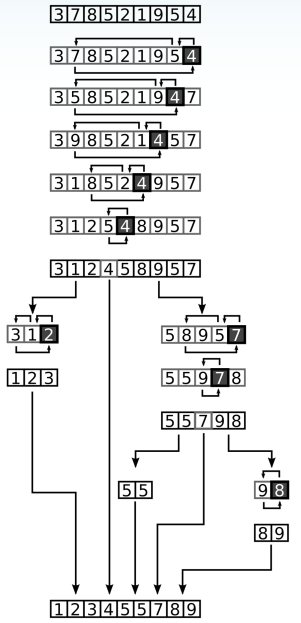
6.506: Algorithm Engineering



Lecture 3
Cache-Oblivious Algorithms and Data Structures

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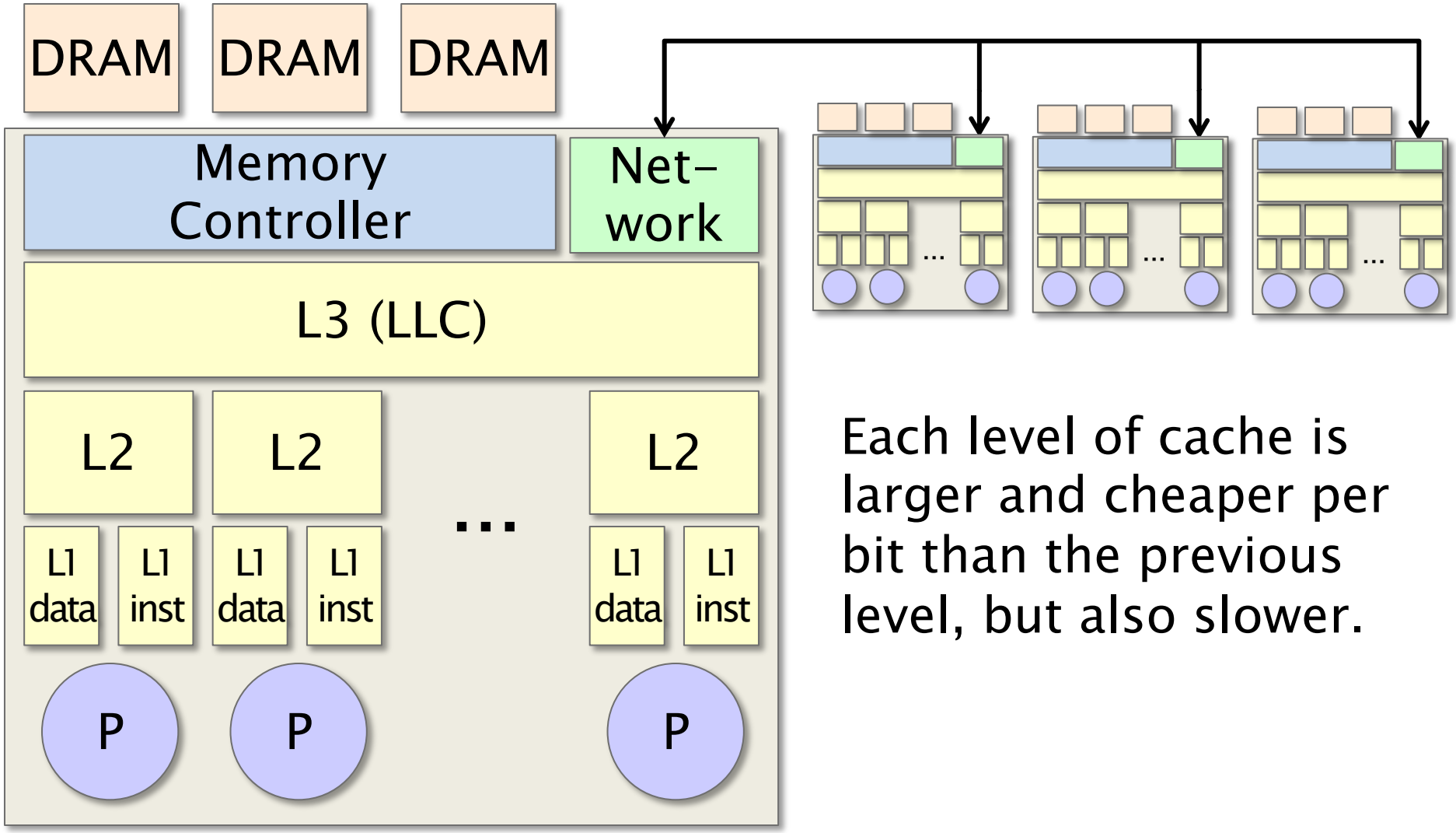
February 14, 2023

Multicore Cache Hierarchy



Each level of cache is larger and cheaper per bit than the previous level, but also slower.

Cache Specs for Typical High-End Multicore

Level	Size/core	Associativity	Latency (cycles)
DRAM	up to 160 GiB		85–240
L3	1.375 MiB	11	50–70
L2	1 MiB	16	14
L1-D	32 KiB	8	4–5
L1-I	32 KiB	8	5

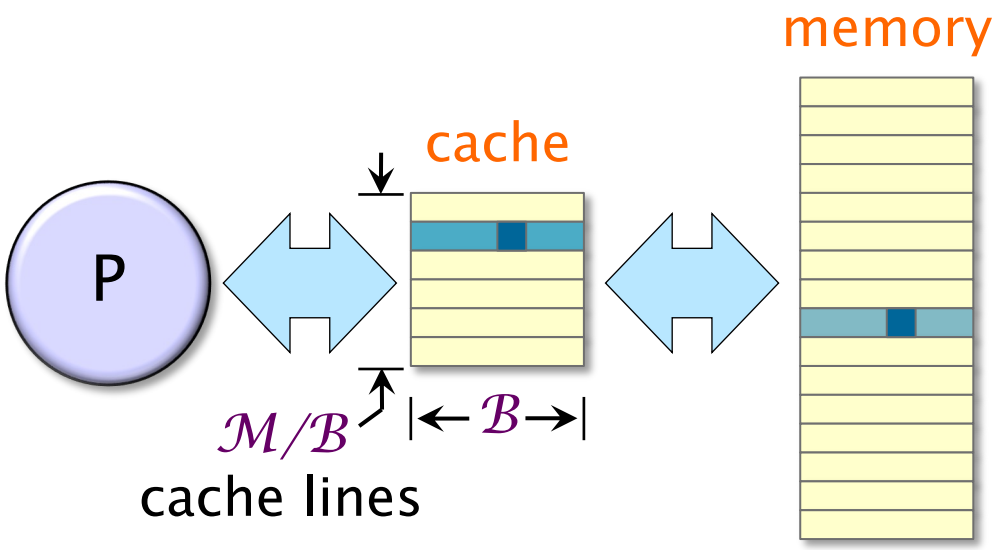
Intel Xeon Platinum 8280L (Cascade Lake)

- Launched April 2019 for $17,906 — cheaper now.
- 2.7 GHz clock, Turbo Boost up to 4 GHz
- 28 cores/chip + 2-way hyperthreading
- 2190 GFLOPS
- 64 B cache lines/blocks
- Up to 8-way multiprocessing

Ideal-Cache Model

Parameters

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

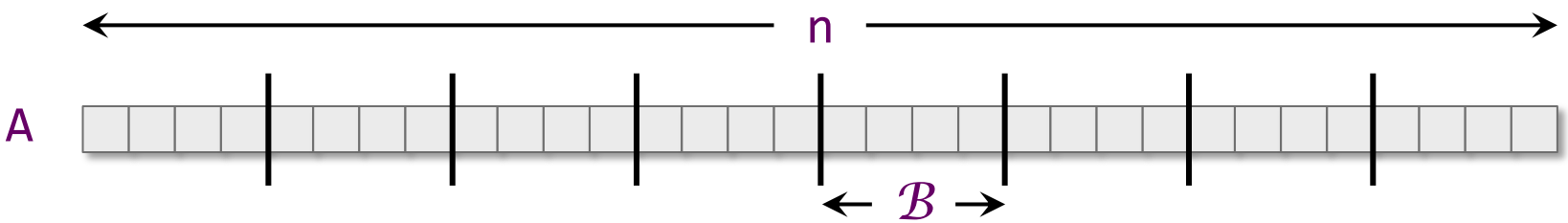


Performance Measures

- work T (ordinary running time)
- cache misses Q

Reading an Array Sequentially

```
sum = 0;
for (int i=0; i<n; ++i)
  sum += A[i];
```



Cache misses: $Q(n) = \Theta(n/\mathcal{B})$

Segment Caching Lemma

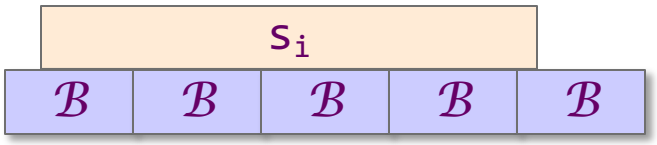
Lemma. Suppose that a program reads a set of r data segments, where the ith segment consists of s_i contiguous bytes in memory, and suppose that

$$\sum_{i=1}^{r} s_i = N < \mathcal{M}/3 \text{ and } N/r \geq \mathcal{B} .$$

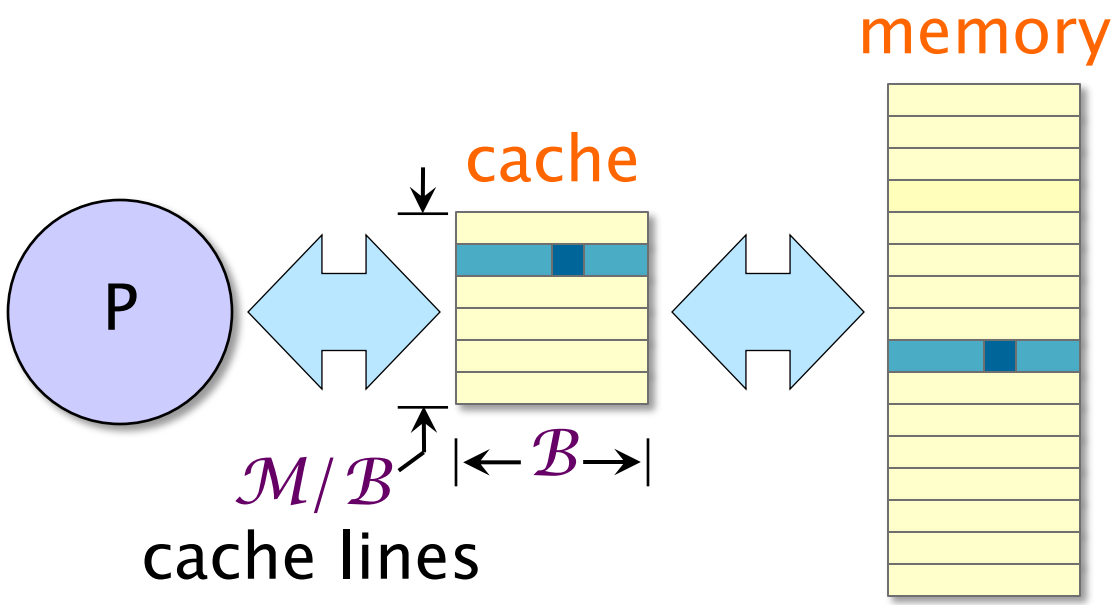
Then all the segments fit into cache, and the number of misses to read them all is at most $3N/\mathcal{B}$.

Proof. A single segment s_i incurs at most $s_i/\mathcal{B} + 2$ misses, and hence we have

$$\begin{aligned}\sum_{i=1}^{r}(s_i/\mathcal{B} + 2) &= N/\mathcal{B} + 2r \\ &= N/\mathcal{B} + (2r\mathcal{B})/\mathcal{B} \\ &\leq N/\mathcal{B} + 2N/\mathcal{B} \\ &= 3N/\mathcal{B} .\end{aligned}$$



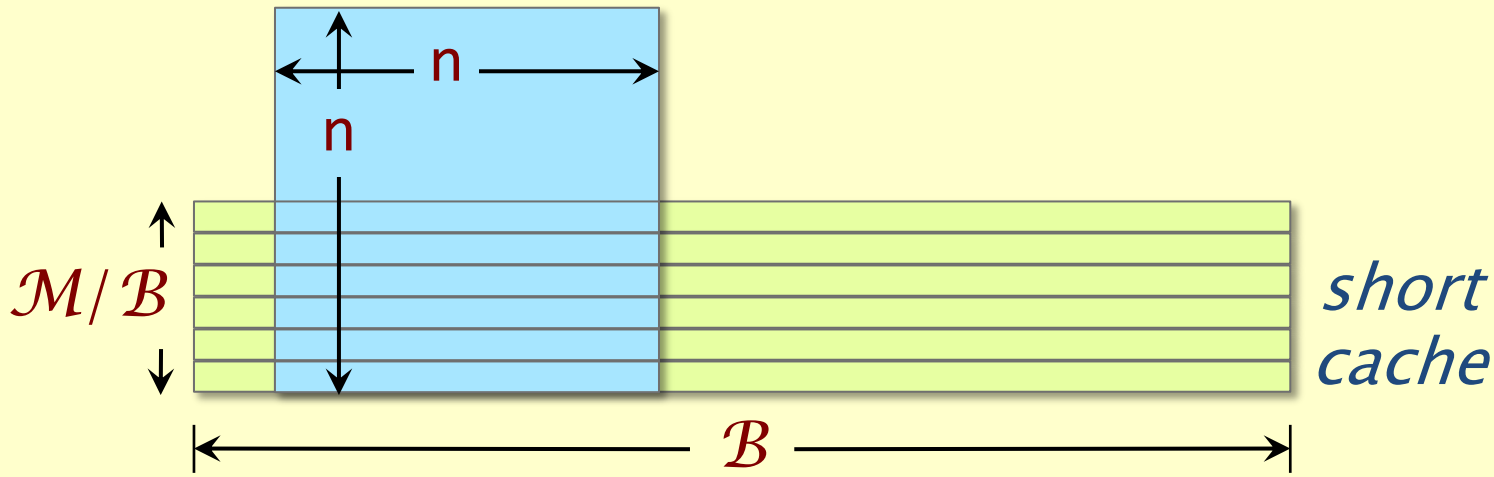
Tall Caches



Tall-cache assumption
$\mathcal{B}^2 < c\mathcal{M}$ for some sufficiently small constant $c \leq 1$.

Example: Intel Xeon Platinum 8280L
- Cache-line length $\mathcal{B} = 64$ bytes.
- L1-cache size $\mathcal{M} = 32$ kibibytes.

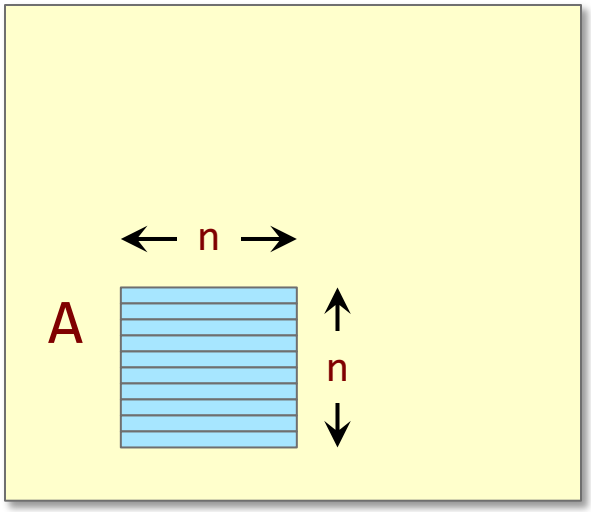
What's Wrong with Short Caches?



Tall-cache assumption
$\mathcal{B}^2 < c\mathcal{M}$ for some sufficiently small constant $c \leq 1$.

An $n \times n$ submatrix stored in row-major order may not fit in a short cache even if $n^2 < c\mathcal{M}$!

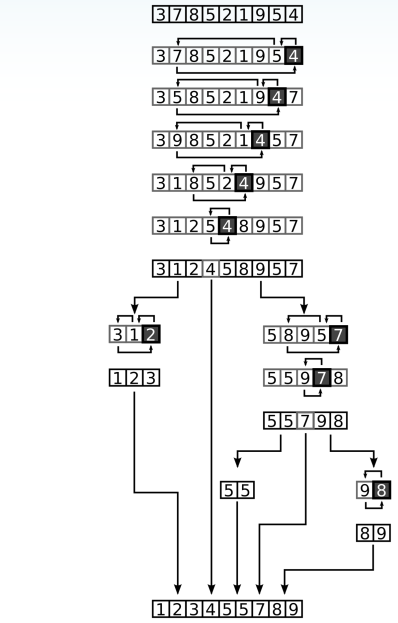
Submatrix Caching Lemma



Lemma. Suppose that an $n \times n$ submatrix A is read into a tall cache satisfying $\mathcal{B}^2 < c\mathcal{M}$, where $c < 1/3$ is constant, and suppose that $c\mathcal{M} \leq n^2 < \mathcal{M}/3$. Then A fits into the cache, and the number of misses to read all of A's elements is at most $3n^2/\mathcal{B}$.

Proof. We have $r = n$, $s_i = n$, $N = n^2$. Since $\mathcal{B}^2 < c\mathcal{M} \leq n^2$, we have $\mathcal{B} \leq n = N/r$. And since $N < \mathcal{M}/3$, the segment caching lemma applies. ■

Cache Analysis of Matrix Multiplication



Multiply Square Matrices

```
void Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i=0; i < n; i++)
    for (int64_t j=0; j < n; j++)
      for (int64_t k=0; k < n; k++)
        C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

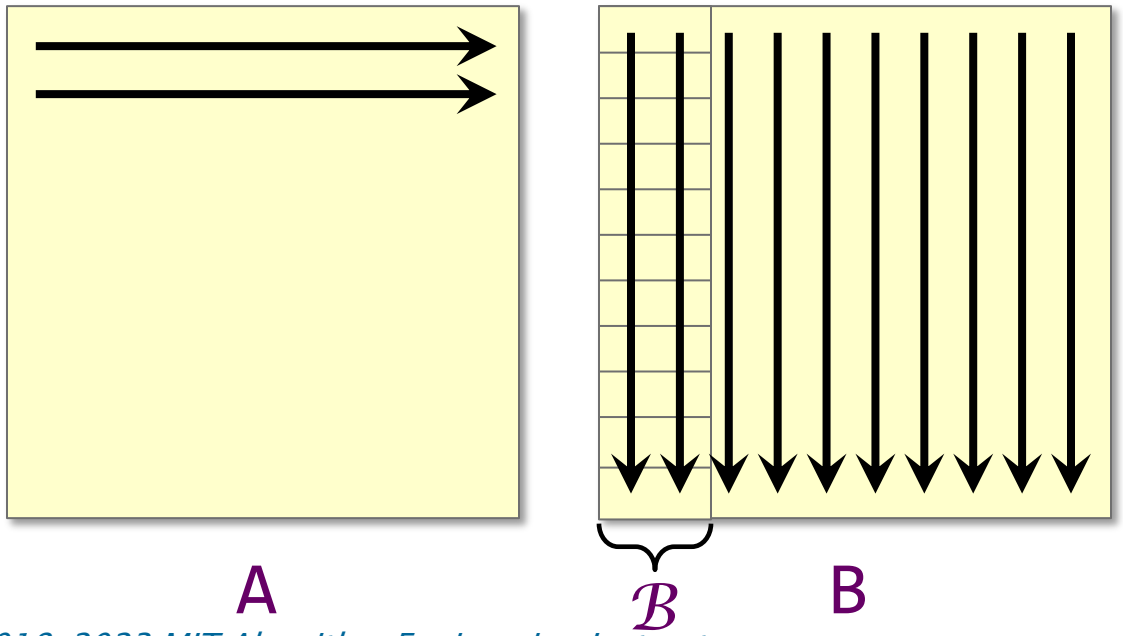
Analysis of work

$T(n) = \Theta(n^3)$.

Analysis of Cache Misses

```
void Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i=0; i < n; i++)
    for (int64_t j=0; j < n; j++)
      for (int64_t k=0; k < n; k++)
        C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

Assume row major and tall cache



Case 1

$n \geq \mathcal{M}/\mathcal{B}$.

Analyze matrix B.

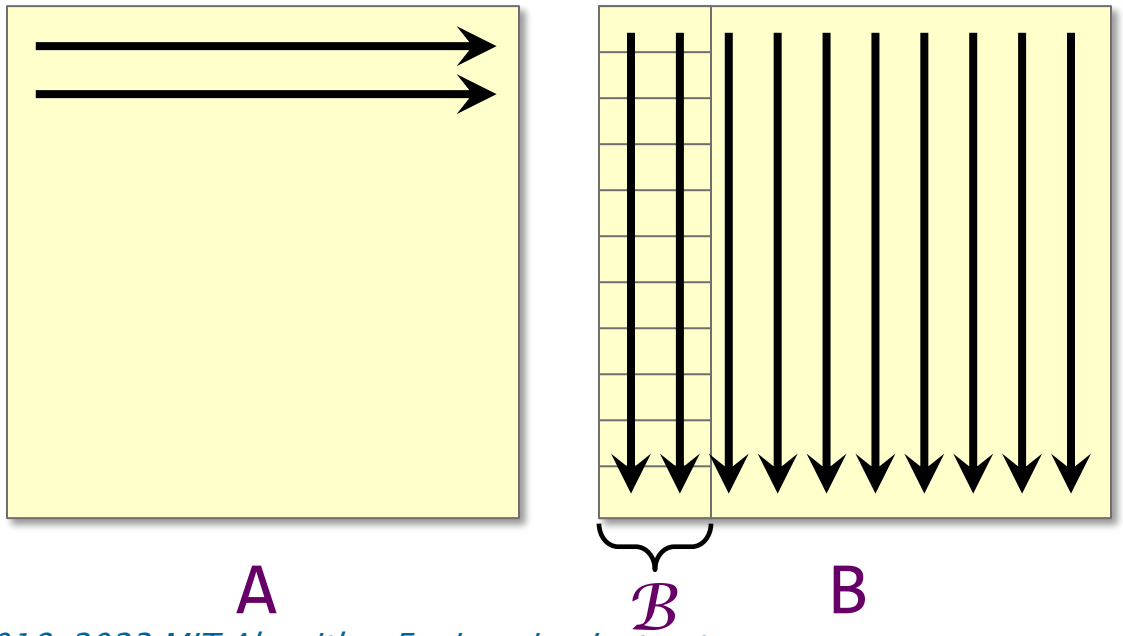
Assume LRU.

$Q(n) = \Theta(n^3)$, since matrix B misses on every access.

Analysis of Cache Misses

```
void Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i=0; i < n; i++)
    for (int64_t j=0; j < n; j++)
      for (int64_t k=0; k < n; k++)
        C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

Assume row major and tall cache



Case 2

$\mathcal{M}^{1/2} \leq n < \mathcal{M}/\mathcal{B}$.

Analyze matrix B.

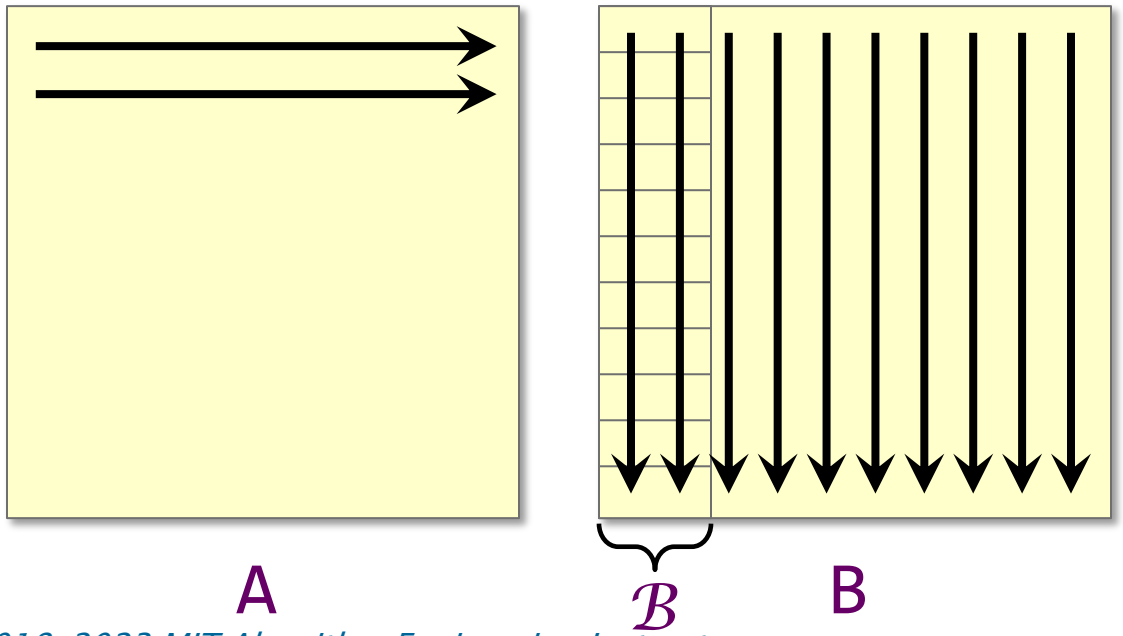
Assume LRU.

$Q(n) = n \cdot \Theta(n^2/\mathcal{B}) = \Theta(n^3/\mathcal{B})$, since matrix B can exploit spatial locality.

Analysis of Cache Misses

```
void Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i=0; i < n; i++)
    for (int64_t j=0; j < n; j++)
      for (int64_t k=0; k < n; k++)
        C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

Assume row major and tall cache



Case 3

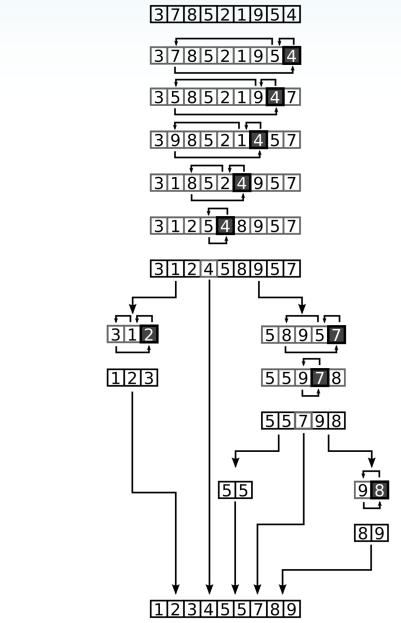
$n < c\mathcal{M}^{1/2}$.

Analyze matrix B.

Assume LRU.

$Q(n) = \Theta(n^2/\mathcal{B})$, by the submatrix caching lemma.

TILING

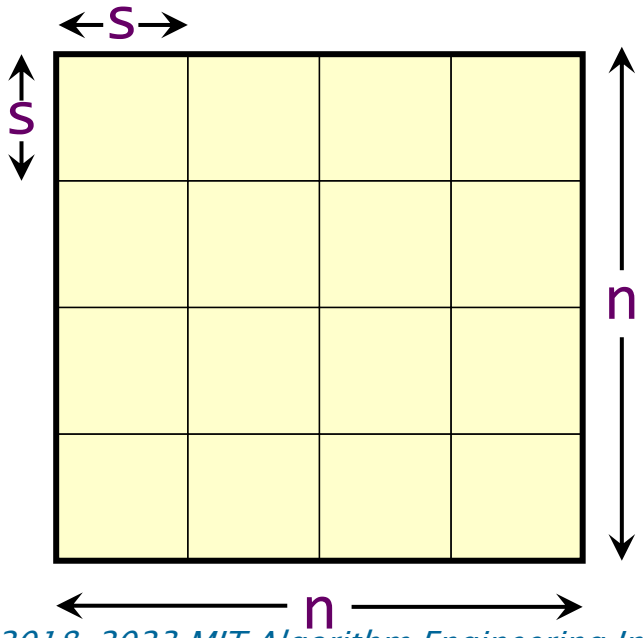


Tiled Matrix Multiplication

```
void Tiled_Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i1=0; i1<n/s; i1+=s)
    for (int64_t j1=0; j1<n/s; j1+=s)
      for (int64_t k1=0; k1<n/s; k1+=s)
        for (int64_t i=i1; i<i1+s && i<n; i++)
          for (int64_t j=j1; j<j1+s && j<n; j++)
            for (int64_t k=k1; k<k1+s && k<n; k++)
              C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

outer nest

inner nest



Analysis of work

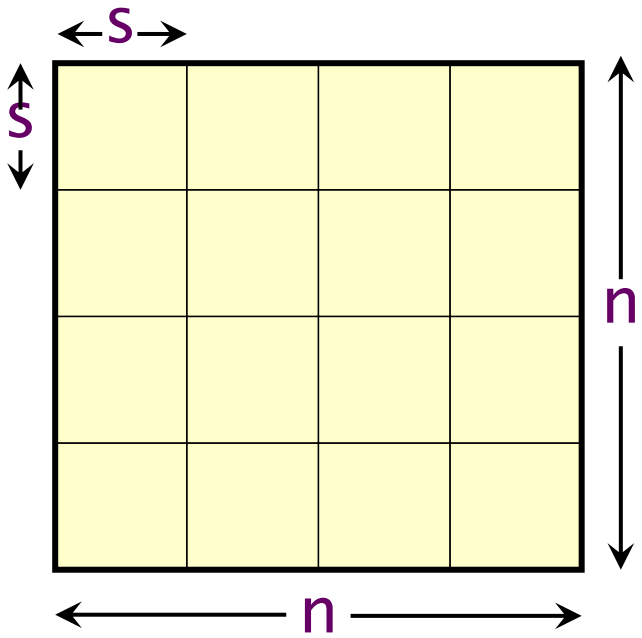
- Work $T(n) = \Theta((n/s)^3(s^3))$
  $= \Theta(n^3)$.

Tiled Matrix Multiplication

```
void Tiled_Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i1=0; i1<n/s; i1+=s)
    for (int64_t j1=0; j1<n/s; j1+=s)
      for (int64_t k1=0; k1<n/s; k1+=s)
        for (int64_t i=i1; i<i1+s && i<n; i++)
          for (int64_t j=j1; j<j1+s && j<n; j++)
            for (int64_t k=k1; k<k1+s && k<n; k++)
              C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

outer nest

inner nest



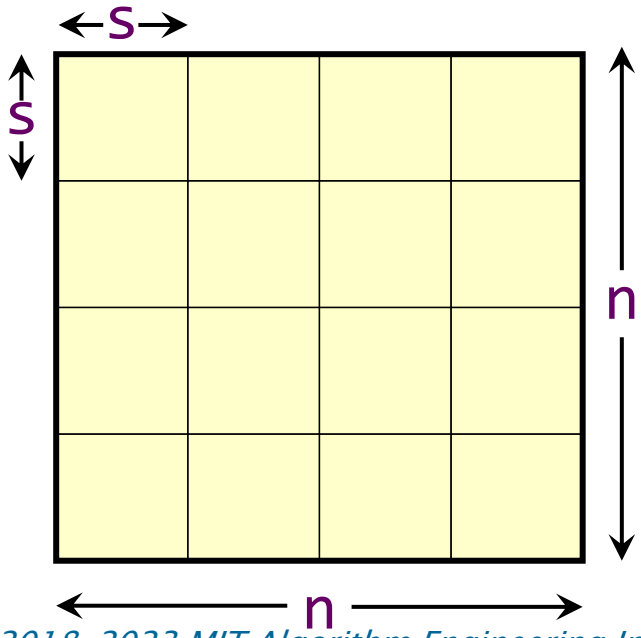
Analysis of cache misses

- Tune s so that the tiles just fit into cache $\Rightarrow s = \Theta(\mathcal{M}^{1/2})$.
- Submatrix caching lemma implies $\Theta(s^2/\mathcal{B})$ misses per tile.
- $Q(n) = \Theta((n/s)^3(s^2/\mathcal{B}))$
  $= \Theta(n^3/\mathcal{B}\mathcal{M}^{1/2})$.
- Optimal [HK81].

Tiled Matrix Multiplication

```
void Tiled_Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i
    for (int
      for (
        fo
          for
            for (
              C[i*n+j] +=
}
```

Voodoo!



Analysis of cache misses

- Tune s so that the tiles just fit into cache $\Rightarrow s = \Theta(\mathcal{M}^{1/2})$.
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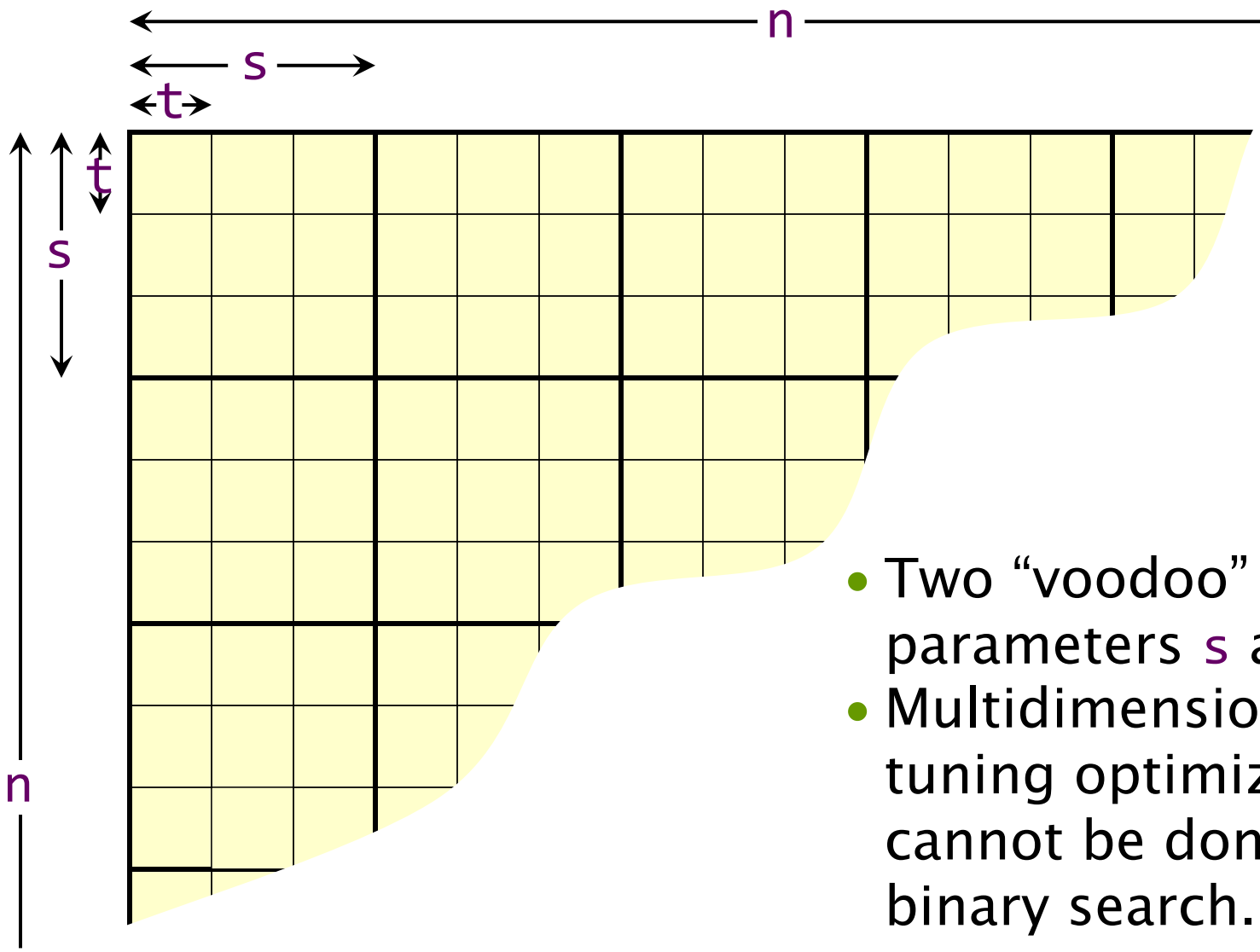
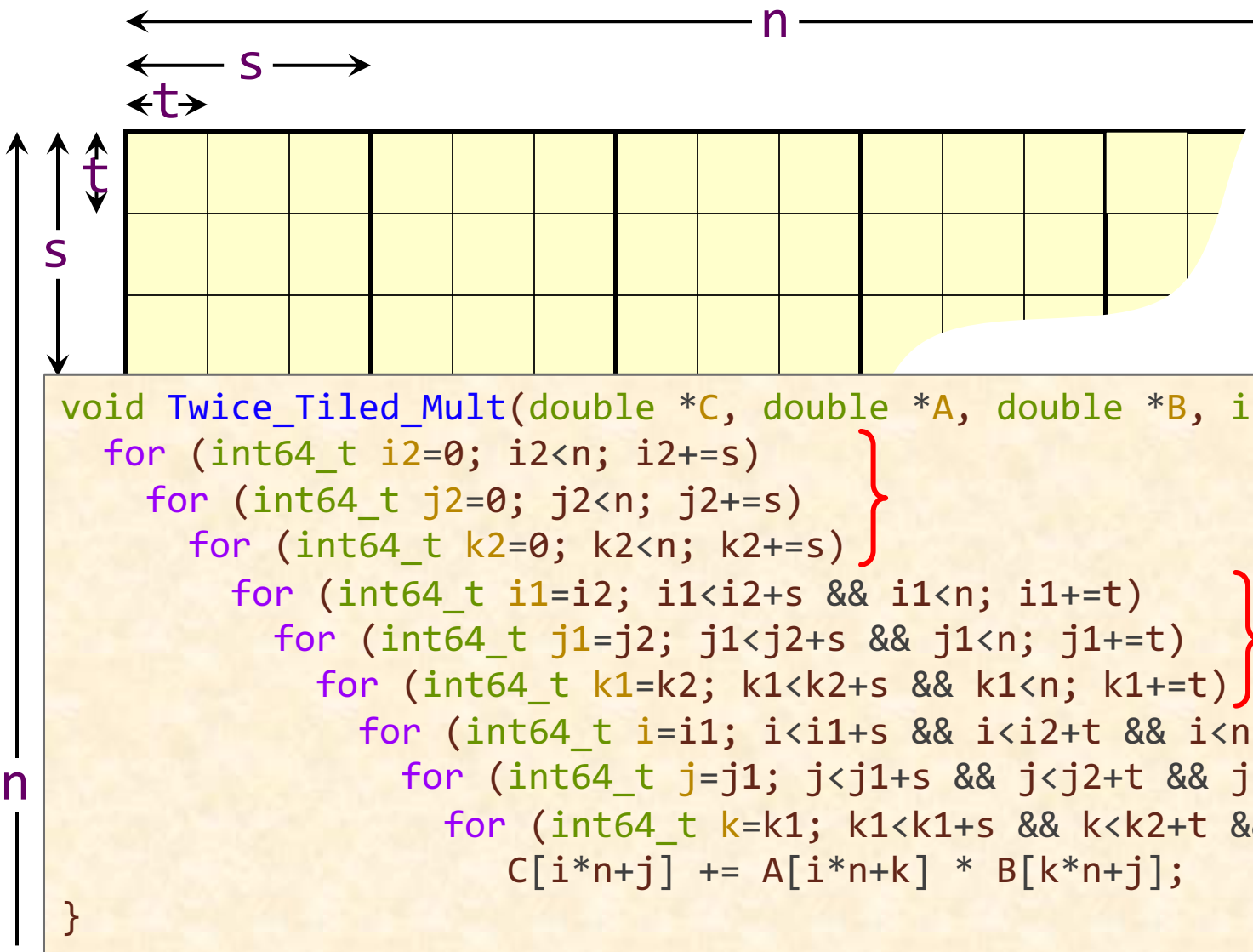
- $Q(n) = \Theta((n/s)^3(s^2/\mathcal{B}))$
  $= \Theta(n^3/\mathcal{B}\mathcal{M}^{1/2})$.
- Optimal [HK81].

Two-Level Cache



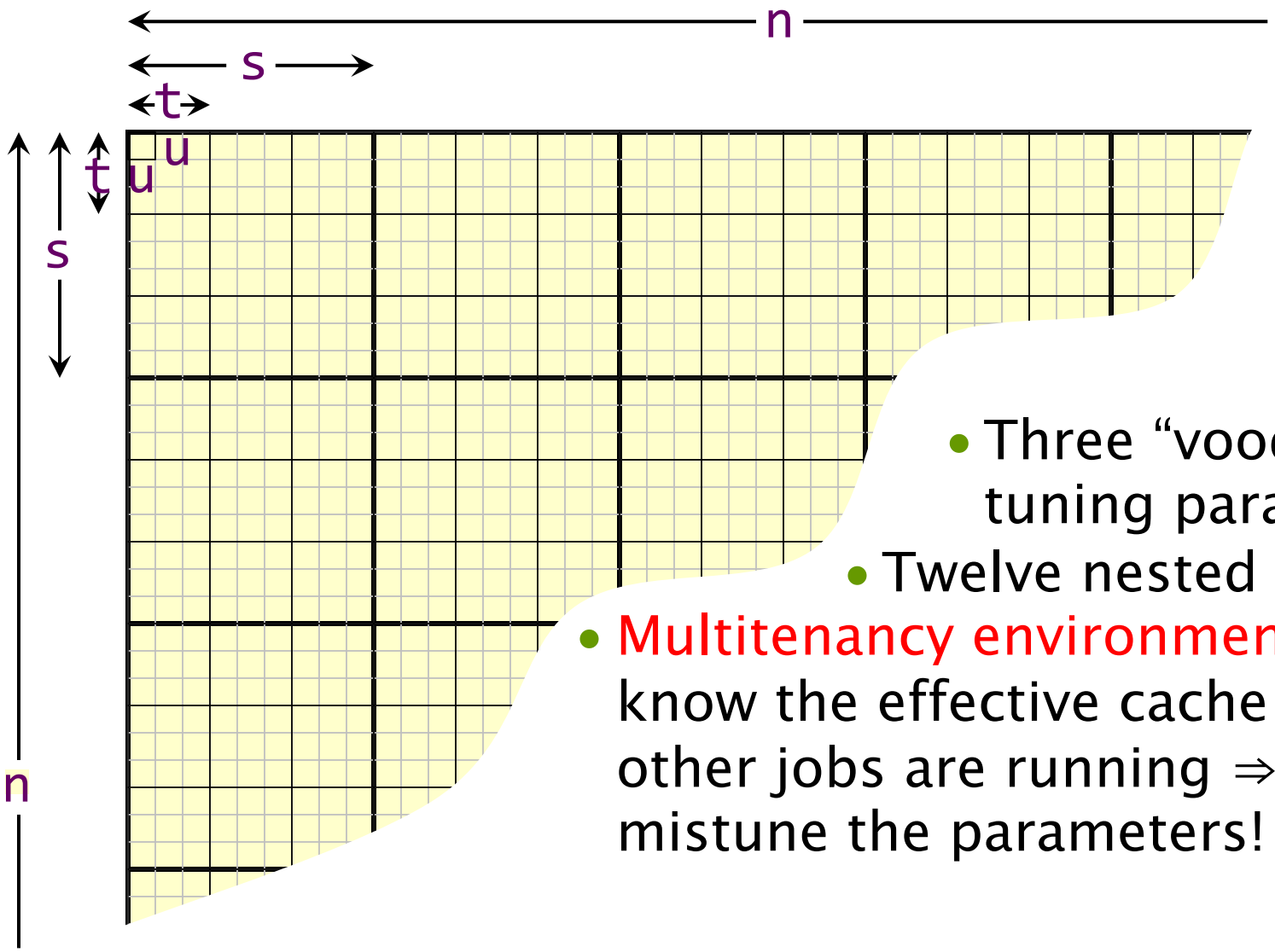
- Two “voodoo” tuning parameters `s` and `t`.
- Multidimensional tuning optimization cannot be done with binary search.

Two-Level Cache



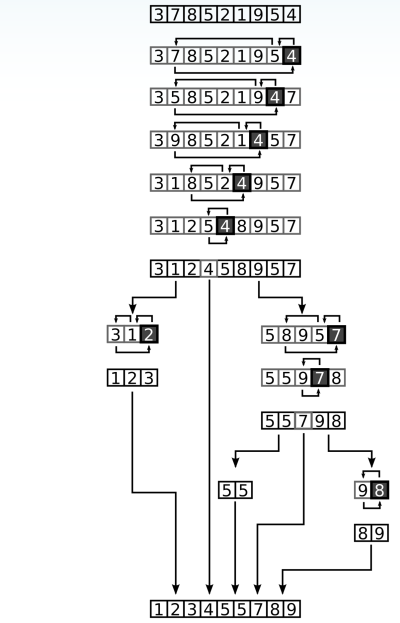

```
void Twice_Tiled_Mult(double *C, double *A, double *B, int64_t n) {
  for (int64_t i2=0; i2<n; i2+=s)
    for (int64_t j2=0; j2<n; j2+=s)
      for (int64_t k2=0; k2<n; k2+=s)
        for (int64_t i1=i2; i1<i2+s && i1<n; i1+=t)
          for (int64_t j1=j2; j1<j2+s && j1<n; j1+=t)
            for (int64_t k1=k2; k1<k2+s && k1<n; k1+=t)
              for (int64_t i=i1; i<i1+s && i<i2+t && i<n; i++)
                for (int64_t j=j1; j<j1+s && j<j2+t && j<n; j++)
                  for (int64_t k=k1; k1<k1+s && k<k2+t && k<n; k++)
                    C[i*n+j] += A[i*n+k] * B[k*n+j];
}
```

Three-Level Cache



- Three "voodoo" tuning parameters.
- Twelve nested `for` loops.
- Multitenancy environment: Don't know the effective cache size when other jobs are running ⇒ easy to mistune the parameters!

Divide & Conquer



Recursive Matrix Multiplication

Divide-and-conquer on $n \times n$ matrices.

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

$$= \begin{bmatrix} A_{11}B_{11} & A_{11}B_{12} \\ A_{21}B_{11} & A_{21}B_{12} \end{bmatrix} + \begin{bmatrix} A_{12}B_{21} & A_{12}B_{22} \\ A_{22}B_{21} & A_{22}B_{22} \end{bmatrix}$$

8 multiply-adds of $(n/2) \times (n/2)$ matrices.

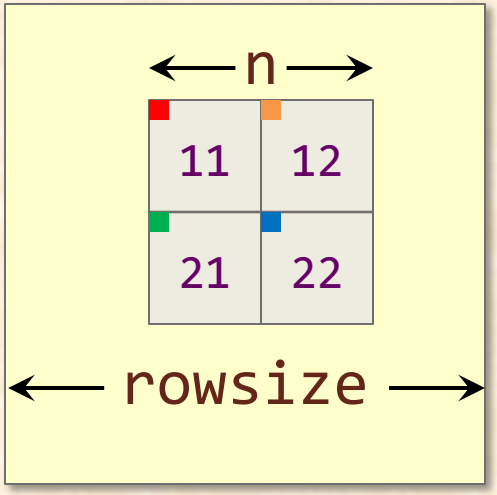
Recursive Code

```
// Assume that n is an exact power of 2.
void Rec_Mult(double *C, double *A, double *B,
              int64_t n, int64_t rowsize) {
  if (n == 1)
    C[0] += A[0] * B[0];
  else {
    int64_t d11 = 0;
    int64_t d12 = n/2;
    int64_t d21 = (n/2) * rowsize;
    int64_t d22 = (n/2) * (rowsize+1);

    Rec_Mult(C+d11, A+d11, B+d11, n/2, rowsize);
    Rec_Mult(C+d11, A+d12, B+d21, n/2, rowsize);
    Rec_Mult(C+d12, A+d11, B+d12, n/2, rowsize);
    Rec_Mult(C+d12, A+d12, B+d22, n/2, rowsize);
    Rec_Mult(C+d21, A+d21, B+d11, n/2, rowsize);
    Rec_Mult(C+d21, A+d22, B+d21, n/2, rowsize);
    Rec_Mult(C+d22, A+d21, B+d12, n/2, rowsize);
    Rec_Mult(C+d22, A+d22, B+d22, n/2, rowsize);
  }
}
```

Coarsen base case to overcome function-call overheads.

Recursive Code

```
// Assume that n is an exact power of 2.
void Rec_Mult(double *C, double *A, double *B,
              int64_t n, int64_t rowsize) {
  if (n == 1)
    C[0] += A[0] * B[0];
  else {
    int64_t d11 = 0;
    int64_t d12 = n/2;
    int64_t d21 = (n/2) * rowsize;
    int64_t d22 = (n/2) * (rowsize+1);

    Rec_Mult(C+d11, A+d11, B+d11, n/2, rowsize);
    Rec_Mult(C+d11, A+d12, B+d21, n/2, rowsize);
    Rec_Mult(C+d12, A+d11, B+d12, n/2, rowsize);
    Rec_Mult(C+d12, A+d12, B+d22, n/2, rowsize);
    Rec_Mult(C+d21, A+d21, B+d11, n/2, rowsize);
    Rec_Mult(C+d21, A+d22, B+d21, n/2, rowsize);
    Rec_Mult(C+d22, A+d21, B+d12, n/2, rowsize);
    Rec_Mult(C+d22, A+d22, B+d22, n/2, rowsize);
  }
}
```



Analysis of Work

```
// Assume that n is an exact power of 2.
void Rec_Mult(double *C, double *A, double *B,
              int64_t n, int64_t rowsize) {
  if (n == 1)
    C[0] += A[0] * B[0];
  else {
    int64_t d11 = 0;
    int64_t d12 = n/2;
    int64_t d21 = (n/2) * rowsize;
    int64_t d22 = (n/2) * (rowsize+1);

    Rec_Mult(C+d11, A+d11, B+d11, n/2, rowsize);
    Rec_Mult(C+d11, A+d12, B+d21, n/2, rowsize);
    Rec_Mult(C+d12, A+d11, B+d12, n/2, rowsize);
    Rec_Mult(C+d12, A+d12, B+d22, n/2, rowsize);
    Rec_Mult(C+d21, A+d21, B+d11, n/2, rowsize);
    Rec_Mult(C+d21, A+d22, B+d21, n/2, rowsize);
    Rec_Mult(C+d22, A+d21, B+d12, n/2, rowsize);
    Rec_Mult(C+d22, A+d22, B+d22, n/2, rowsize);
  }
}
```

$$\begin{aligned} T(n) &= 8\,T(n/2) + \Theta(1) \\ &= \Theta(n^3) \end{aligned}$$

Analysis of Work

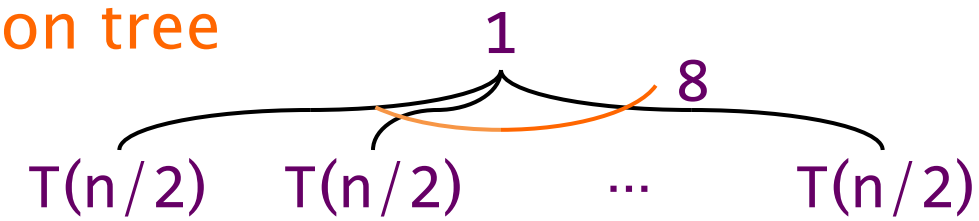
$$T(n) = 8T(n/2) + 1$$

recursion tree $T(n)$

Analysis of Work

$$T(n) = 8T(n/2) + 1$$

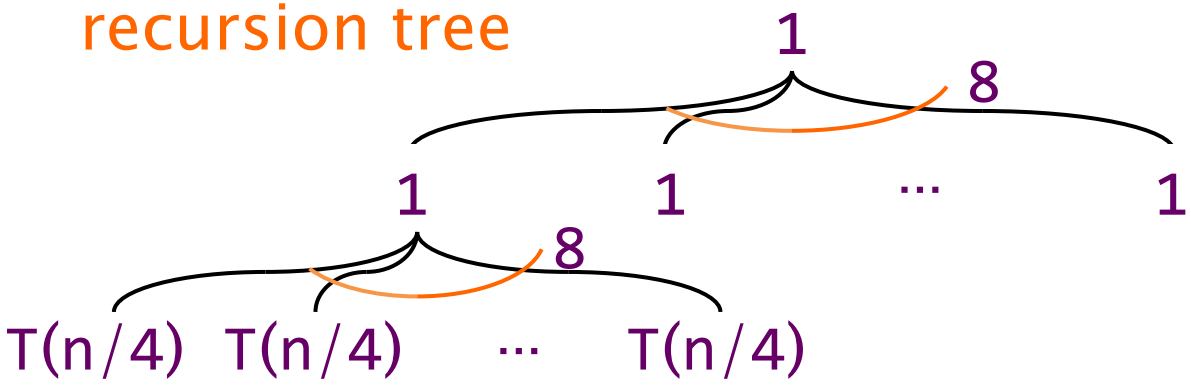
recursion tree



Analysis of Work

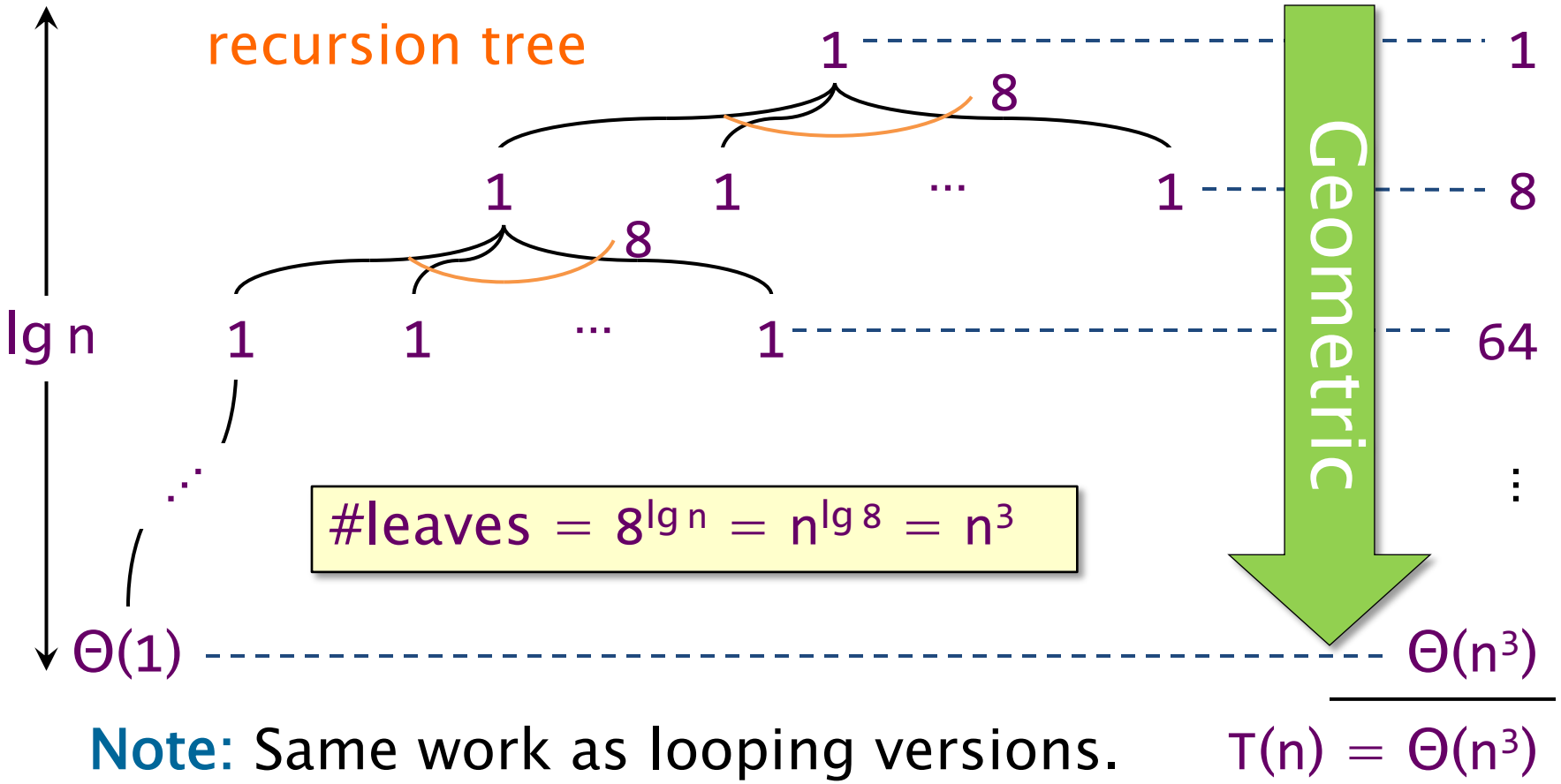
$$T(n) = 8T(n/2) + 1$$

recursion tree



Analysis of Work

$$T(n) = 8T(n/2) + 1$$



Note: Same work as looping versions.

$$T(n) = \Theta(n^3)$$

Analysis of Cache Misses

```
// Assume that n is an exact power of 2.
void Rec_Mult(double *C, double *A, double *B,
              int64_t n, int64_t rowsize) {
  if (n == 1)
    C[0] += A[0] * B[0];
  else {
    int64_t d11 = 0;
    int64_t d12 = n/2;
    int64_t d21 = (n/2) * rowsize;
    int64_t d22 = (n/2) * (rowsize+1);

    Rec_Mult(C+d11, A+d11, B+d11, n/2, rowsize);
    Rec_Mult(C+d11, A+d12, B+d21, n/2, rowsize);
    Rec_Mult(C+d12, A+d11, B+d12, n/2, rowsize);
    Rec_Mult(C+d12, A+d12, B+d22, n/2, rowsize);
    Rec_Mult(C+d21, A+d21, B+d11, n/2, rowsize);
    Rec_Mult(C+d21, A+d22, B+d21, n/2, rowsize);
    Rec_Mult(C+d22, A+d21, B+d12, n/2, rowsize);
    Rec_Mult(C+d22, A+d22, B+d22, n/2, rowsize);
  }
}
```

Submatrix caching lemma

$$Q(n) = \begin{cases} \Theta(n^2/\mathcal{B}) \text{ if } n^2 < c\mathcal{M} \text{ for suff. small const } c \le 1, \\ 8\,Q(n/2) + \Theta(1) \text{ otherwise.} \end{cases}$$

Analysis of Cache Misses

$$Q(n) = \begin{cases} \Theta(n^2/\mathcal{B}) \text{ if } n^2 < c\mathcal{M} \text{ for suff. small const } c \le 1, \\ 8\,Q(n/2) + 1 \text{ otherwise.} \end{cases}$$

recursion tree $Q(n)$

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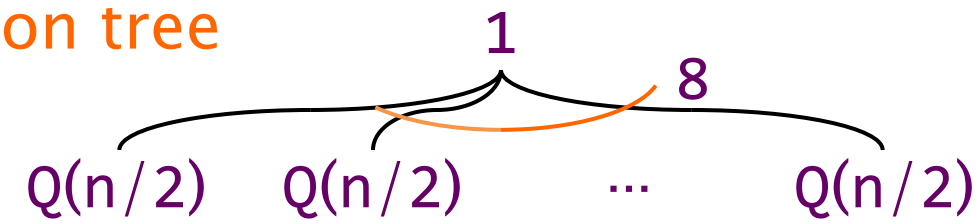
recursion tree



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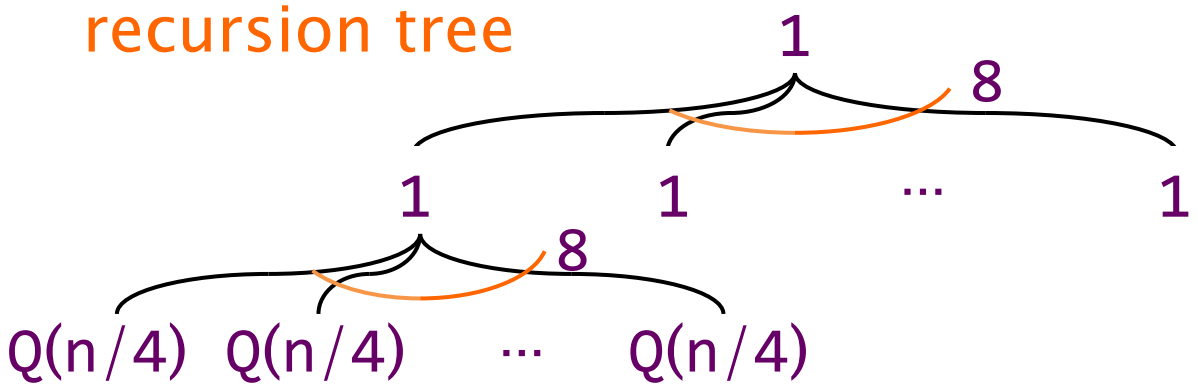

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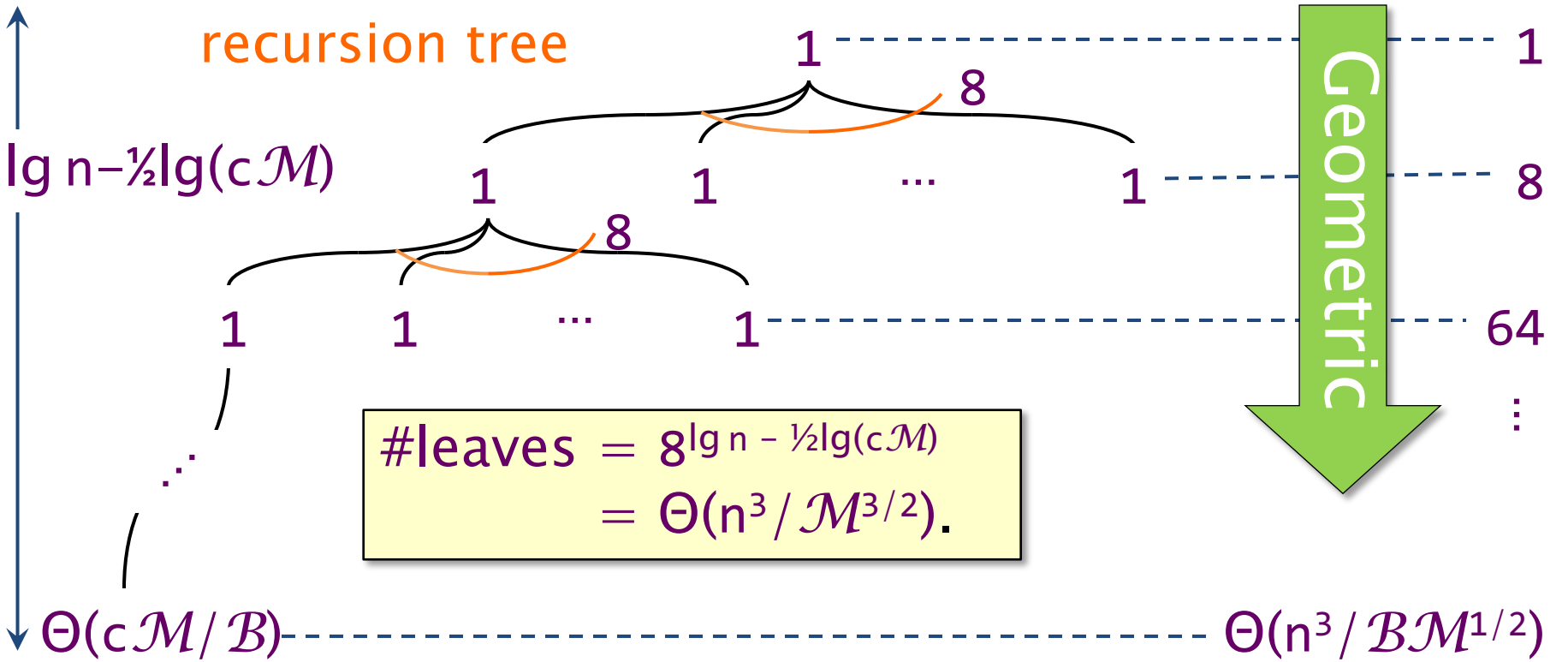


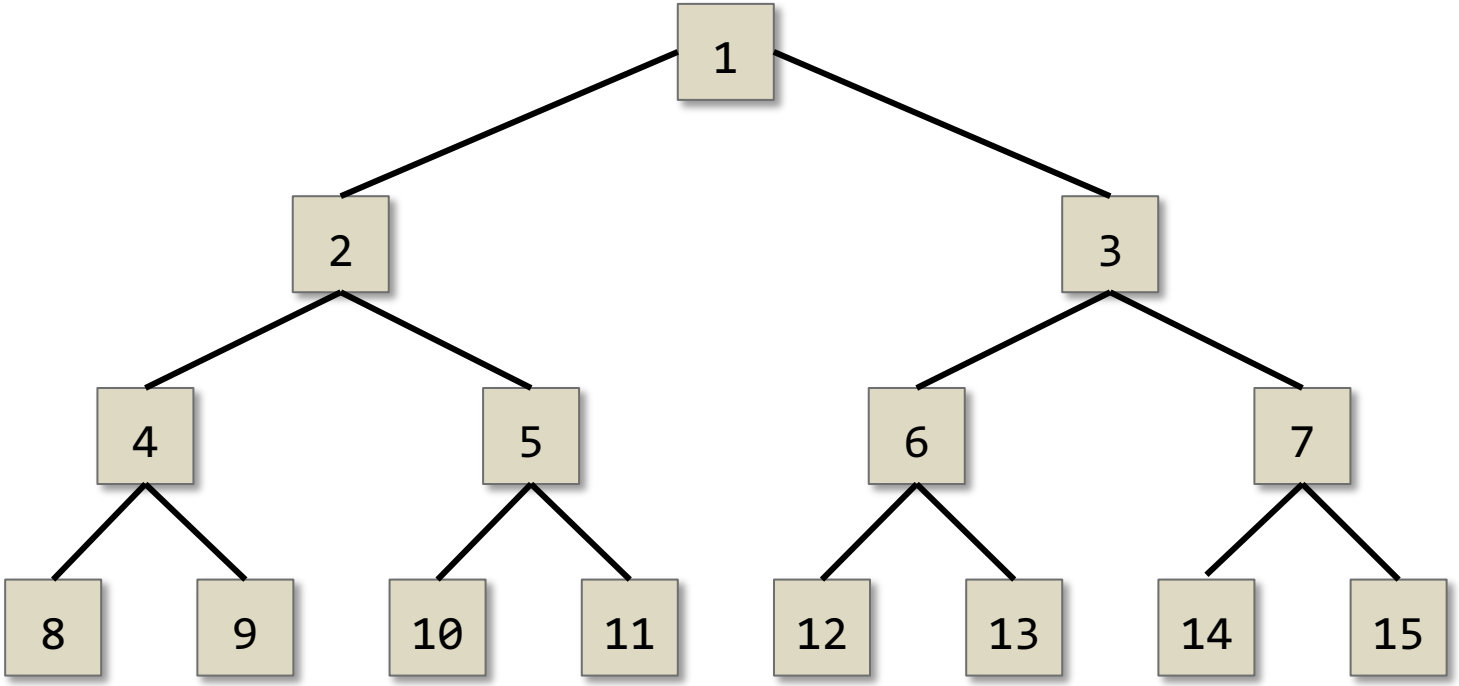
Same cache misses as with tiling!

$$Q(n) = \Theta(n^3/\mathcal{B}\mathcal{M}^{1/2})$$

Cache-Oblivious Algorithms

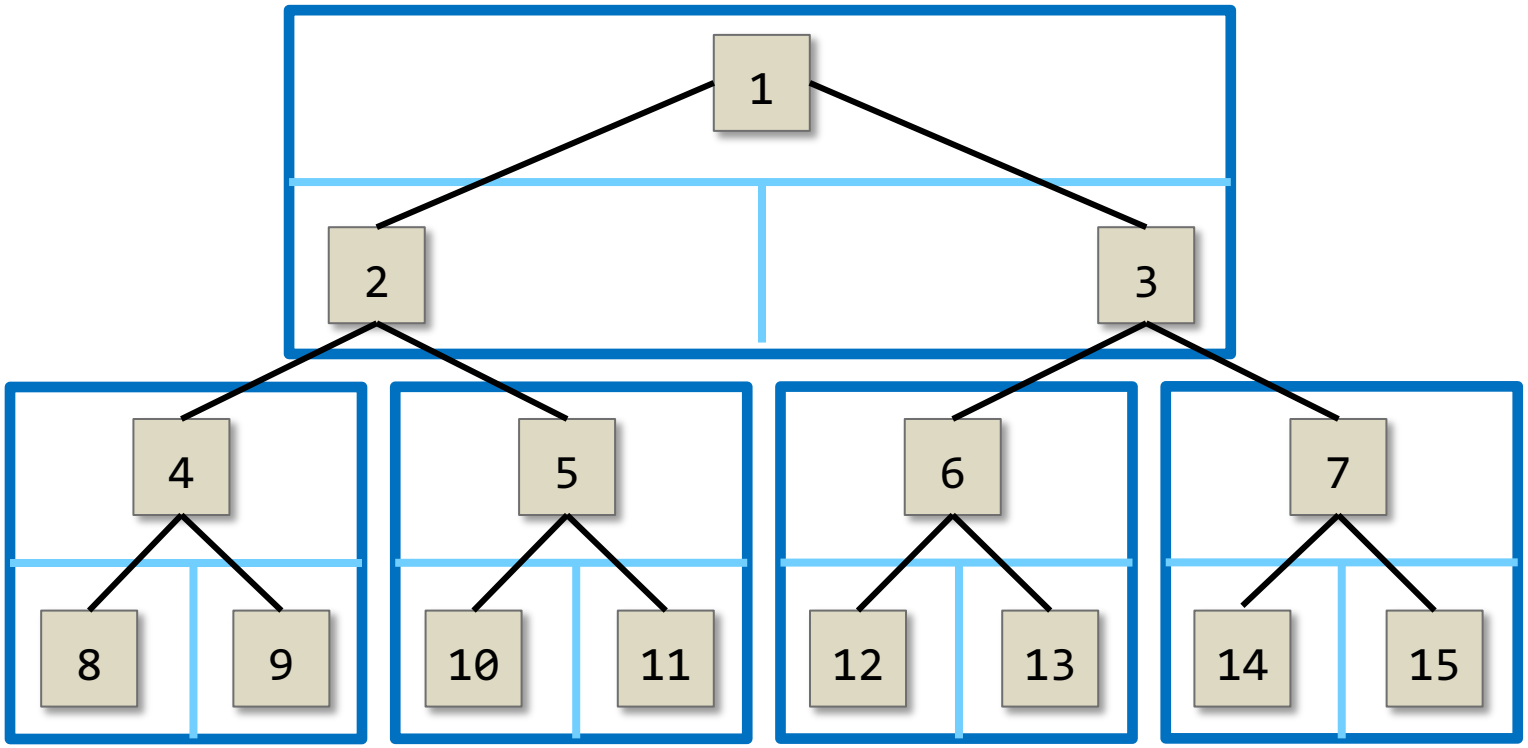
- **Cache-oblivious algorithms** [FLPR99]
- No voodoo tuning parameters.
- No explicit knowledge of caches.
- Passively autotune.
- Handle multilevel caches automatically.
- Good in multitenancy environments.

Cache-Aware Search Tree (Static)



Cache misses: $Q(n) = \Theta(\lg n)$

Cache-Oblivious Search Tree (Static)



1	2	3	4	8	9	5	10	12	6	12	13	7	14	15

Cache misses: $Q(n) = \Theta(\log_{\mathcal{B}} n)$

Other C–O Algorithms

Matrix Transposition/Addition $\Theta(1+mn/\mathcal{B})$

Straightforward recursive algorithm.

Strassen's Algorithm $\Theta(n + n^2/\mathcal{B} + n^{\lg 7}/\mathcal{B}\mathcal{M}^{(\lg 7)/2 - 1})$

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

Recursive algorithm due to Sivan Toledo [T97].

C-O Data Structures

Ordered-File Maintenance

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

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

B-Trees

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

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

Priority Queues

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

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

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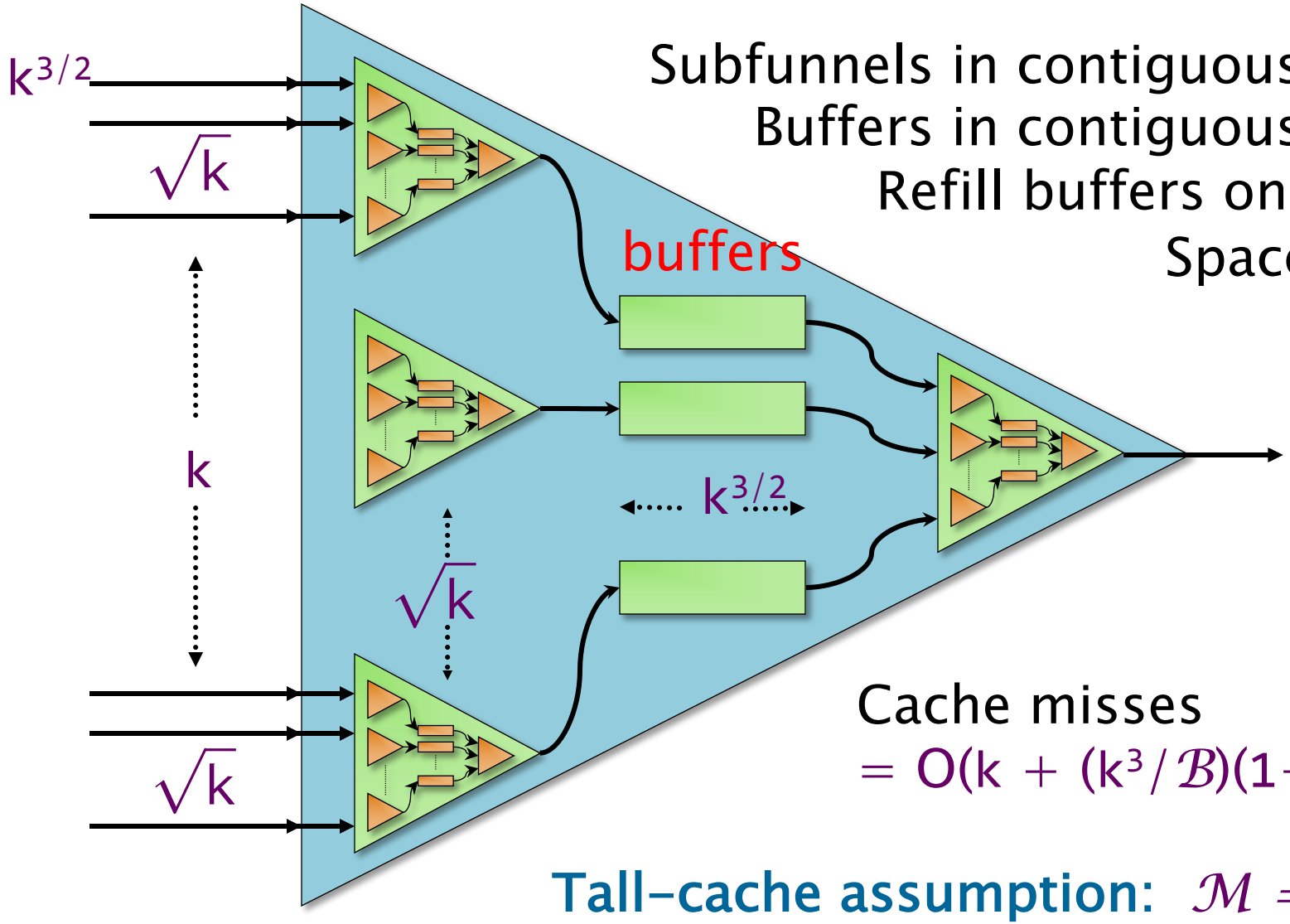
Construction of a k-funnel



Subfunnels in contiguous storage.
Buffers in contiguous storage.
Refill buffers on demand.
Space $= O(k^2)$.

Cache misses
$= O(k + (k^3/\mathcal{B})(1+\log_{\mathcal{M}} k))$.

Tall-cache assumption: $\mathcal{M} = \Omega(\mathcal{B}^2)$.