and a third "inverted" trapezoid (gray) that must execute in series after the two upright trapezoids.

Parallel Looping v. Parallel D&C

Memory Bandwidth



Impediments to Speedup

✓ Insufficient parallelism ✓ Scheduling overhead ✓ Lack of memory bandwidth \square Contention (locking and true/false sharing) Cilkscale can diagnose the first two problems. Q. How can we diagnose lack of memory bandwidth? A. Run P identical copies of the serial projection in parallel — if you have enough memory. Tools exist to detect lock contention in an execution, but not the *potential* for lock contention. Potential for true and false

sharing is even harder to detect, although you shouldn't have true sharing if you're code is free of determinacy races.

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CACHE-OBLIVIOUS SORTING (OMITTED)



WRAP-UP

Other C-O Algorithms

Matrix Transposition/Addition

 $\Theta(1+mn/B)$

Straightforward recursive algorithm.

Strassen's Algorithm $\Theta(n + n^2/\mathcal{B} + n^{\lg 7}/\mathcal{BM}^{(\lg 7)/2 - 1})$ Straightforward recursive algorithm.

Fast Fourier Transform $\Theta(1 + (n/\mathcal{B})(1 + \log_{\mathcal{M}}n))$ Variant of Cooley-Tukey [CT65] using cache-oblivious
matrix transpose.

LUP-Decomposition

 $\Theta(1 + n^2/\mathcal{B} + n^3/\mathcal{BM}^{1/2})$

Recursive algorithm due to Sivan Toledo [T97].

C-O Data Structures

Ordered-File Maintenance

 $O(1 + (\lg^2 n) / B)$

INSERT/DELETE anywhere in file while maintaining O(1)sized gaps. Amortized bound [BDFC00], later improved in [BCDFC02].

B-TreesINSERT/DELETE: $O(1+log_{\mathcal{B}+1}n+(lg^2n)/\mathcal{B})$ SEARCH:SEARCH: $O(1+log_{\mathcal{B}+1}n)$ TRAVERSE: $O(1+k/\mathcal{B})$

Solution [BDFC00] with later simplifications [BDIW02], [BFJ02].

Priority Queues

 $O(1+(1/B)\log_{M/B}(n/B))$

Funnel-based solution [BF02]. General scheme based on buffer trees [ABDHMM02] supports INSERT/DELETE.

CACHE-OBLIVIOUS SORTING

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This unit on sorting was not covered in lecture, but it has been taught in 6.172 in the past. It contains several instructive examples.

Merging Two Sorted Arrays



```
void merge_sort(int64_t *B, int64_t *A, int64_t n) {
    if (n==1) {
        B[0] = A[0];
    } else {
        int64_t C[n];
        cilk_spawn merge_sort(C, A, n/2);
            merge_sort(C+n/2, A+n/2, n-n/2);
        cilk_sync;
        merge(B, C, n/2, C+n/2, n-n/2);
    }
}
```



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        cilk_spawn merge_sort(C, A, n/2);
            merge_sort(C+n/2, A+n/2, n-n/2);
        cilk_sync;
        merge(B, C, n/2, C+n/2, n-n/2);
    }
}
```





Work of Merge Sort



Solve $W(n) = 2W(n/2) + \Theta(n)$.

W(n)





Solve $W(n) = 2W(n/2) + \Theta(n)$.



Solve $W(n) = 2W(n/2) + \Theta(n)$.









Solve $W(n) = 2W(n/2) + \Theta(n)$.





Now with Caching

Merge subroutine

 $Q(n) = \Theta(n/B)$.

Merge sort

 $Q(n) = \begin{cases} \Theta(n/\mathcal{B}) & \text{if } n \leq c\mathcal{M}, \text{ constant } c \leq 1; \\ 2Q(n/2) + \Theta(n/\mathcal{B}) & \text{otherwise.} \end{cases}$

 $Q(n) = \begin{cases} \Theta(n/B) & \text{if } n \leq c\mathcal{M}, \text{ constant } c \leq 1; \\ 2Q(n/2) + \Theta(n/B) & \text{otherwise.} \end{cases}$

Recursion tree

Q(n)

 $Q(n) = \begin{cases} \Theta(n/\mathcal{B}) & \text{if } n \leq c\mathcal{M}, \text{ constant } c \leq 1; \\ 2Q(n/2) + \Theta(n/\mathcal{B}) & \text{otherwise.} \end{cases}$

Recursion tree



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Recursion tree



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Recursion tree



 $Q(n) = \begin{cases} \Theta(n/B) & \text{if } n \le c\mathcal{M}, \text{ constant } c \le 1; \\ 2Q(n/2) + \Theta(n/B) & \text{otherwise.} \end{cases}$

Recursion tree



Bottom Line for Merge Sort

 $\begin{aligned} \mathsf{Q}(\mathsf{n}) &= \begin{cases} \Theta(\mathsf{n}/\mathcal{B}) & \text{if } \mathsf{n} \leq \mathsf{c}\mathcal{M}, \text{ constant } \mathsf{c} \leq \mathsf{1}; \\ 2\mathsf{Q}(\mathsf{n}/2) + \Theta(\mathsf{n}/\mathcal{B}) & \text{otherwise}; \end{cases} \\ &= \Theta((\mathsf{n}/\mathcal{B}) \lg(\mathsf{n}/\mathcal{M})). \end{aligned}$

- For $n \gg \mathcal{M}$, we have $\lg(n/\mathcal{M}) \approx \lg n$, and thus $W(n)/Q(n) \approx \Theta(\mathcal{B})$.
- For $n \approx \mathcal{M}$, we have $\lg(n/\mathcal{M}) \approx \Theta(1)$, and thus $W(n)/Q(n) \approx \Theta(\mathcal{B} \lg n)$.

Multiway Merging

IDEA: Merge R < n subarrays with a tournament.



Multiway Merging

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Multiway Merging

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Multiway Merging

IDEA: Merge R < n subarrays with a tournament.



Work of Multiway Merge Sort

$$W(n) = \begin{cases} \Theta(1) & \text{if } n = 1; \\ R \cdot W(n/R) + \Theta(n \lg R) & \text{otherwise.} \end{cases}$$

Recursion tree



Caching Recurrence

Consider the R-way merging of contiguous arrays of total size n. If $R < c\mathcal{M}/\mathcal{B}$, for some sufficiently small constant $c \leq 1$, the entire tournament plus 1 block from each array can fit in cache. $\Rightarrow Q(n) \leq \Theta(n/\mathcal{B})$ for merging.

 $\begin{aligned} & \mathsf{R}\text{-way merge sort} \\ & \mathsf{Q}(\mathsf{n}) \leq \begin{cases} \Theta(\mathsf{n}/\mathcal{B}) & \text{if } \mathsf{n} < \mathsf{c}\mathcal{M}; \\ & \mathsf{R}\text{-}\mathsf{Q}(\mathsf{n}/\mathsf{R}) + \Theta(\mathsf{n}/\mathcal{B}) \\ & \text{otherwise.} \end{aligned}$

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Cache Analysis



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Tuning the Voodoo Parameter

We have

 $Q(n) = \Theta((n/\mathcal{B}) \log_{R}(n/\mathcal{M})),$ which decreases as $R < c\mathcal{M}/\mathcal{B}$ increases. Choosing R as big as possible yields $R = \Theta(\mathcal{M}/\mathcal{B}).$

By the tall-cache assumption $(\mathcal{B}^2 < c\mathcal{M})$ and the fact that $\log_{\mathcal{M}}(n/\mathcal{M}) = \Theta((\lg n)/\lg \mathcal{M})$, we have

 $\begin{aligned} \mathsf{Q}(\mathsf{n}) &= \Theta((\mathsf{n}/\mathcal{B}) \log_{\mathcal{M}/\mathcal{B}}(\mathsf{n}/\mathcal{M})) \\ &= \Theta((\mathsf{n}/\mathcal{B}) \log_{\mathcal{M}}(\mathsf{n}/\mathcal{M})) \\ &= \Theta((\mathsf{n} \lg \mathsf{n})/\mathcal{B} \lg \mathcal{M}) . \end{aligned}$

Hence, we have $W(n)/Q(n) \approx \Theta(\mathcal{B} \lg \mathcal{M})$.

Multiway versus Binary Merge Sort

We have

 $Q_{multiway}(n) = \Theta((n \lg n) / \mathcal{B} \lg \mathcal{M})$

versus

$$\begin{aligned} \mathbf{Q}_{\text{binary}}(\mathbf{n}) &= \Theta((\mathbf{n}/\mathcal{B}) \, |\, \mathbf{g}(\mathbf{n}/\mathcal{M})) \\ &= \Theta((\mathbf{n} \, |\, \mathbf{g} \, \mathbf{n})/\mathcal{B}) , \end{aligned}$$

as long as $n \gg \mathcal{M}$, because then $\lg(n/\mathcal{M}) \approx \lg n$. Thus, multiway merge sort saves a factor of $\Theta(\lg \mathcal{M})$ in cache misses.

Example (ignoring constants)

• L1-cache: $\mathcal{M} = 2^{15} \Rightarrow 15 \times \text{savings}$.

• L2-cache: $\mathcal{M} = 2^{18} \Rightarrow 18 \times \text{ savings.}$

• L3-cache: $\mathcal{M} = 2^{23} \Rightarrow 23 \times \text{savings.}$

Optimal Cache-Oblivious Sorting

Funnelsort [FLPR99]

- 1. Recursively sort $n^{1/3}$ groups of $n^{2/3}$ items.
- 2. Merge the sorted groups with an $n^{1/3}$ -funnel.

A k-funnel merges k³ items in k sorted lists, incurring at most

 $\Theta(\mathbf{k} + (\mathbf{k}^3/\mathcal{B})(\mathbf{1} + \log_{\mathcal{M}} \mathbf{k}))$

cache misses. Thus, funnelsort incurs

$$\begin{split} \mathsf{Q}(\mathsf{n}) &\leq \mathsf{n}^{1/3}\mathsf{Q}(\mathsf{n}^{2/3}) + \Theta(\mathsf{n}^{1/3} + (\mathsf{n}/\mathsf{b})(1 + \log_{\mathcal{M}}\mathsf{n})) \\ &= \Theta(1 + (\mathsf{n}/\mathcal{B})(1 + \log_{\mathcal{M}}\mathsf{n})) \,, \end{split}$$

cache misses, which is asymptotically optimal [AV88].

Construction of a k-funnel



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