6.172 Performance Engineering of Software Systems

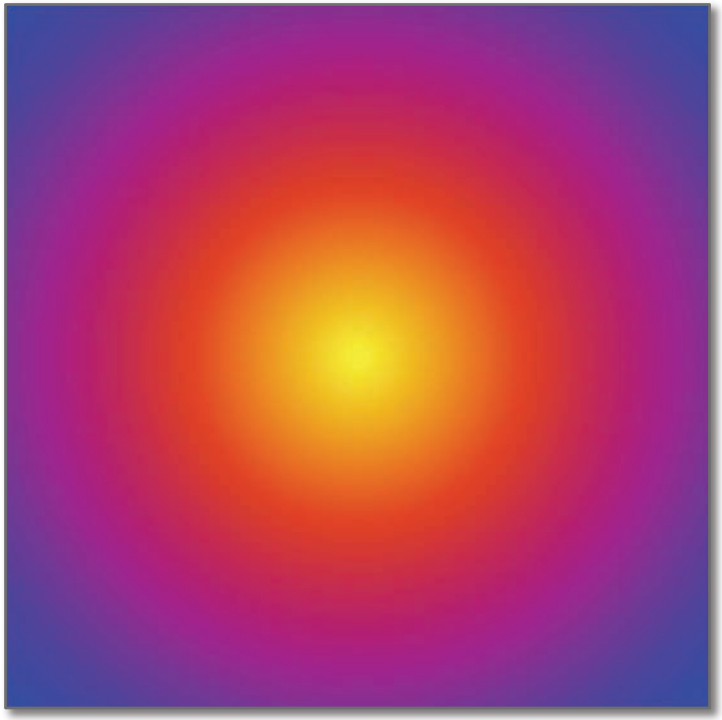
LECTURE 15

Cache-Oblivious Algorithms

Julian Shun

Simulation of Heat Diffusion

Heat Diffusion



2D heat equation

Let `u(t, x, y)` = temperature at time `t` of point `(x, y)`.

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} \quad \frac{\partial^2 u}{\partial y^2} \right.$$

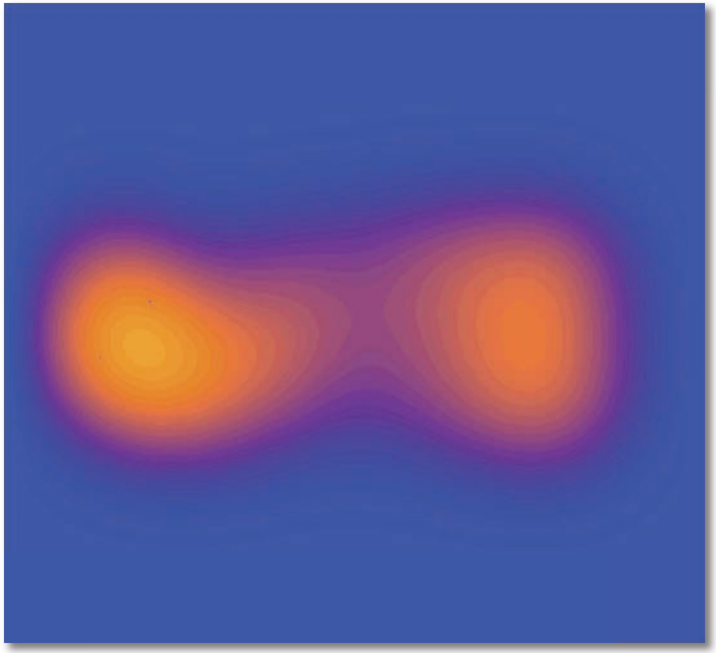
α is the *thermal diffusivity*.

Acknowledgment

Some of the slides in this presentation were inspired by originals due to Matteo Frigo.

2D Heat-Diffusion Simulation

Before



After

1D Heat Equation

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

Finite-Difference Approximation

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

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

$$\frac{\partial}{\partial x} u\ t\ \ x\ ) \approx \frac{u\ t\ \ x\ +\Delta x/2\ ) - u\ t\ \ x - \Delta x/2}{\Delta x},$$

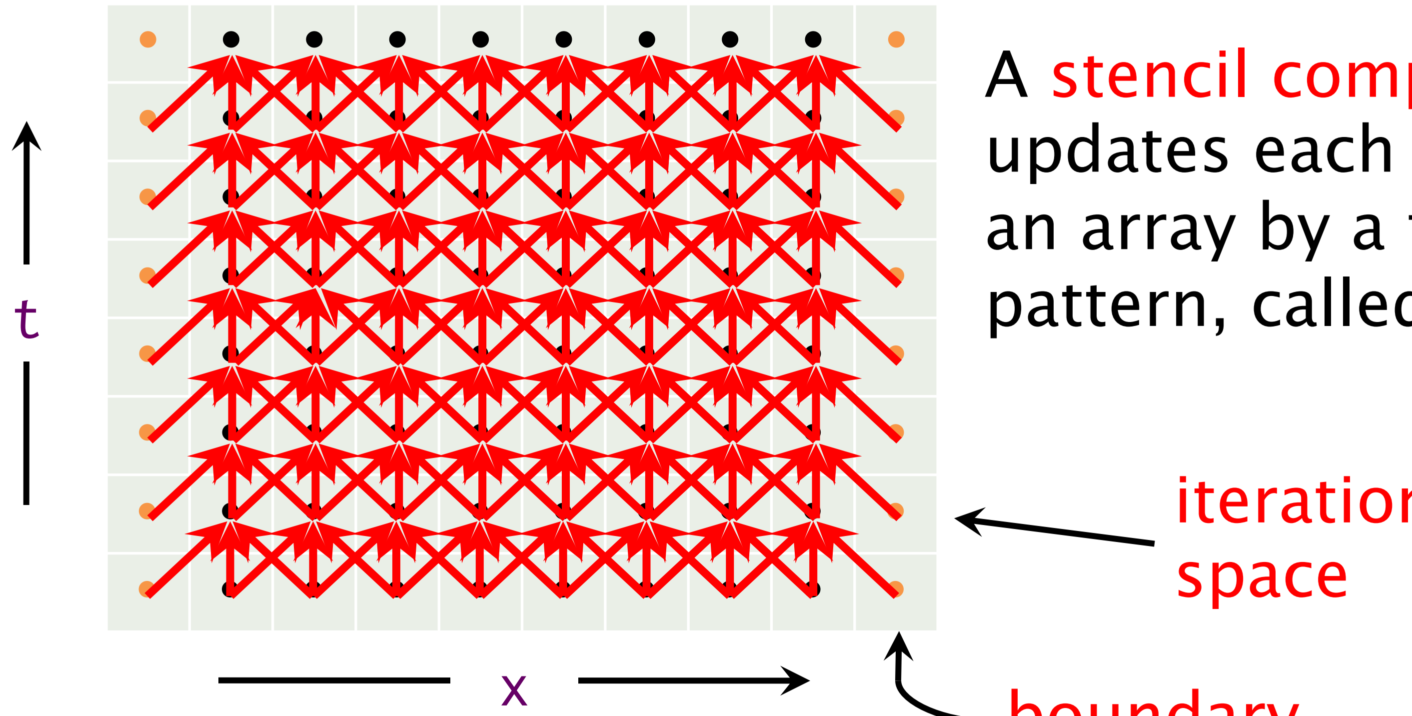
$$\frac{\partial^2}{\partial x^2} u\ t\ \ x \quad \approx \quad \frac{\frac{\partial}{\partial x} u\ t\ \ x\ +\Delta x/2\ ) - \frac{\partial}{\partial x} u\ t\ \ x - \Delta x/2}{\Delta x}$$

The 1D heat equation thus reduces to

$$\frac{u\ t\ +\Delta t\ \ x\ ) - u\ t\ \ x}{\Delta t} = \alpha \left(\frac{u\ t\ \ x\ +\Delta x\ ) - 2u\ t\ \ x \quad u\ t\ \ x - \Delta x}{(\Delta x\ ^2} \right).$$

3-Point Stencil

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



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

Update rule

$\Delta t = 1,\ \Delta x = 1$

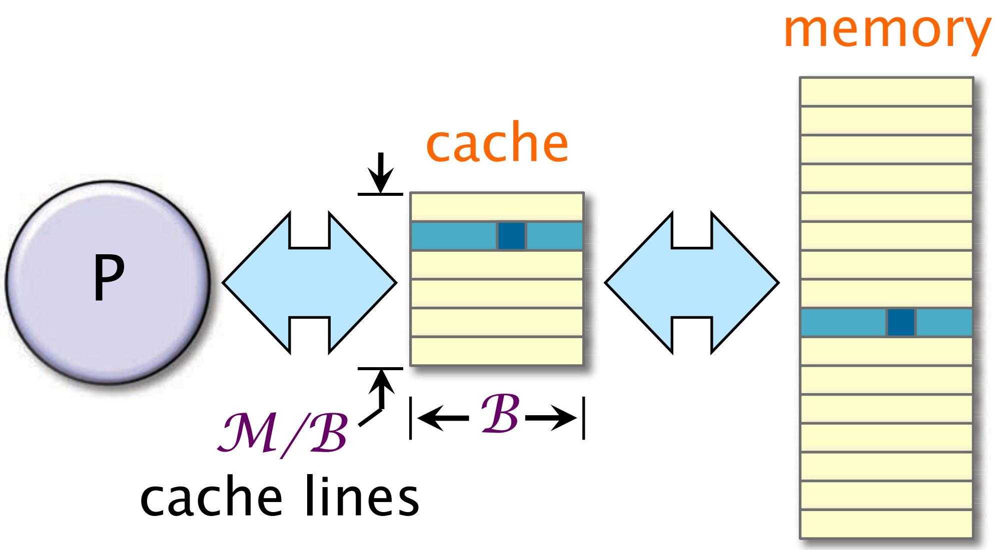
```
u[t+1][x] = u[t][x] + ALPHA
                * (u[t][x+1] - 2*u[t][x] + u[t][x-1]);
```

Cache-Oblivious Stencil Computations

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

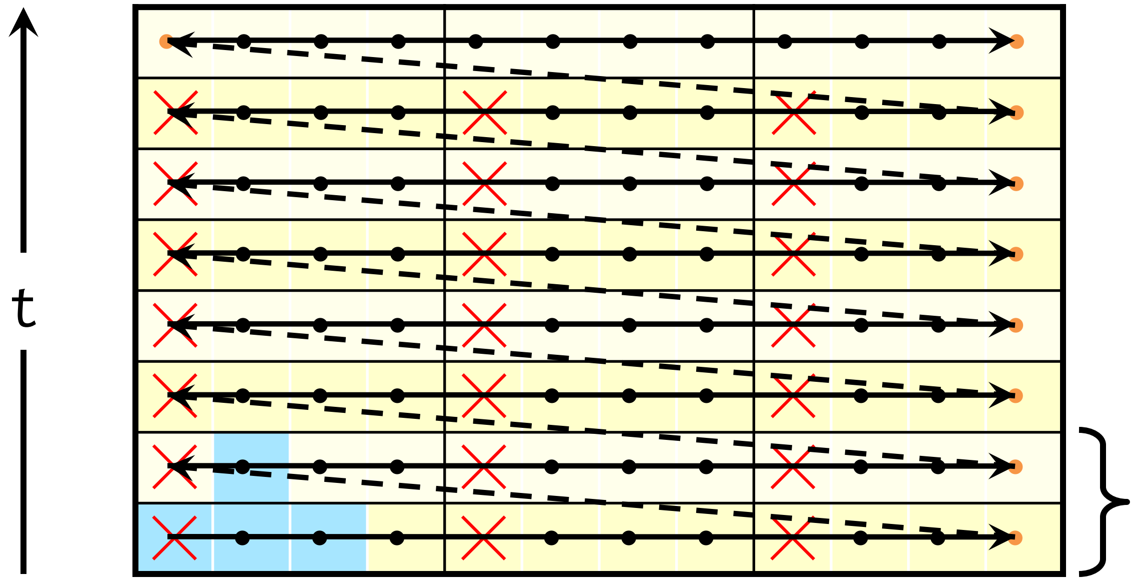
- work `W` (ordinary running time)
- cache misses `Q`

Cache Behavior of Looping

```
double u[2][N]; // even-odd trick

static inline double kernel(double * w) {
    return w[0] + ALPHA * (w[-1] - 2*w[0] + w[1]);
}

for (size_t t = 1; t < T-1; ++t) { // time loop
  for(size_t x = 1; x < N-1; ++x)  // space loop
    u[(t+1)%2][x] = kernel( &u[t%2][x] );
```

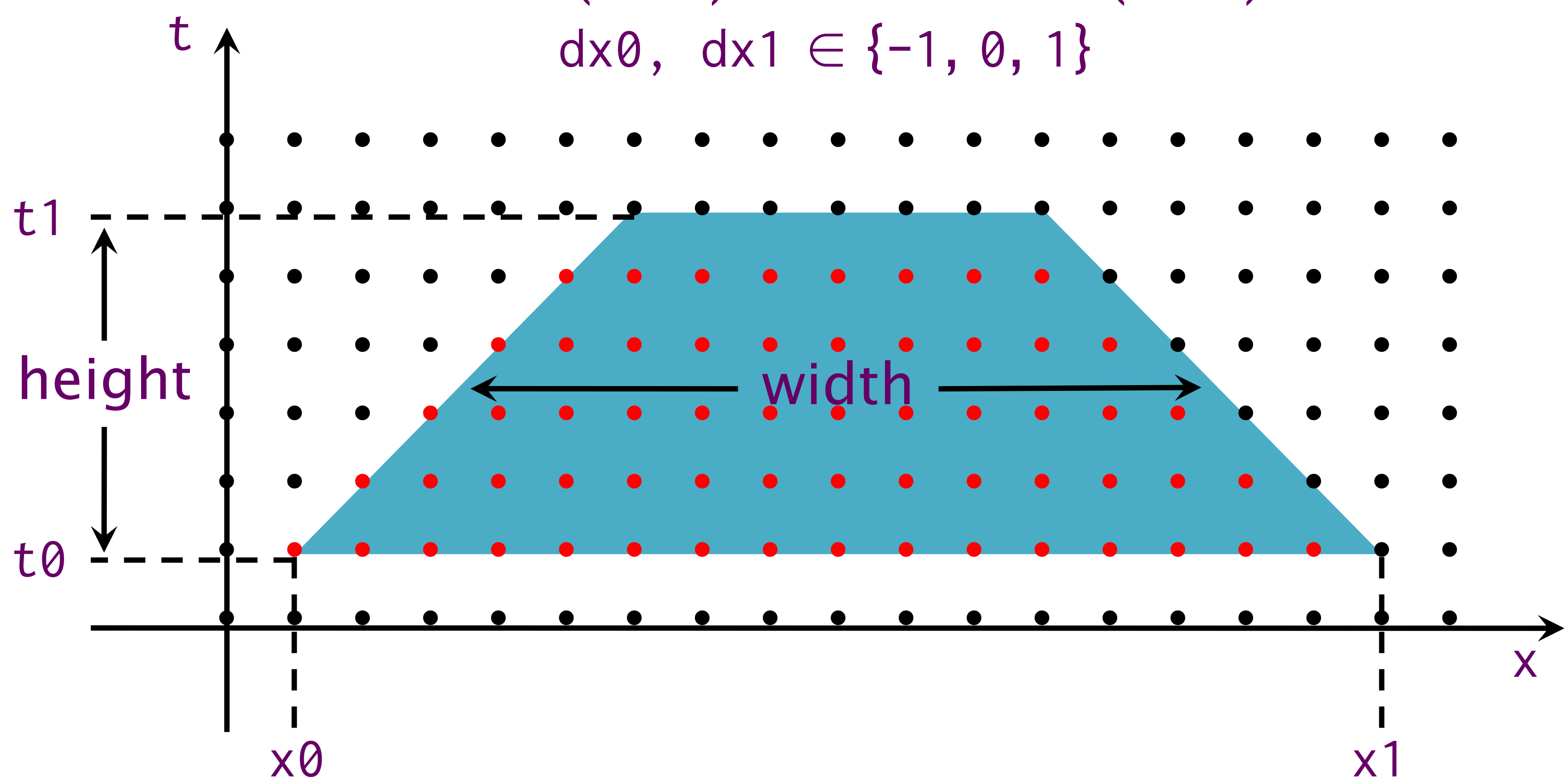


Assuming LRU, if $N > \mathcal{M}$, then $Q = \Theta(NT/\mathcal{B})$.

Cache-Oblivious 3-Point Stencil

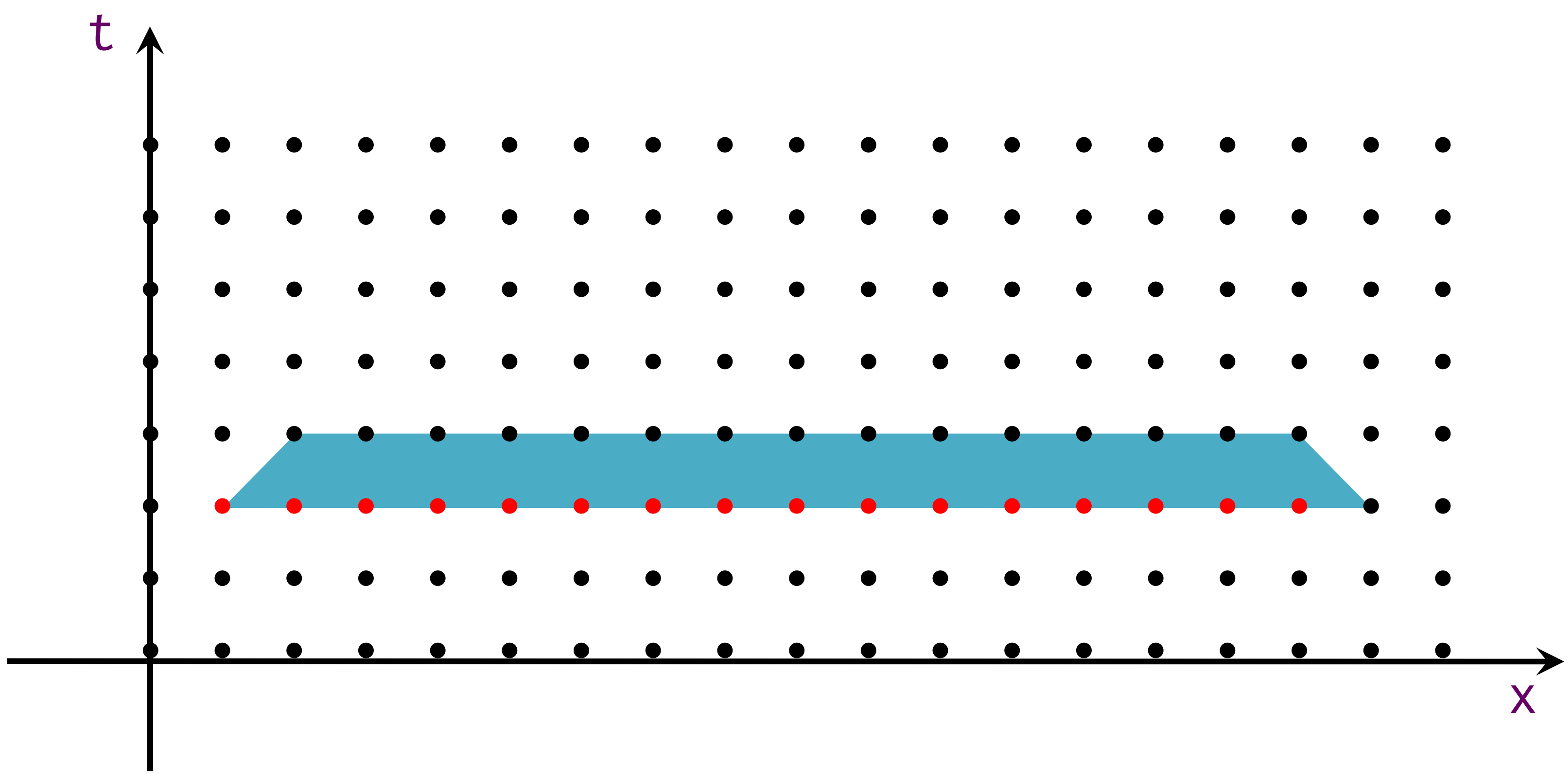
Recursively traverse trapezoidal regions of space-time points `(t,x)` such that

$$t0 \le t < t1$$
$$x0+dx0(t-t0) \le x < x1+dx1(t-t0)$$
$$dx0,\ dx1 \in \{-1,\ 0,\ 1\}$$



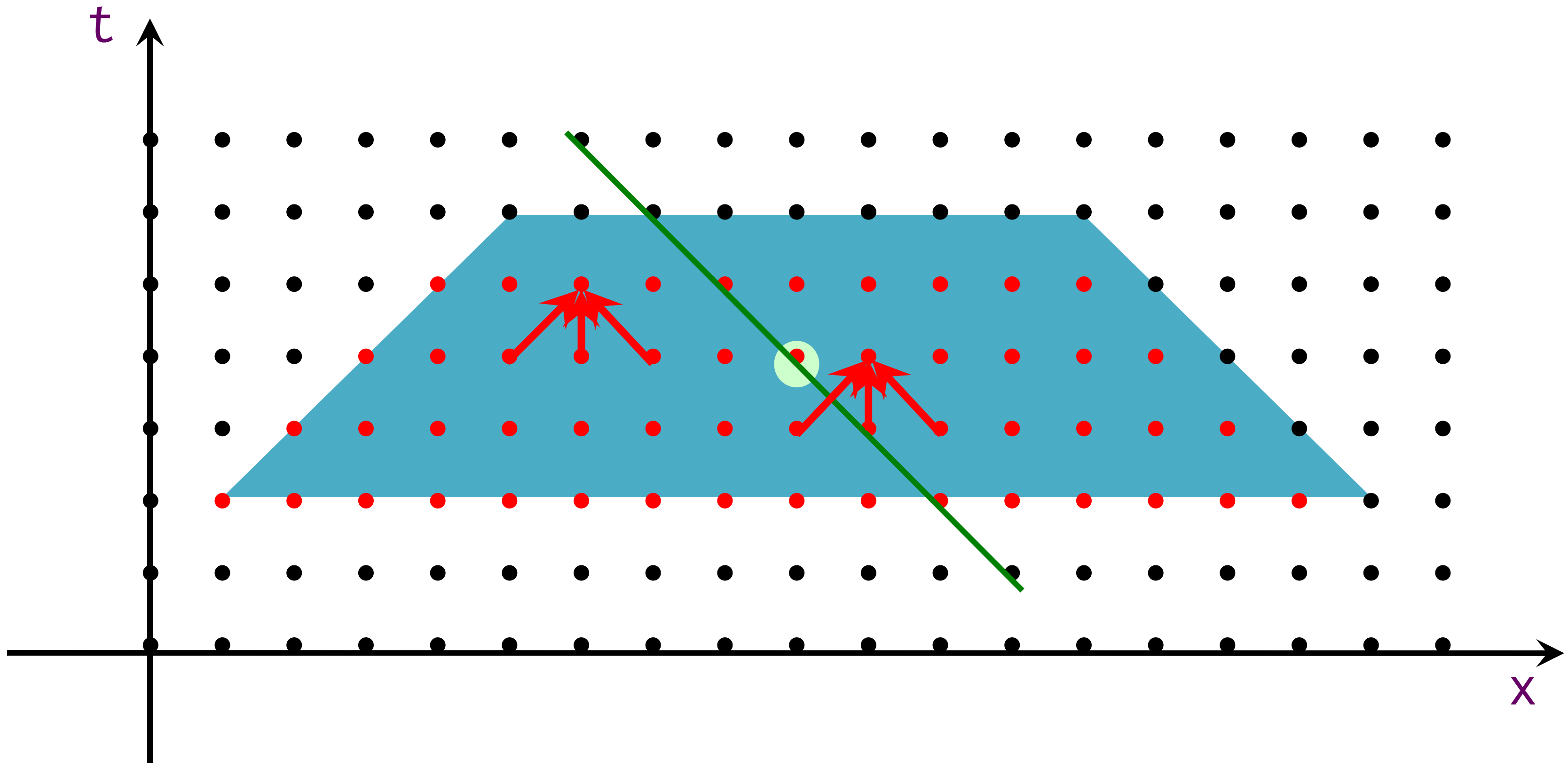
Base Case

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



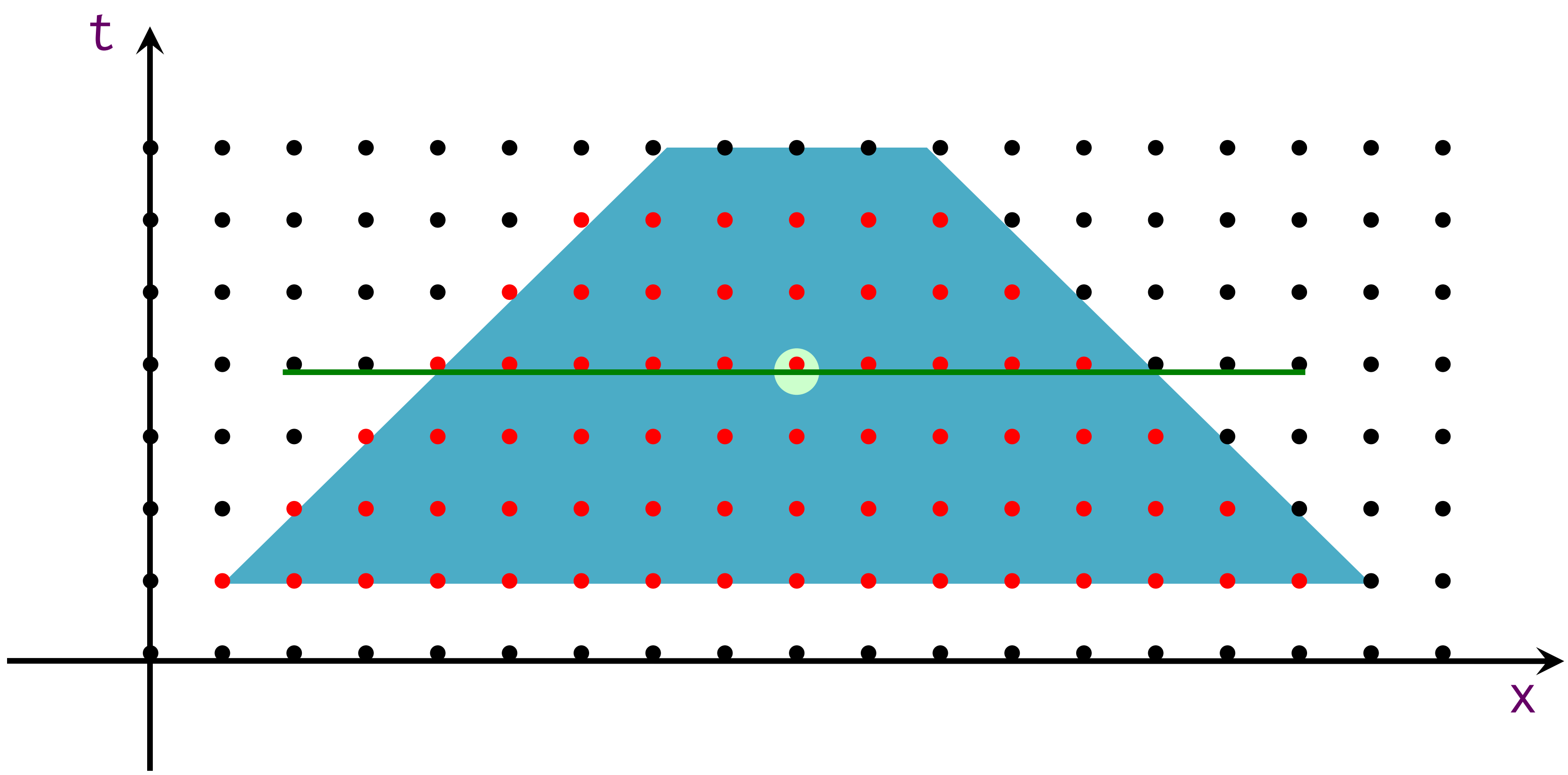
Space Cut

If width ≥ 2·height, cut the trapezoid with a line of slope −1 through the center. Traverse the trapezoid on the left first, and then the one on the right.



Time Cut

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

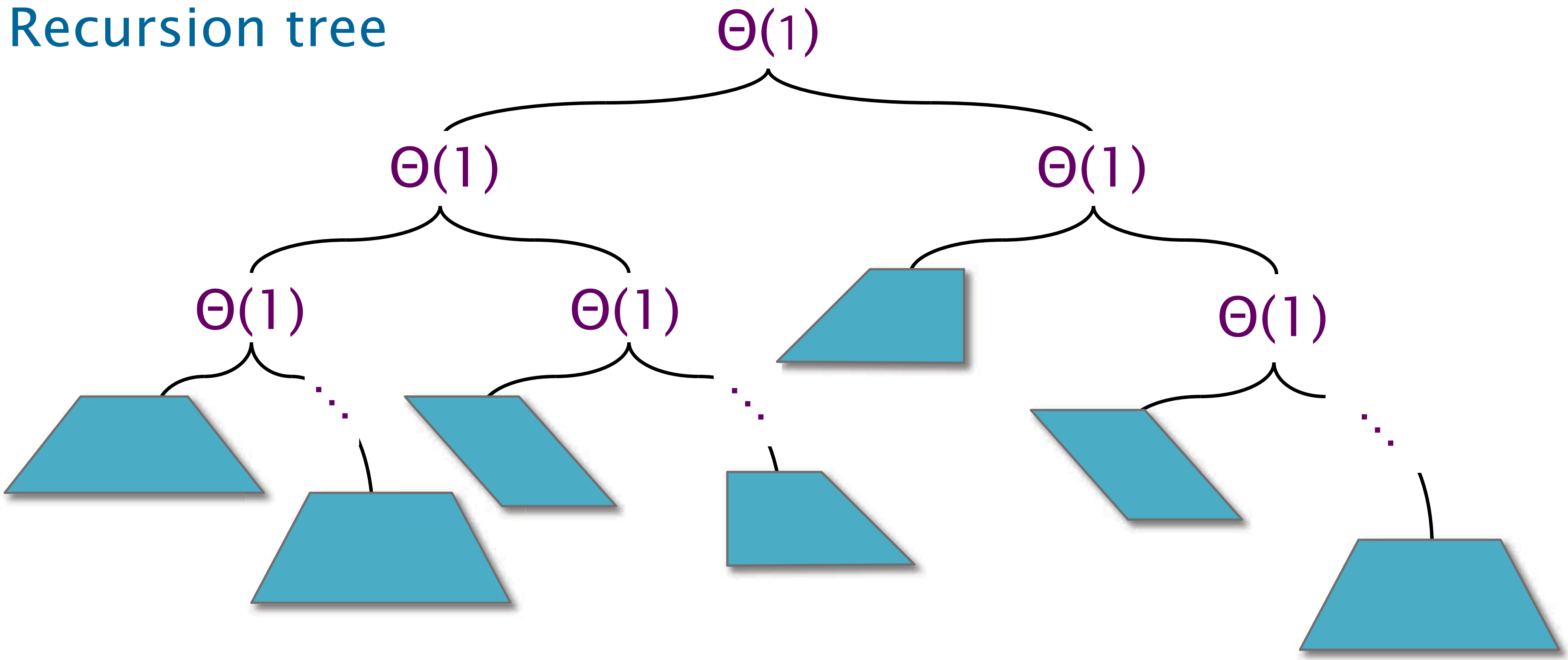


C Implementation

```
void trapezoid(int64_t t0, int64_t t1, int64_t x0, int64_t dx0,
               int64_t x1, int64_t dx1)
{
  int64_t lt = t1 - t0;
  if (lt == 1) { //base case
      for (int64_t x = x0; x < x1; x++)
        u[t1%2][x] = kernel( &u[t0%2][x] );
  } else if (lt > 1) {
    if (2 * (x1 - x0) + (dx1 - dx0) * lt >= 4 * lt) { //space cut
      int64_t xm = (2 * (x0 + x1) + (2 + dx0 + dx1) * lt) / 4;
      trapezoid(t0, t1, x0, dx0, xm, -1);
      trapezoid(t0, t1, xm, -1, x1, dx1);
    } else { //time cut
      int64_t halflt = lt / 2;
      trapezoid(t0, t0 + halflt, x0, dx0, x1, dx1);
      trapezoid(t0 + halflt, t1, x0 + dx0 * halflt, dx0,
                x1 + dx1 * halflt, dx1);
    }
  }
}
```

Cache Analysis

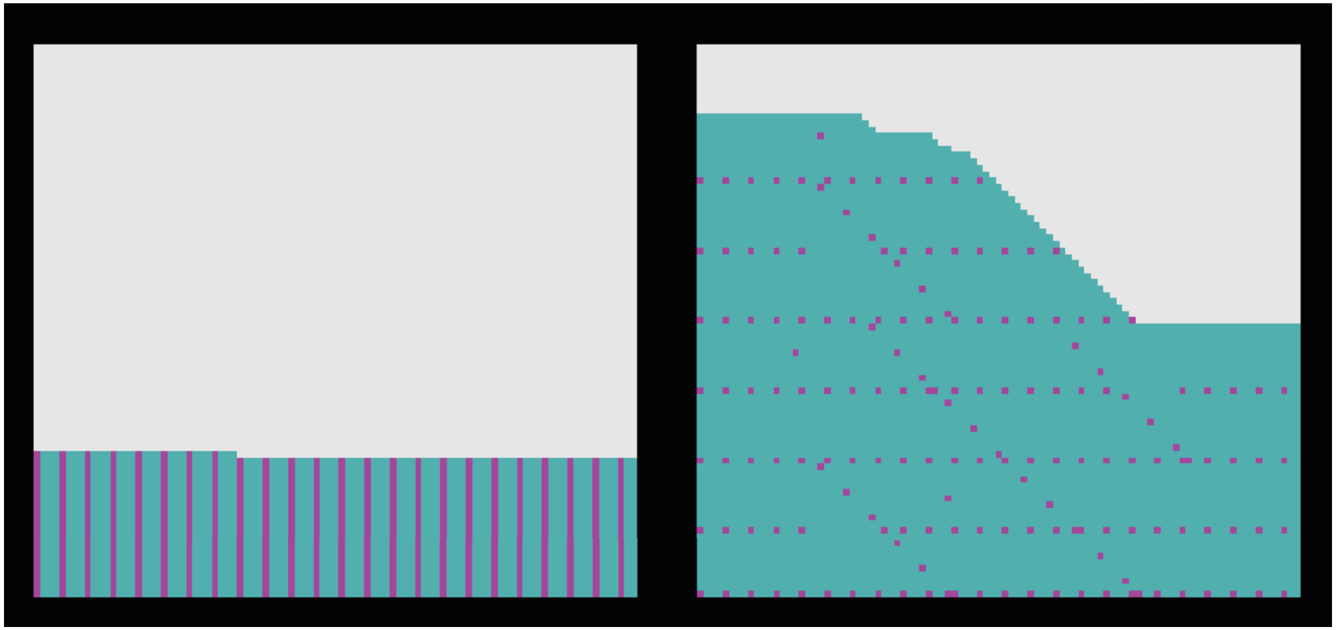
Recursion tree



- Each leaf represents $\Theta(hw)$ points, where $h = \Theta(w)$.
- Each leaf incurs $\Theta(w/\mathcal{B})$ misses, where $w = \Theta(\mathcal{M})$.
- $\Theta(NT/hw)$ leaves.
- #internal nodes = #leaves − 1 do not contribute substantially to Q.
- $Q = \Theta(NT/hw) \cdot \Theta(w/\mathcal{B}) = \Theta(NT/\mathcal{M}^2) \cdot \Theta(\mathcal{M}/\mathcal{B}) = \Theta(NT/\mathcal{M}\mathcal{B})$.
- For d dimensions, $Q = \Theta(NT/\mathcal{M}^{1/d}\mathcal{B})$

Simulation: 3-Point Stencil

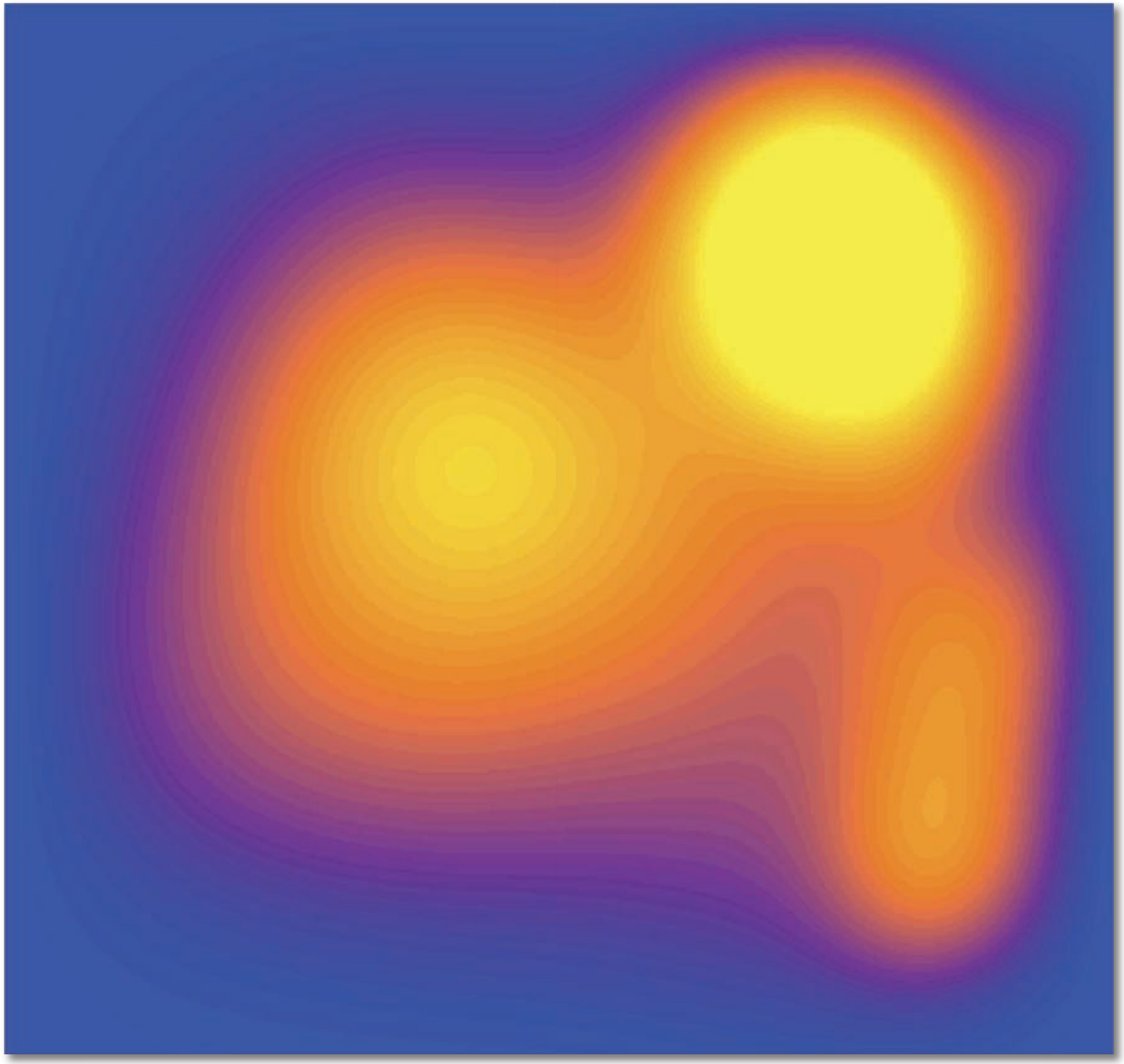
- Rectangular region
  - $N = 95$
  - $T = 87$



Looping Trapezoid

- Fully associative LRU cache
  - $\mathcal{B} = 4$ points
  - $\mathcal{M} = 32$ points
- Cache-hit latency $= 1$ cycle
- Cache-miss latency $= 10$ cycles

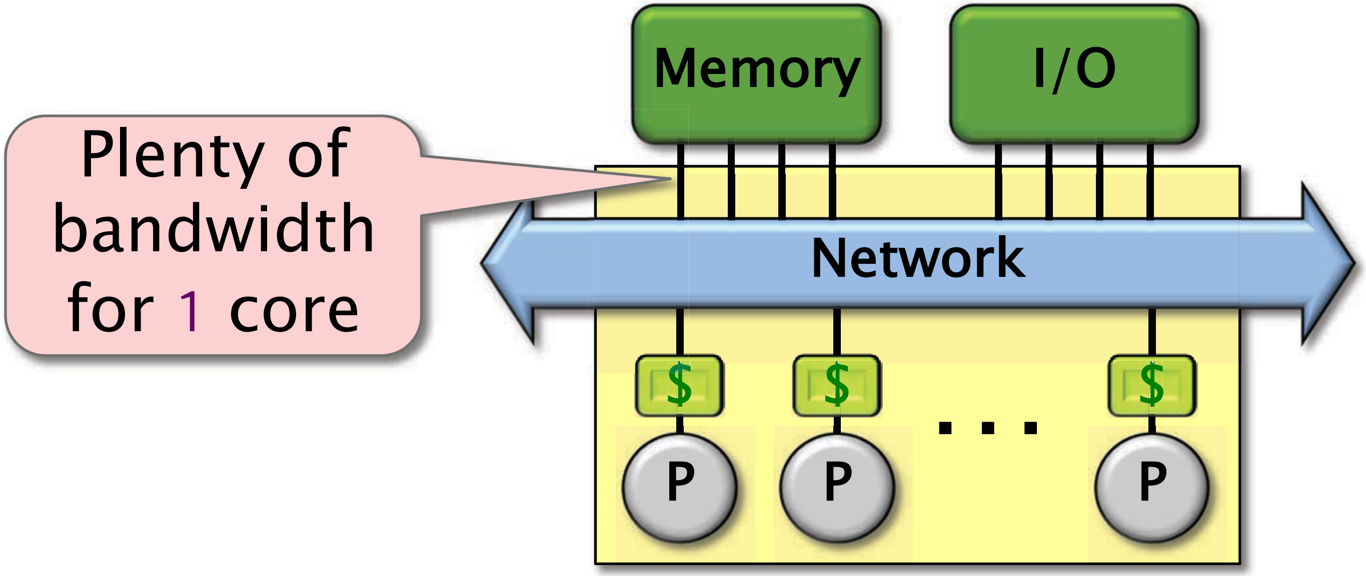
Looping v. Trapezoid on Heat



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. One core cannot saturate the memory bandwidth.



Caching and Parallelism

Cilk and Caching

Theorem. Let Q_P be the number of cache misses in a deterministic Cilk computation when run on P processors, each with a private cache, and let S_P be the number of successful steals during the computation. In the ideal-cache model, we have

$$Q_P = Q_1 + O(S_P \mathcal{M}/\mathcal{B}) \ ,$$

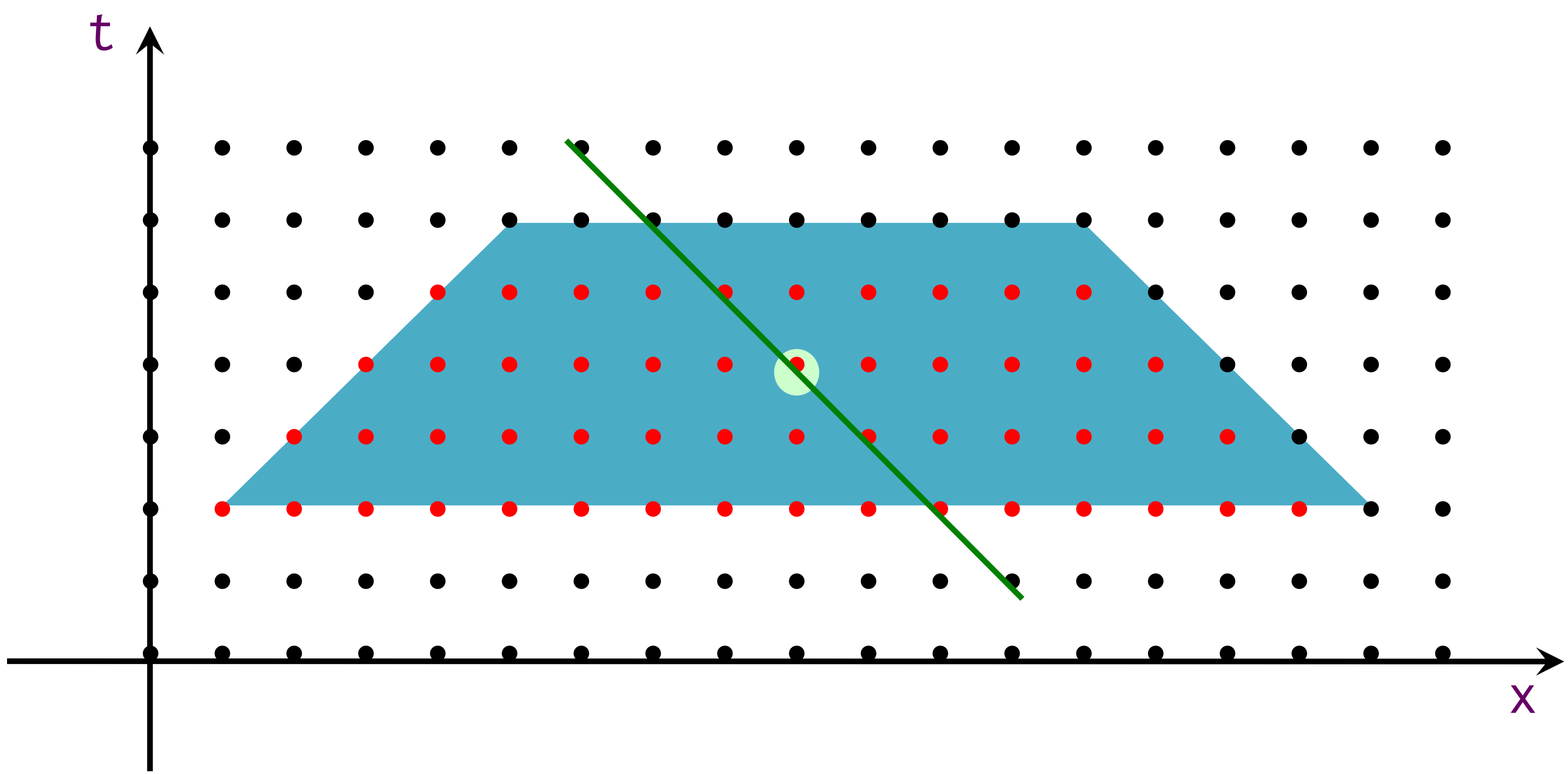
where $\mathcal{M}$ is the cache size and $\mathcal{B}$ is the size of a cache block.

Proof. After a worker steals a continuation, its cache is completely cold in the worst case. But after $\mathcal{M}/\mathcal{B}$ (cold) cache misses, its cache is identical to that in the serial execution. The same is true when a worker resumes a stolen subcomputation after a `cilk_sync`. The number of times these two situations can occur is at most $2S_P$. ■

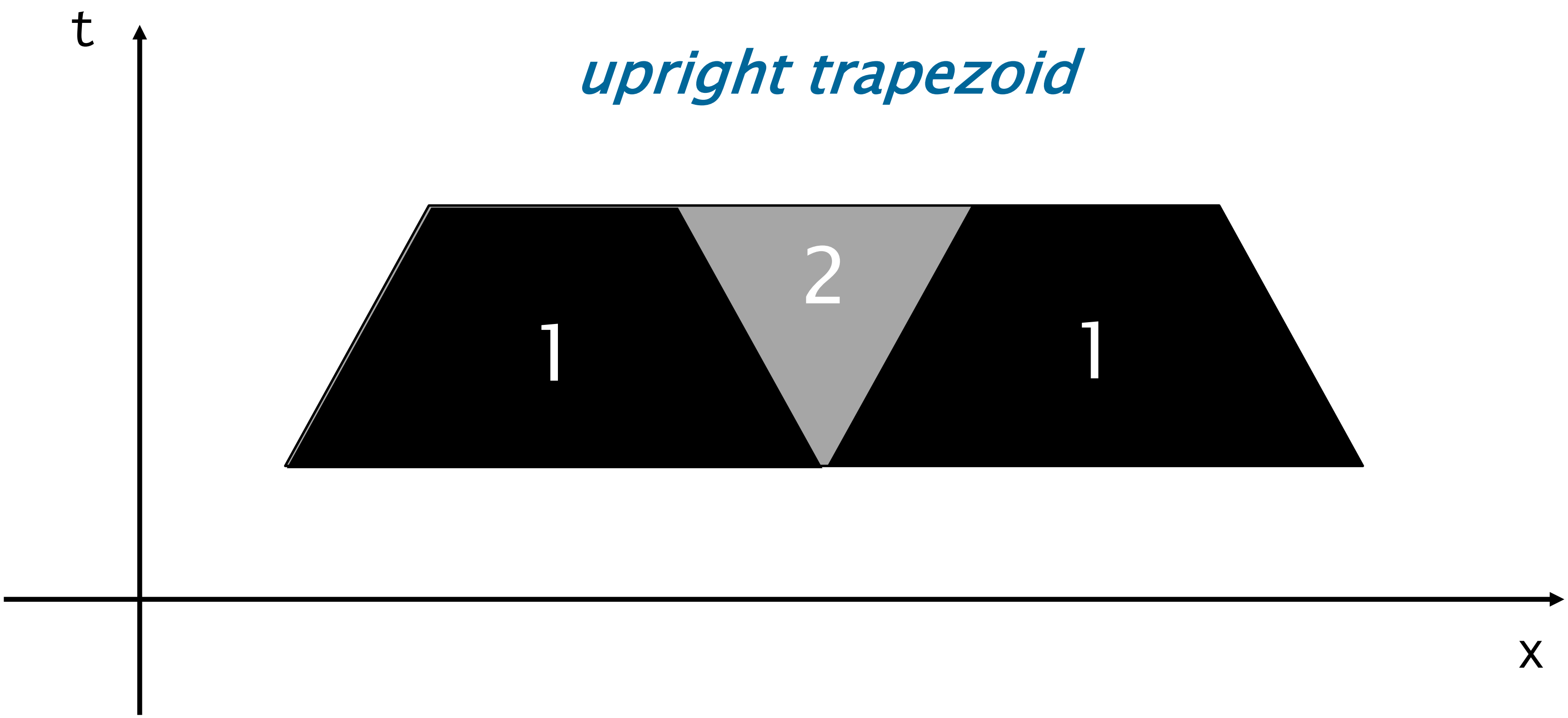
MORAL: Minimizing cache misses in the serial elision essentially minimizes them in parallel executions.

Does this work in parallel?

Space cut: If width ≥ 2·height, cut the trapezoid with a line of slope −1 through the center. Traverse the trapezoid on the left first, and then the one on the right.

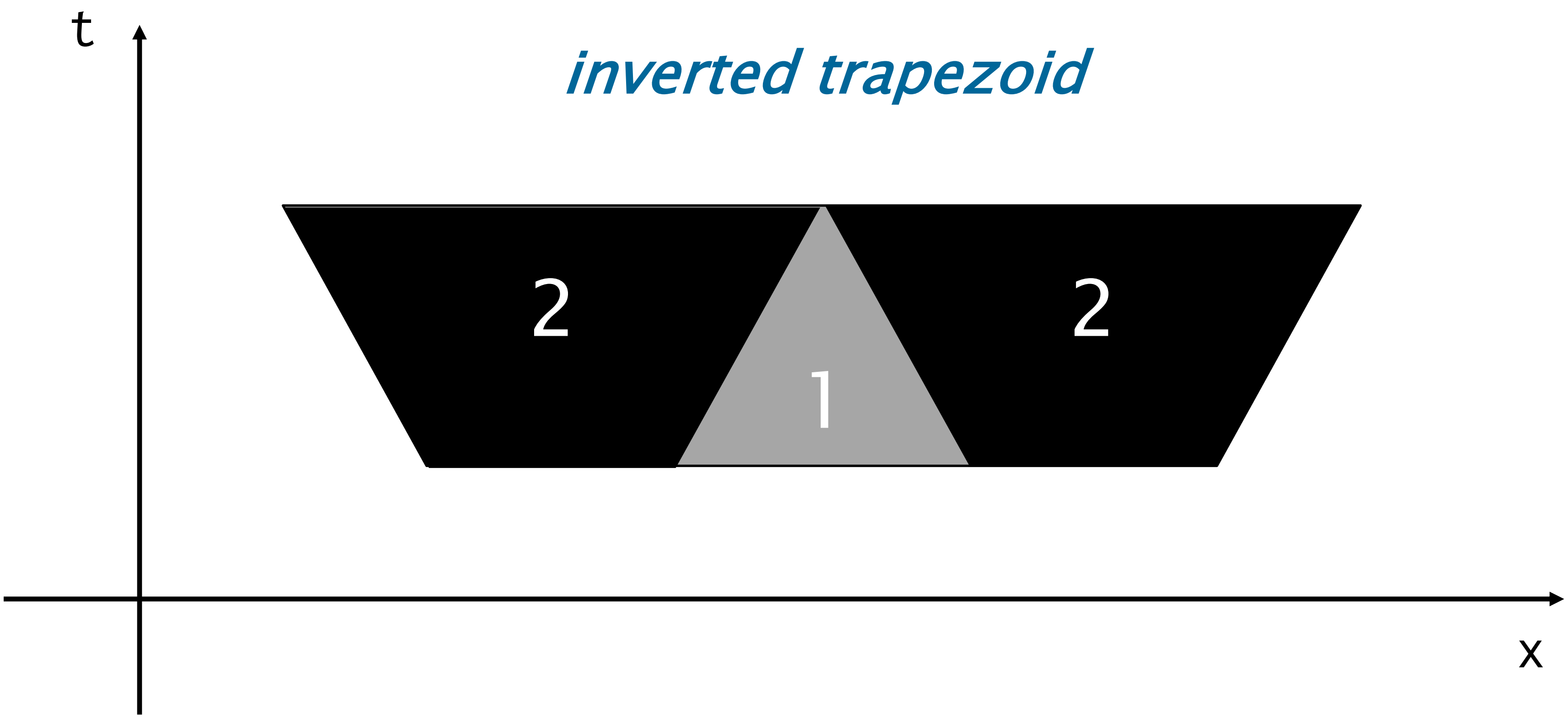


Parallel Space Cuts



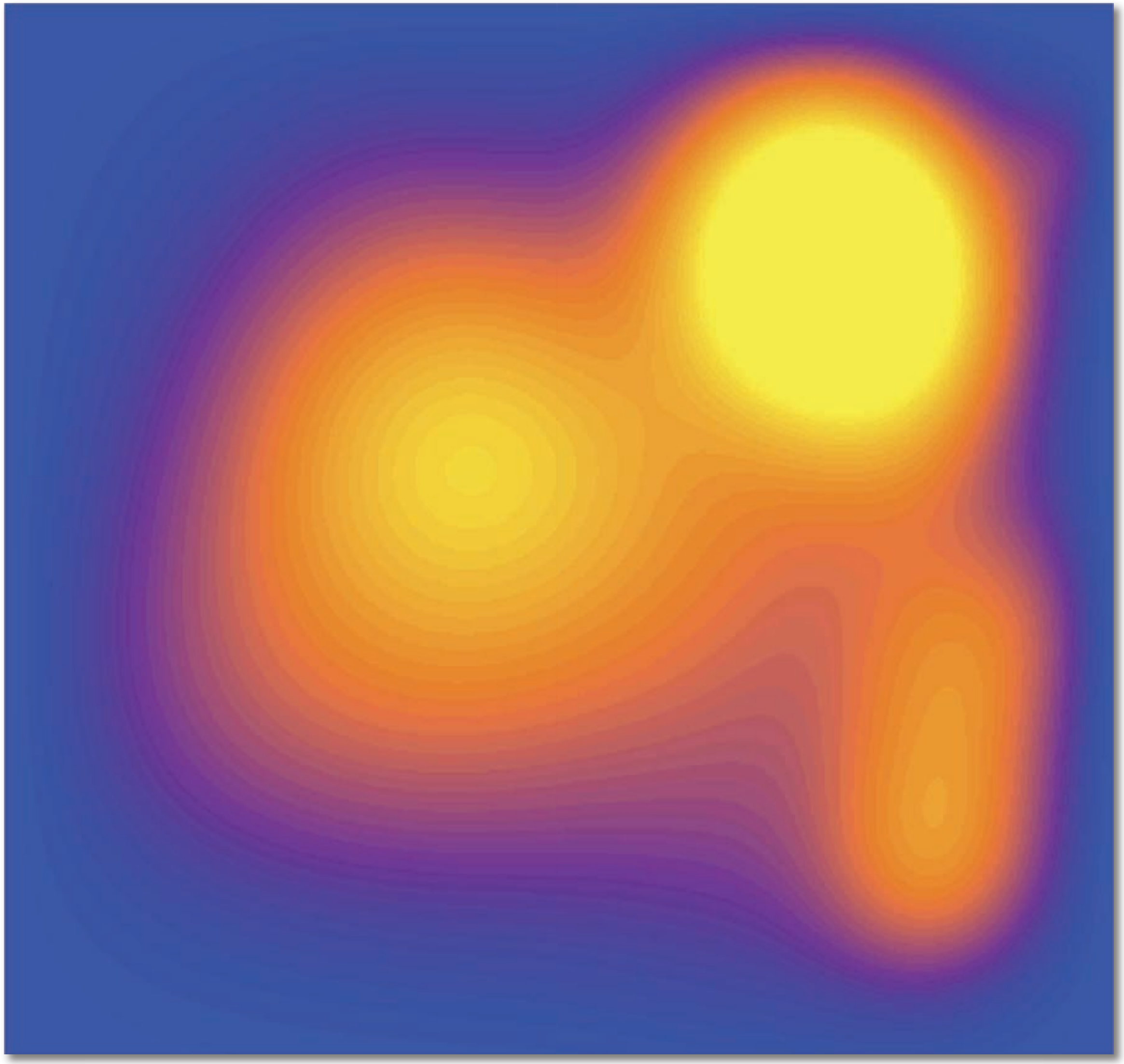
A *parallel space cut* produces two black trapezoids that can be executed in parallel and a third gray trapezoid that executes in series with the black trapezoids.

Parallel Space Cuts



A ***parallel space cut*** produces two black trapezoids that can be executed in parallel and a third gray trapezoid that executes in series with the black trapezoids.

Parallel Looping v. Parallel Trap.



Performance Comparison

Heat equation on a 3000×3000 grid for 1000 time steps (4 processor cores with 8MB LLC)

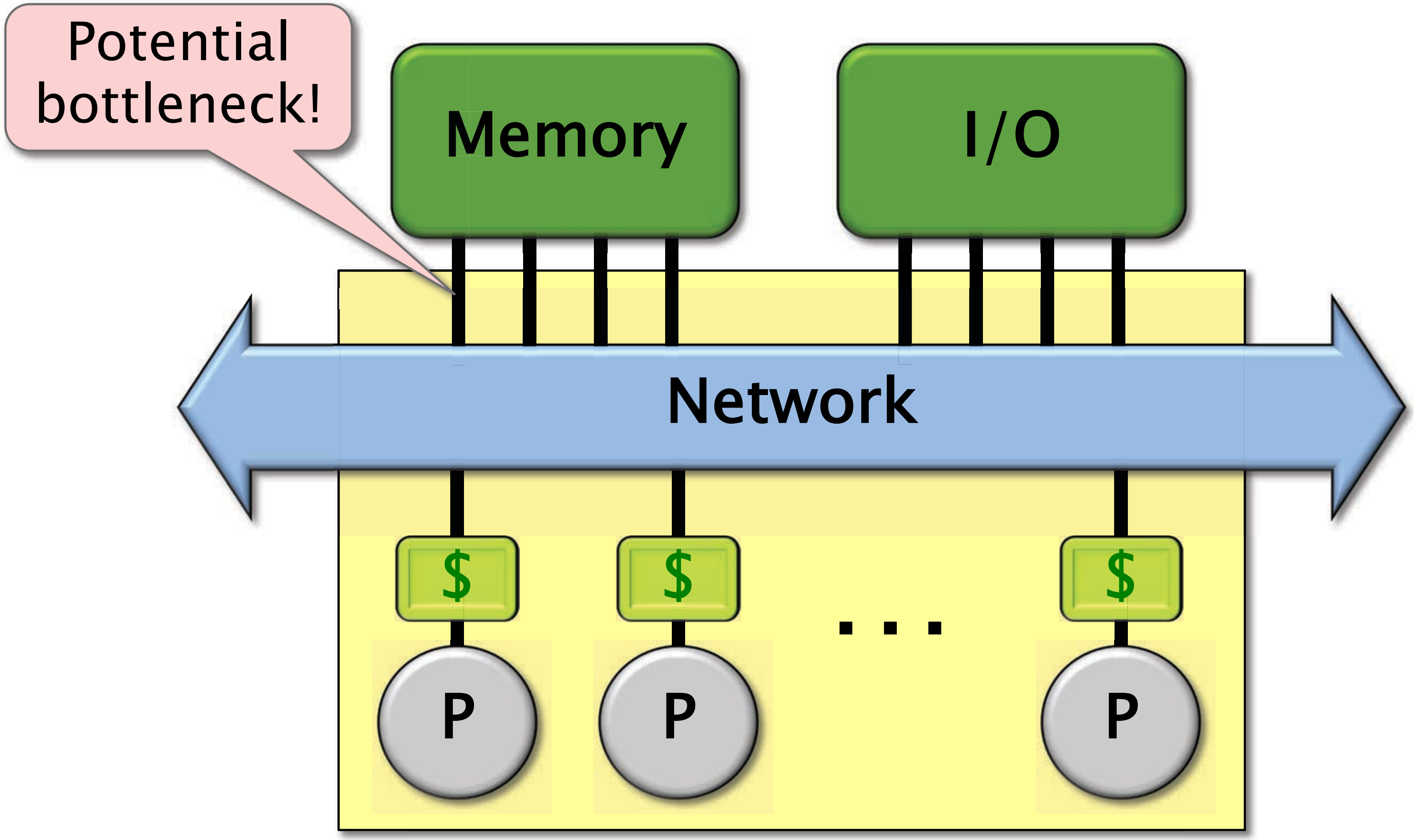
Code	Time
Serial looping	128.95s
Parallel looping	66.97s
Serial trapezoidal	66.76s
Parallel trapezoidal	16.86s

} 1.93x

} 3.96x

The parallel looping code achieves less than half the potential speedup, even though it has far more parallelism.

Memory Bandwidth



Impediments to Speedup

- ☑ Insufficient parallelism
- ☑ Scheduling overhead
- ☑ Lack of memory bandwidth
- ☑ Contention (locking and true/false sharing)

Cilkscale can diagnose the first two problems.

Q. How can we diagnose the third?

A. Run P identical copies of the serial code 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.

CACHE-OBLIVIOUS SORTING

OUTLINE

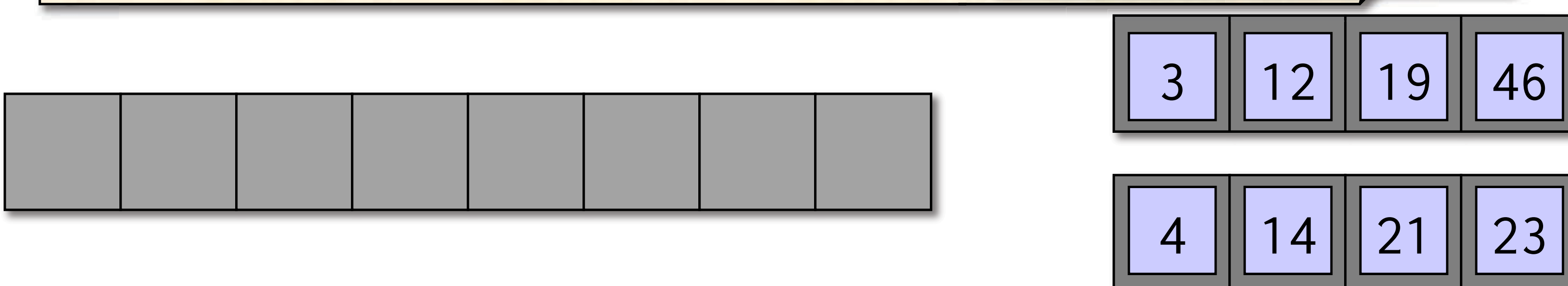
- Simulation of Heat Diffusion
- Cache-Oblivious Stencil Computations
- Caching and Parallelism
- Cache-Oblivious Sorting

Merging Two Sorted Arrays

```c
void merge(int64_t *C, int64_t *A, int64_t na,
           int64_t *B, int64_t nb) {
  while (na>0 && nb>0) {
    if (*A <= *B) {
      *C++ = *A++; na--;
    } else {
      *C++ = *B++; nb--;
    }
  }
  while (na>0) {
    *C++ = *A++; na--;
  }
  while (nb>0) {
    *C++ = *B++; nb--;
  }
}
```

Time to merge n elements = $\Theta(n)$.

Number of cache misses = $\Theta(n/B)$.



Merge Sort

```
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);
  }
}
```

19	3	12	46	33	4	21	14

Merge Sort

```
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);
  }
}
```

19	3	12	46	33	4	21	14

Merge Sort

```
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);
  }
}
```

19 3	12 46	33 4	21 14

Merge Sort

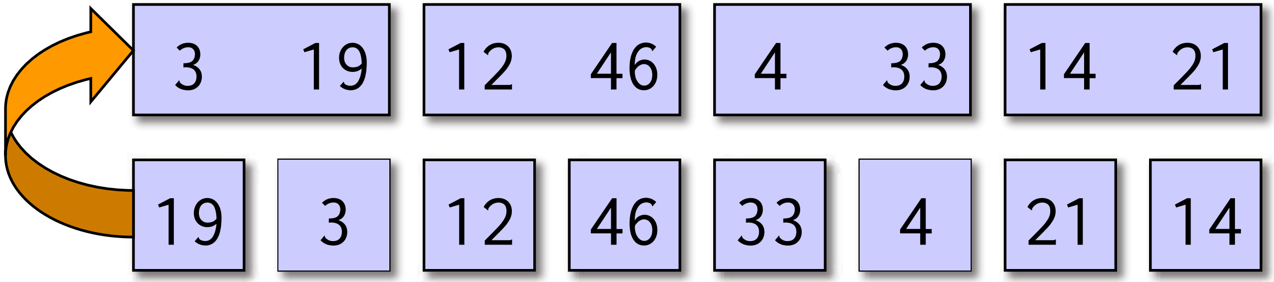
```
void merge_sort(int64_t *B, int64_t *A, int64_t n) {
  if (n==1) {
    B[0] = A[0];
  } else {
    int64_t C[n];
    cilk_spawn merge_sort(C, A, n/2);
               merge_sort(C+n/2, A+n/2, n-n/2);
    cilk_sync;
    merge(B, C, n/2, C+n/2, n-n/2);
  }
}
```

19	3	12	46	33	4	21	14

Merge Sort

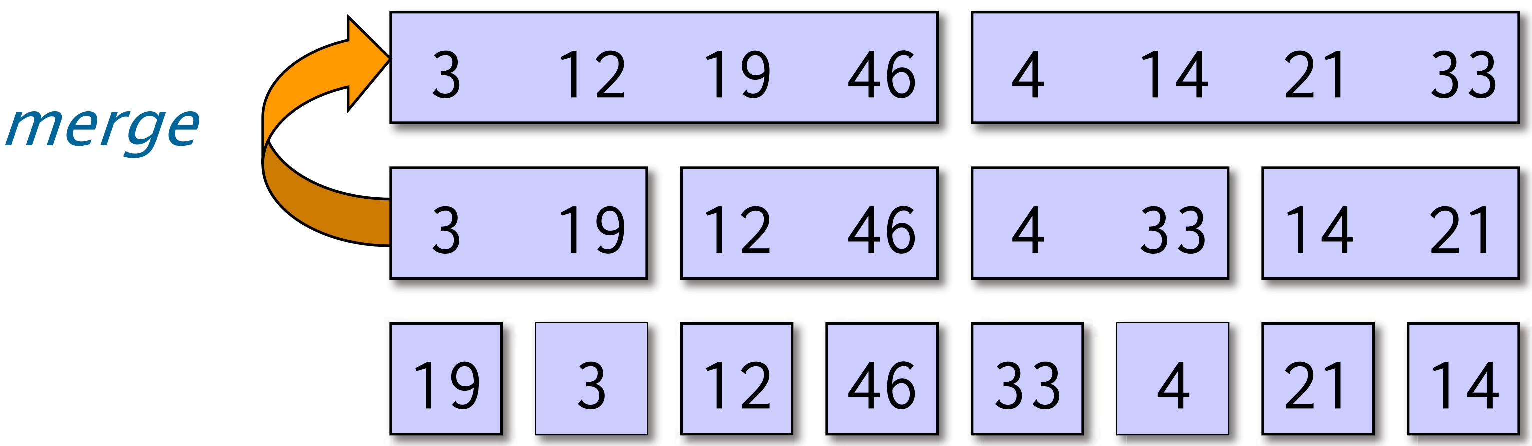
```
void merge_sort(int64_t *B, int64_t *A, int64_t n) {
  if (n==1) {
    B[0] = A[0];
  } else {
    int64_t C[n];
    cilk_spawn merge_sort(C, A, n/2);
               merge_sort(C+n/2, A+n/2, n-n/2);
    cilk_sync;
    merge(B, C, n/2, C+n/2, n-n/2);
  }
}
```

merge



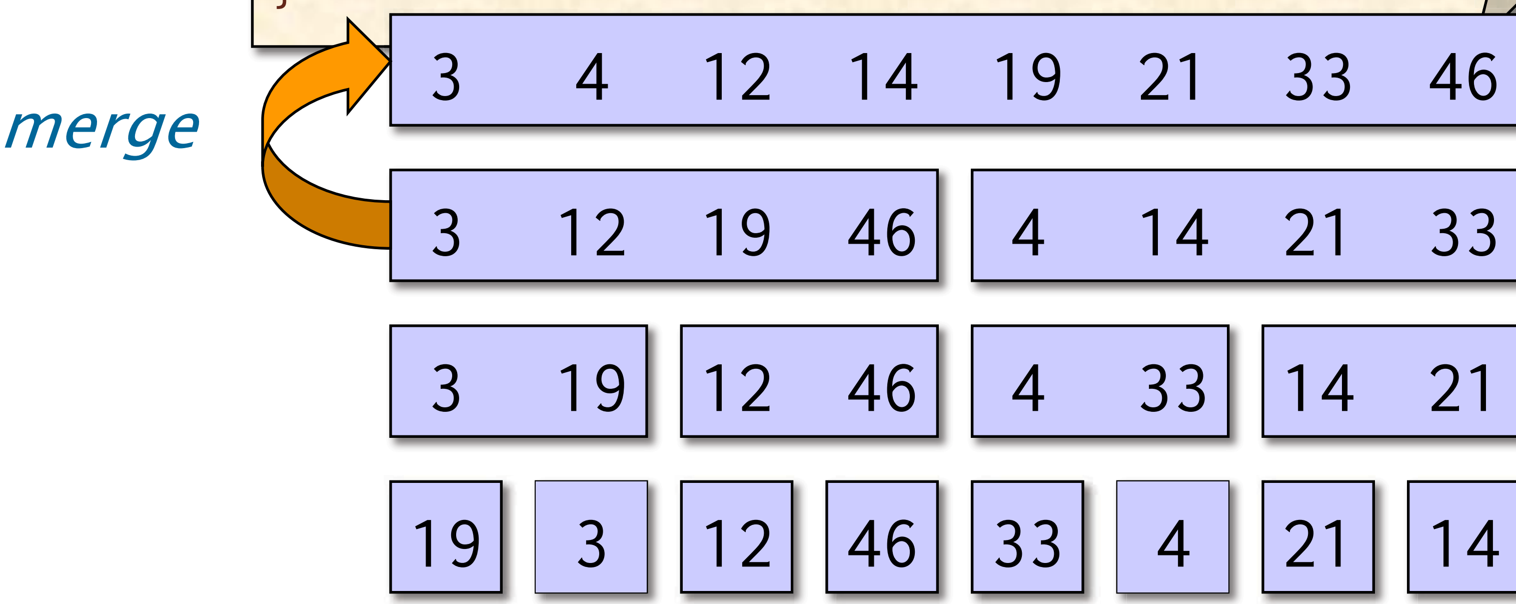
Merge Sort

```
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);
  }
}
```



Merge Sort

```c
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);
  }
}
```



Work of Merge Sort

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

CASE 2

$n^{\log_b a} = n^{\log_2 2} = n$

$f(n) = \Theta(n^{\log_b a} \lg^0 n)$

Work: $W(n) = 2W(n/2) + \Theta(n)$

$= \Theta(n \lg n)$

Recursion Tree

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

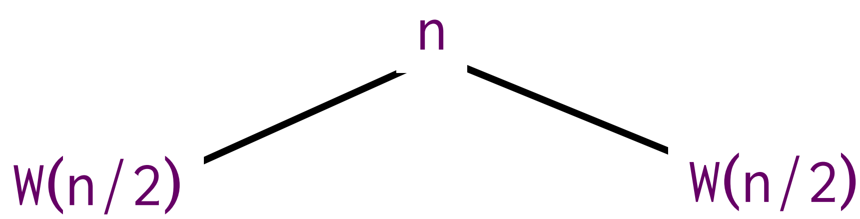
Recursion Tree

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

$$W(n)$$

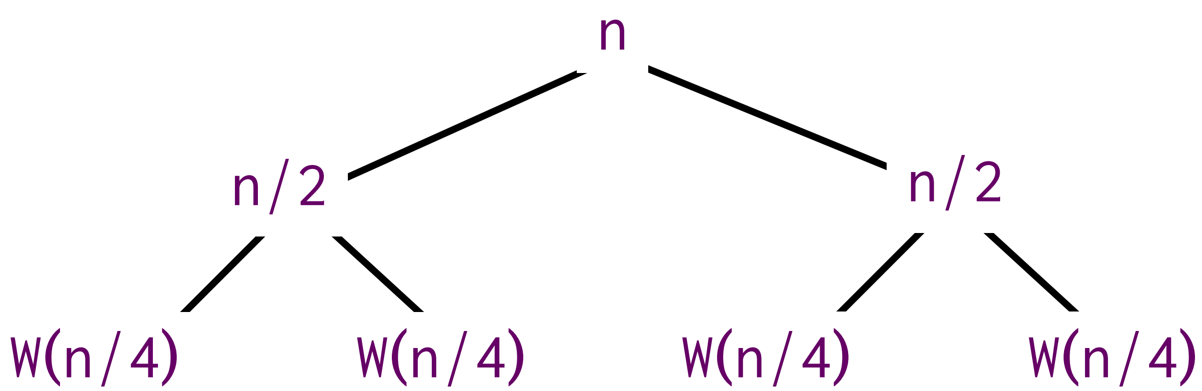
Recursion Tree

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



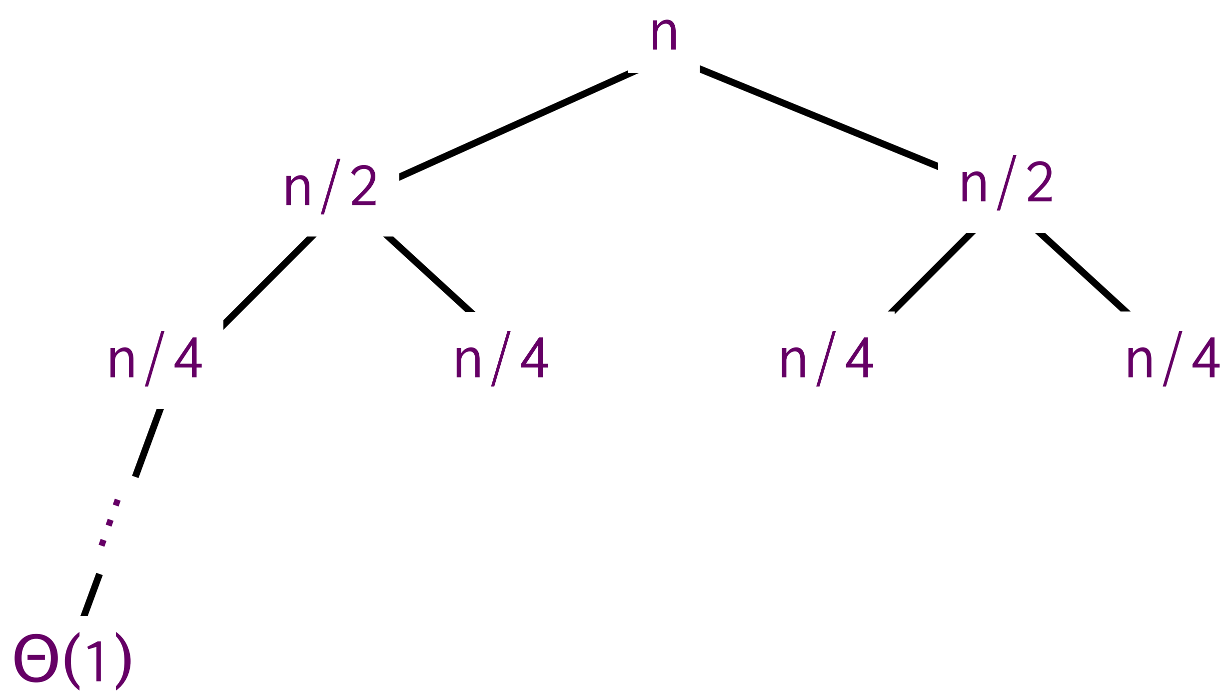
Recursion Tree

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



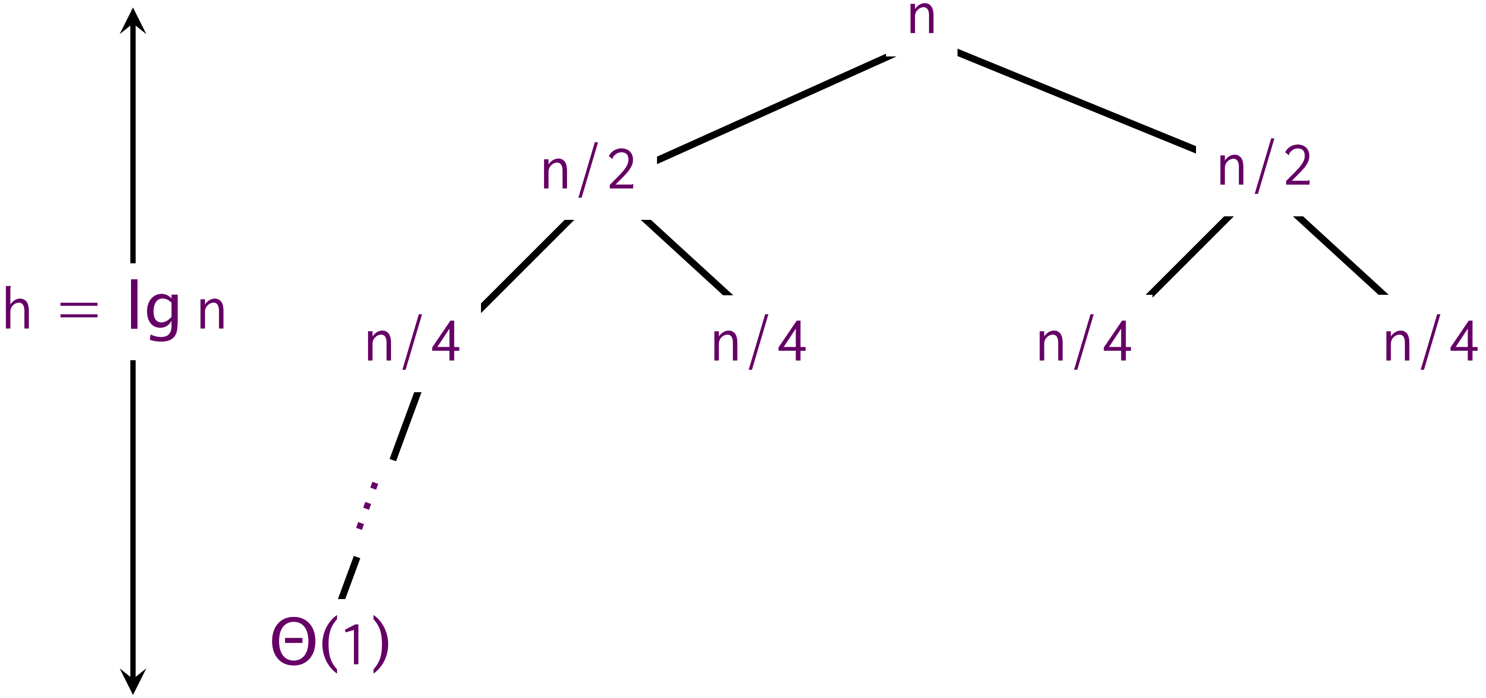
Recursion Tree

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



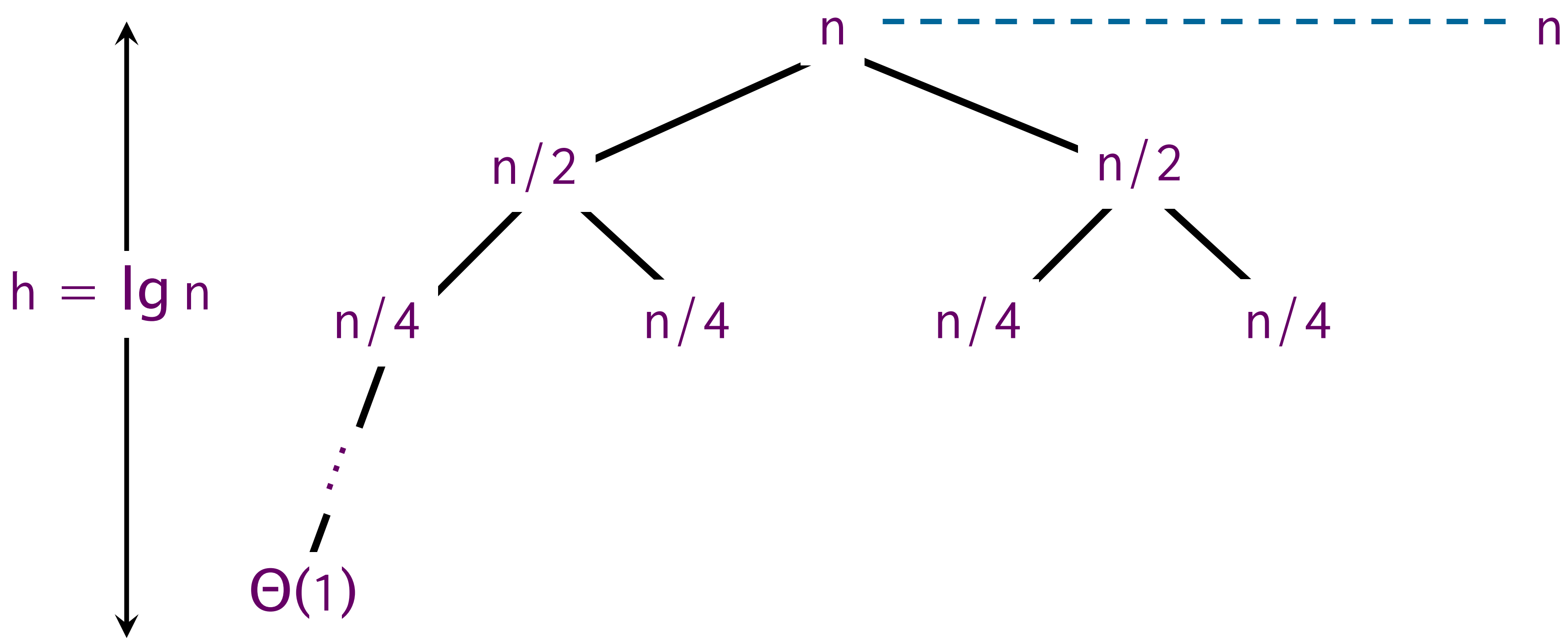
Recursion Tree

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



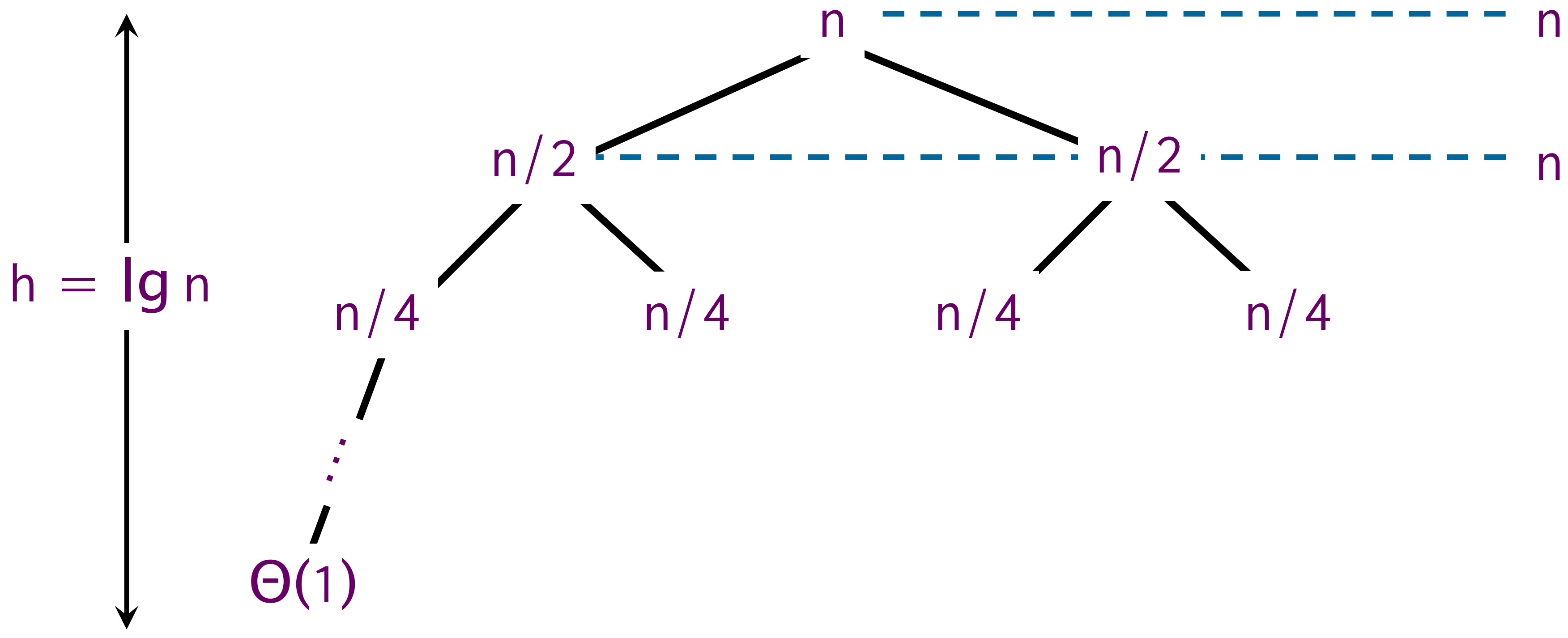
Recursion Tree

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



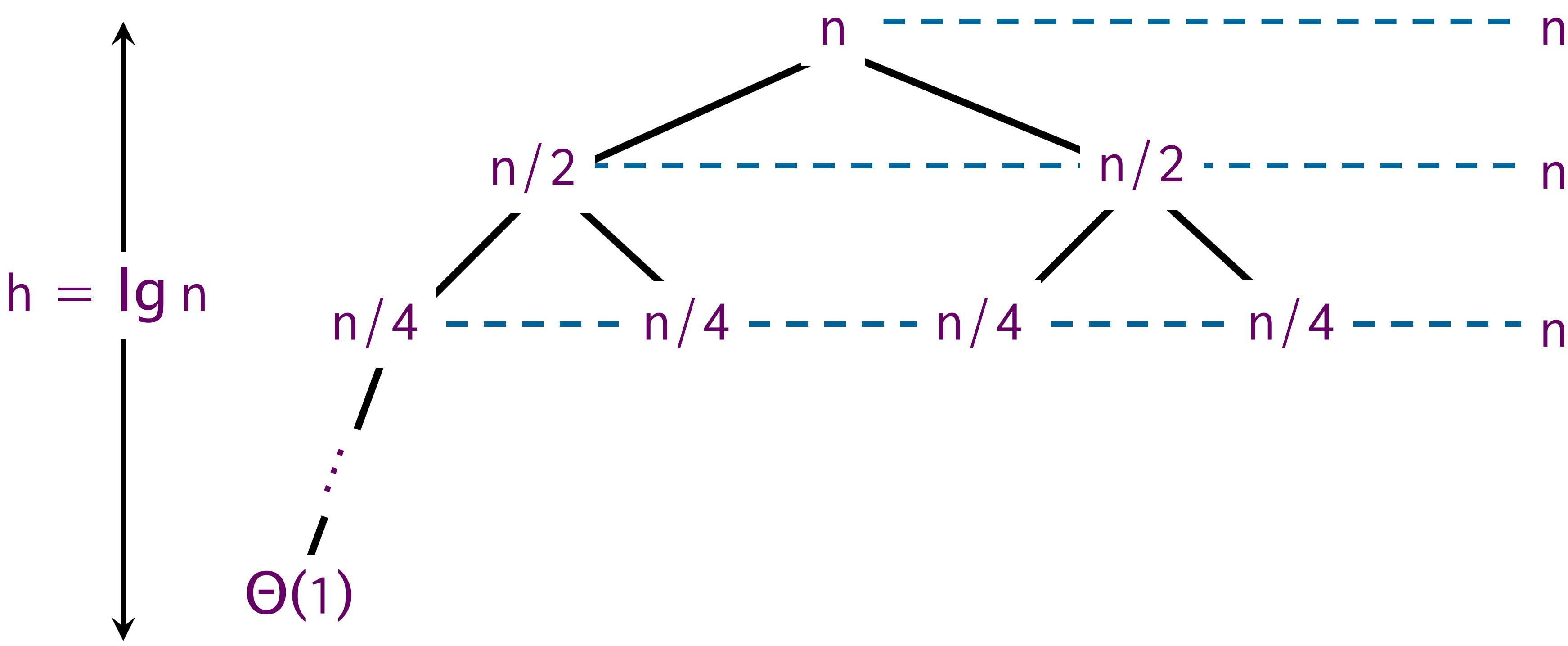
Recursion Tree

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



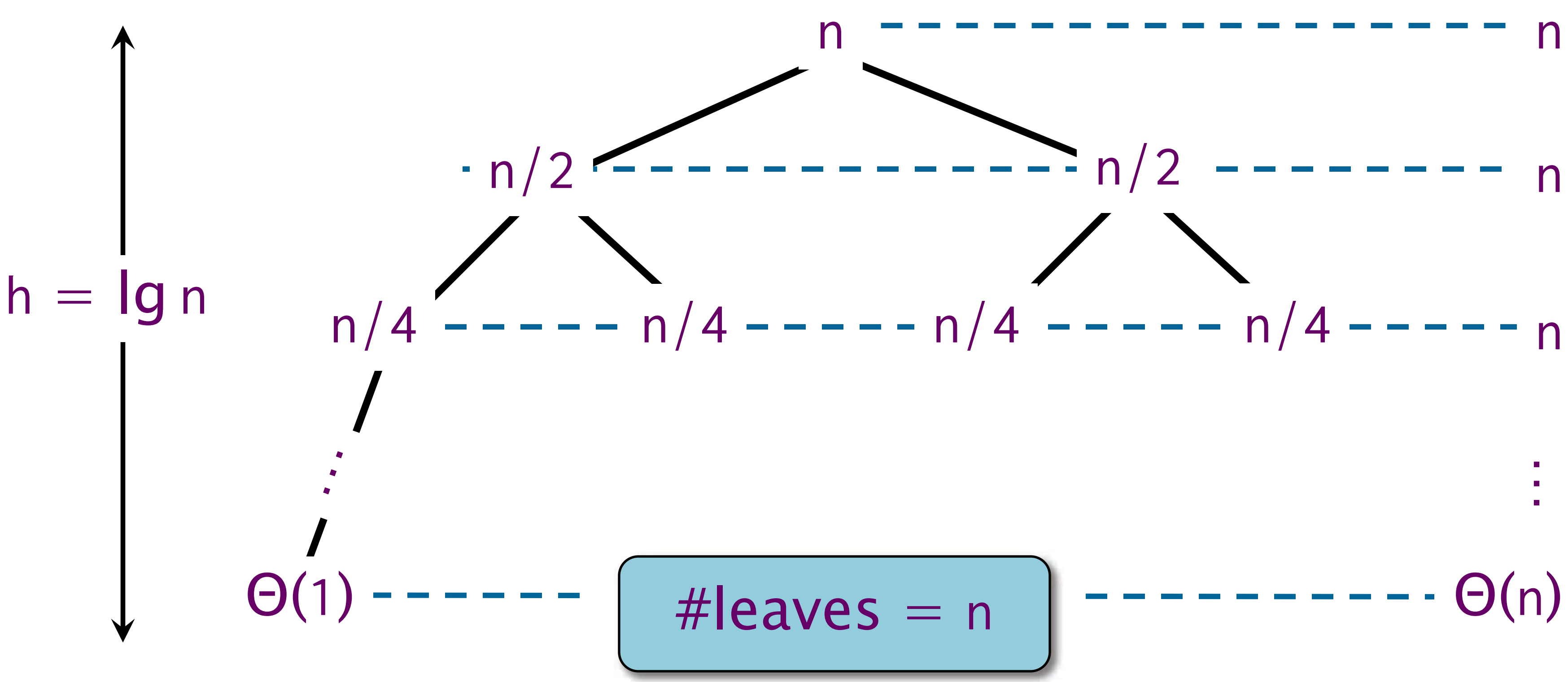
Recursion Tree

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



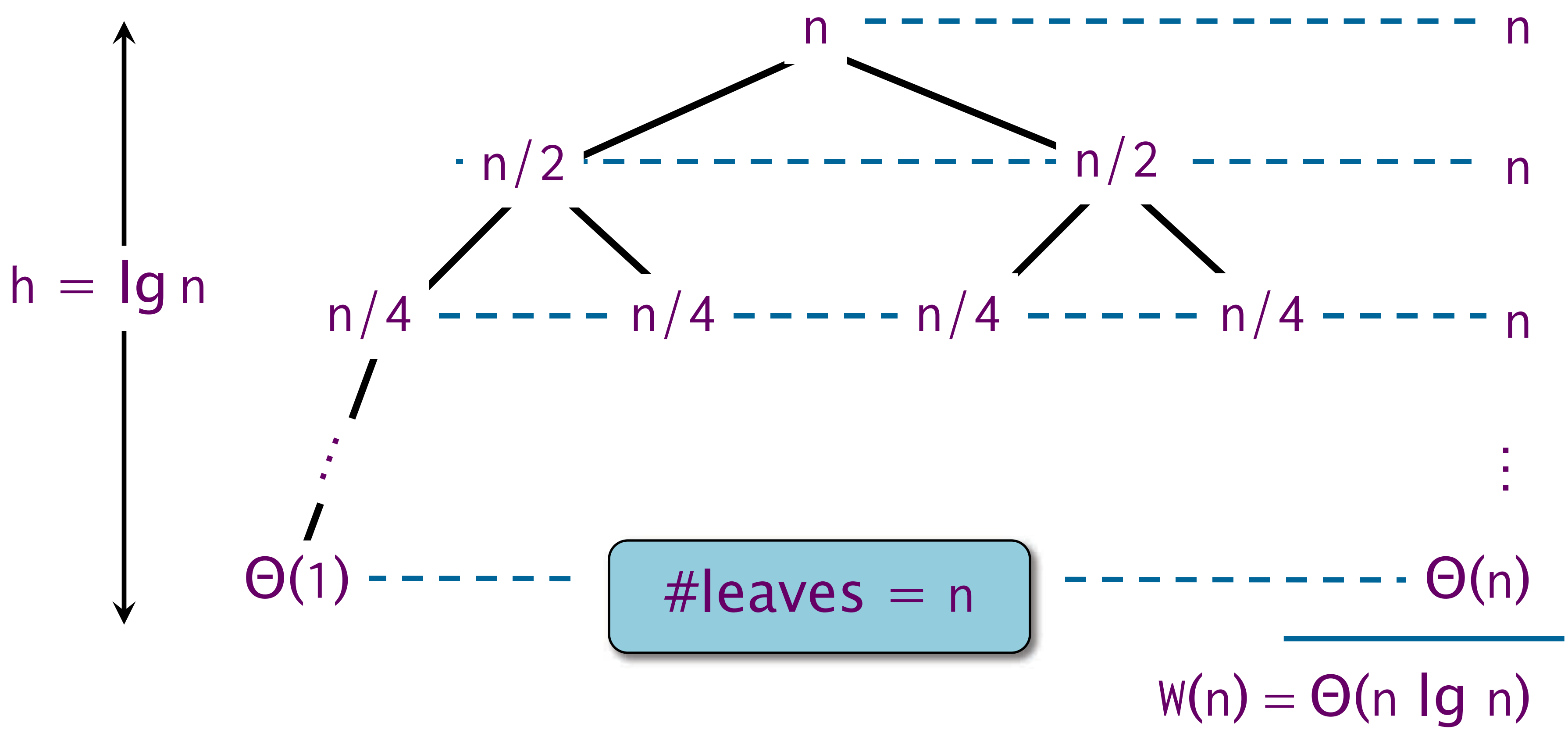
Recursion Tree

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



Recursion Tree

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



Now with Caching

Merge subroutine

$Q(n) = \Theta(n/\mathcal{B})$.

Merge sort

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

Cache Analysis of Merge Sort

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

Recursion tree

$Q(n)$

Cache Analysis of Merge Sort

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

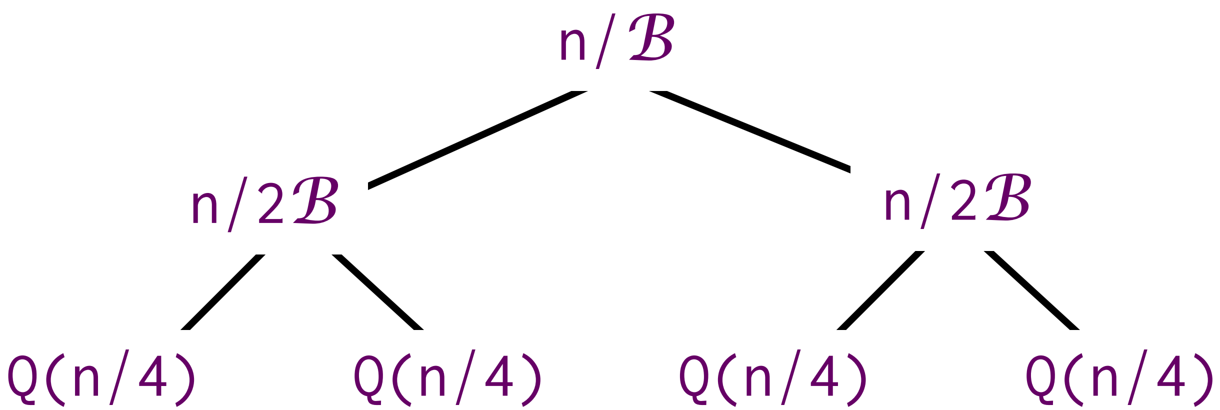
Recursion tree

$$\begin{array}{ccc} & n/\mathcal{B} & \\ \swarrow & & \searrow \\ Q(n/2) & & Q(n/2) \end{array}$$

Cache Analysis of Merge Sort

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

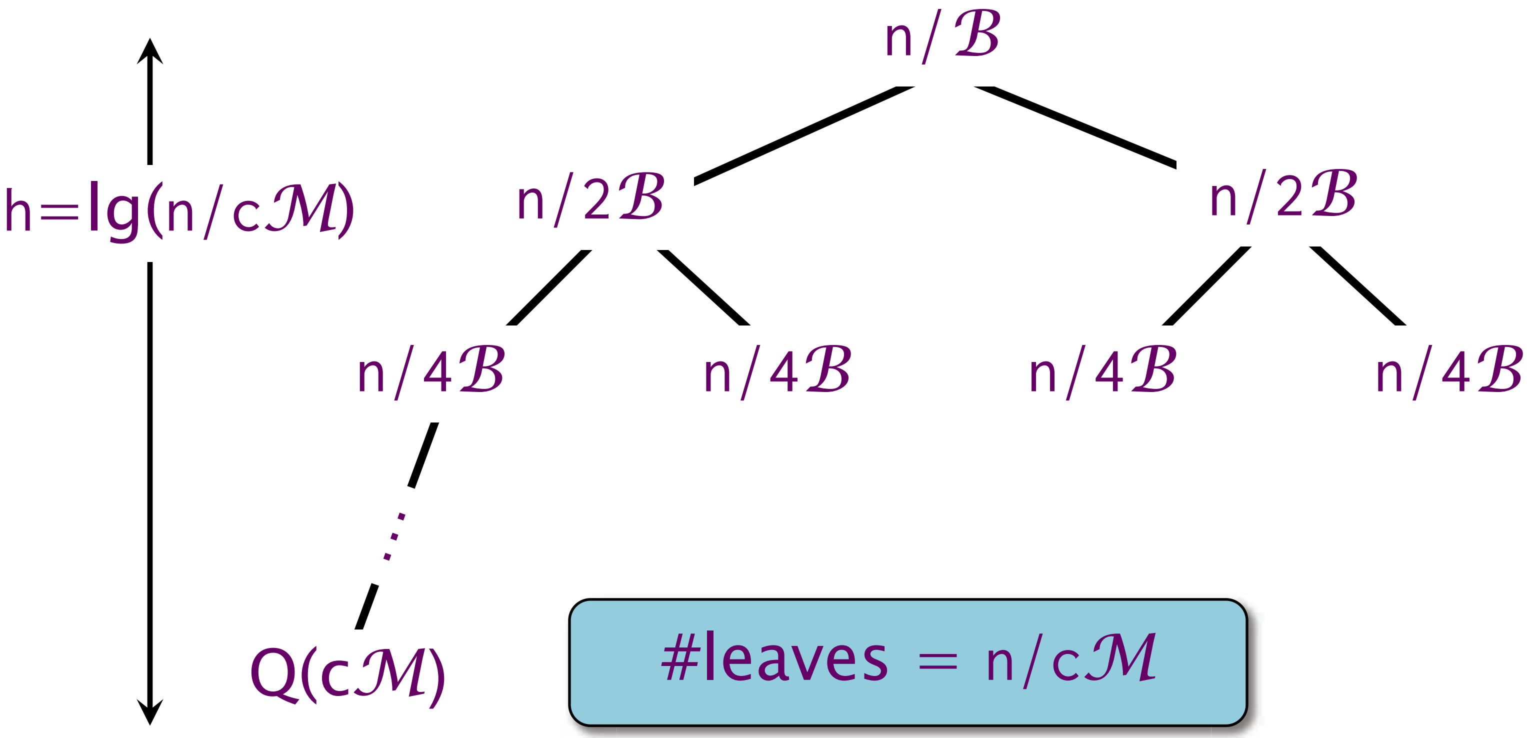
Recursion tree



Cache Analysis of Merge Sort

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

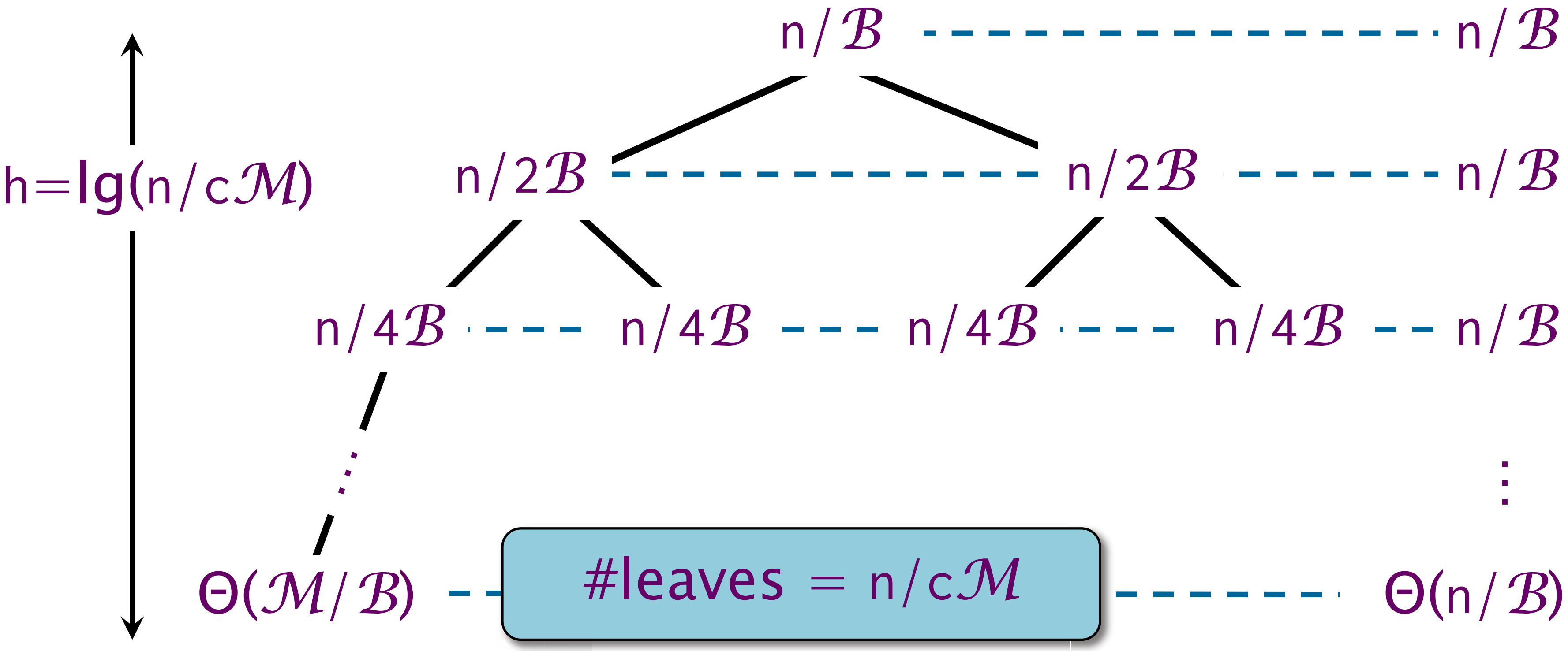
Recursion tree



Cache Analysis of Merge Sort

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

Recursion tree



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

Bottom Line for Merge Sort

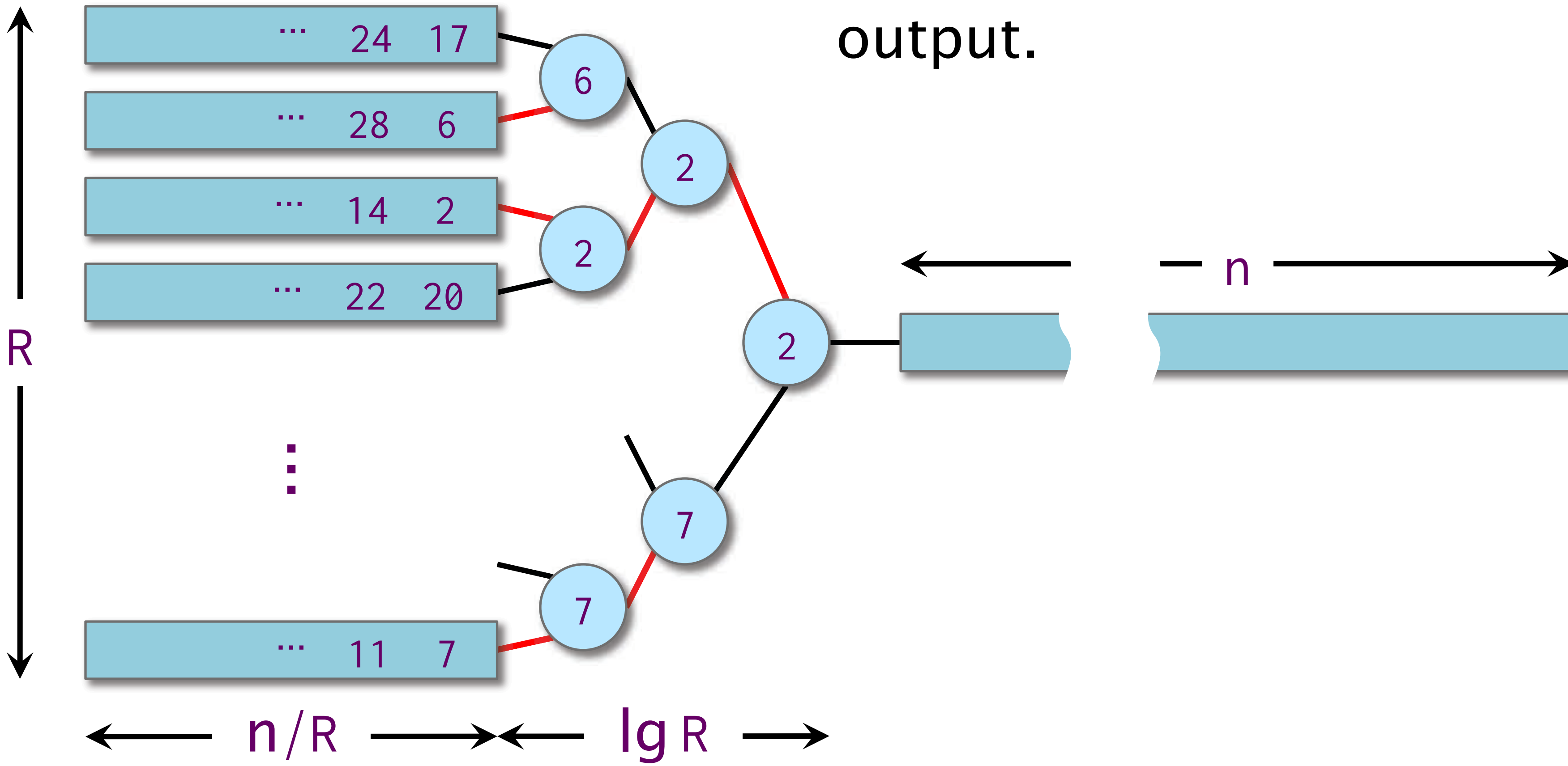
$$Q(n) = \begin{cases} \Theta(n/\mathcal{B}) & \text{if } n \le c\mathcal{M}, \text{ constant } c \le 1; \\ 2Q(n/2) + \Theta(n/\mathcal{B}) & \text{otherwise;} \end{cases}$$
$$= \Theta(\,(n/\mathcal{B}) \lg (n/\mathcal{M})\,)\,.$$

- 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.

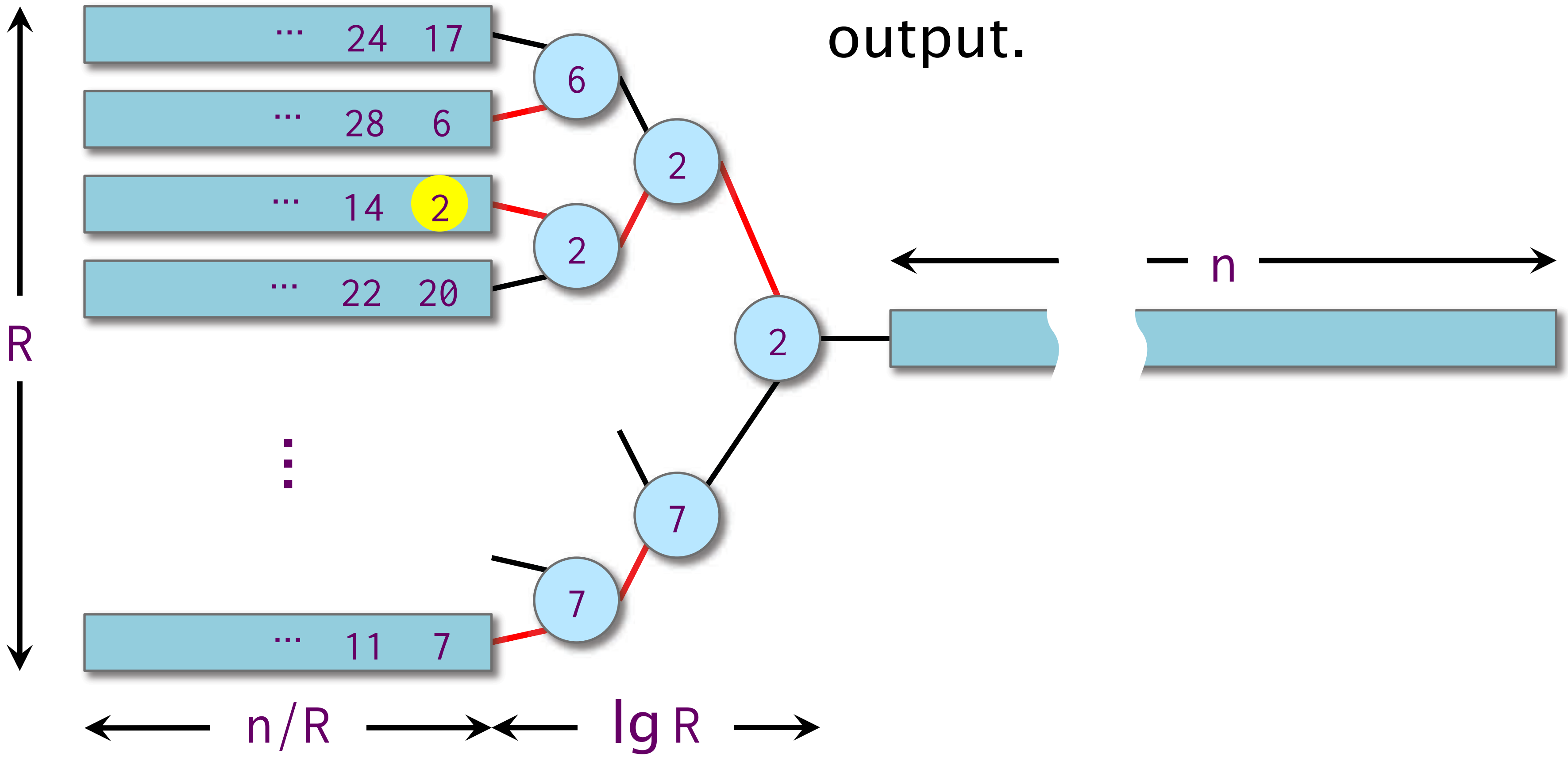
- Tournament takes $\Theta(R)$ work to produce the first output.



Multiway Merging

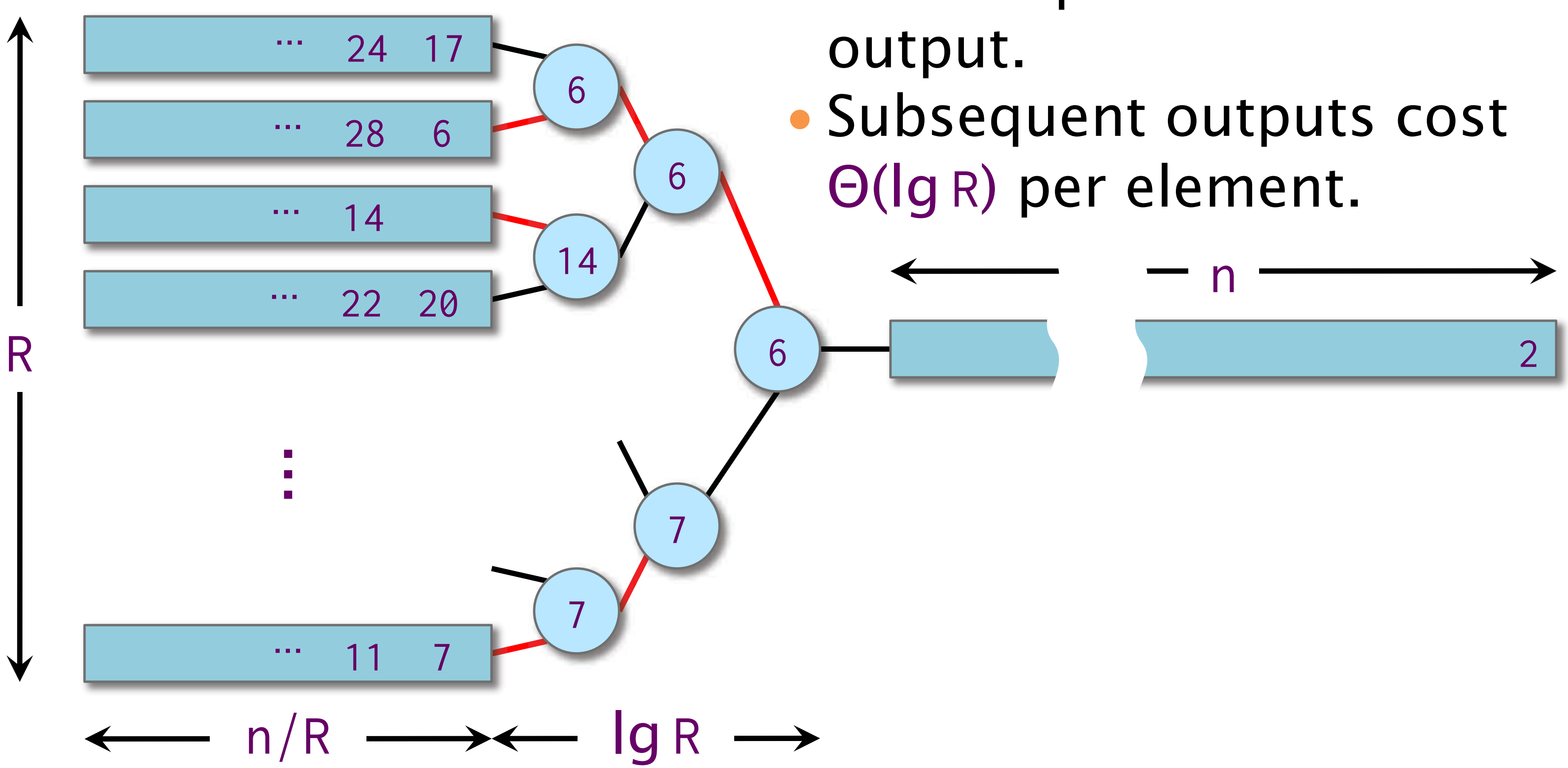
IDEA: Merge $R < n$ subarrays with a tournament.

- Tournament takes $\Theta(R)$ work to produce the first output.



Multiway Merging

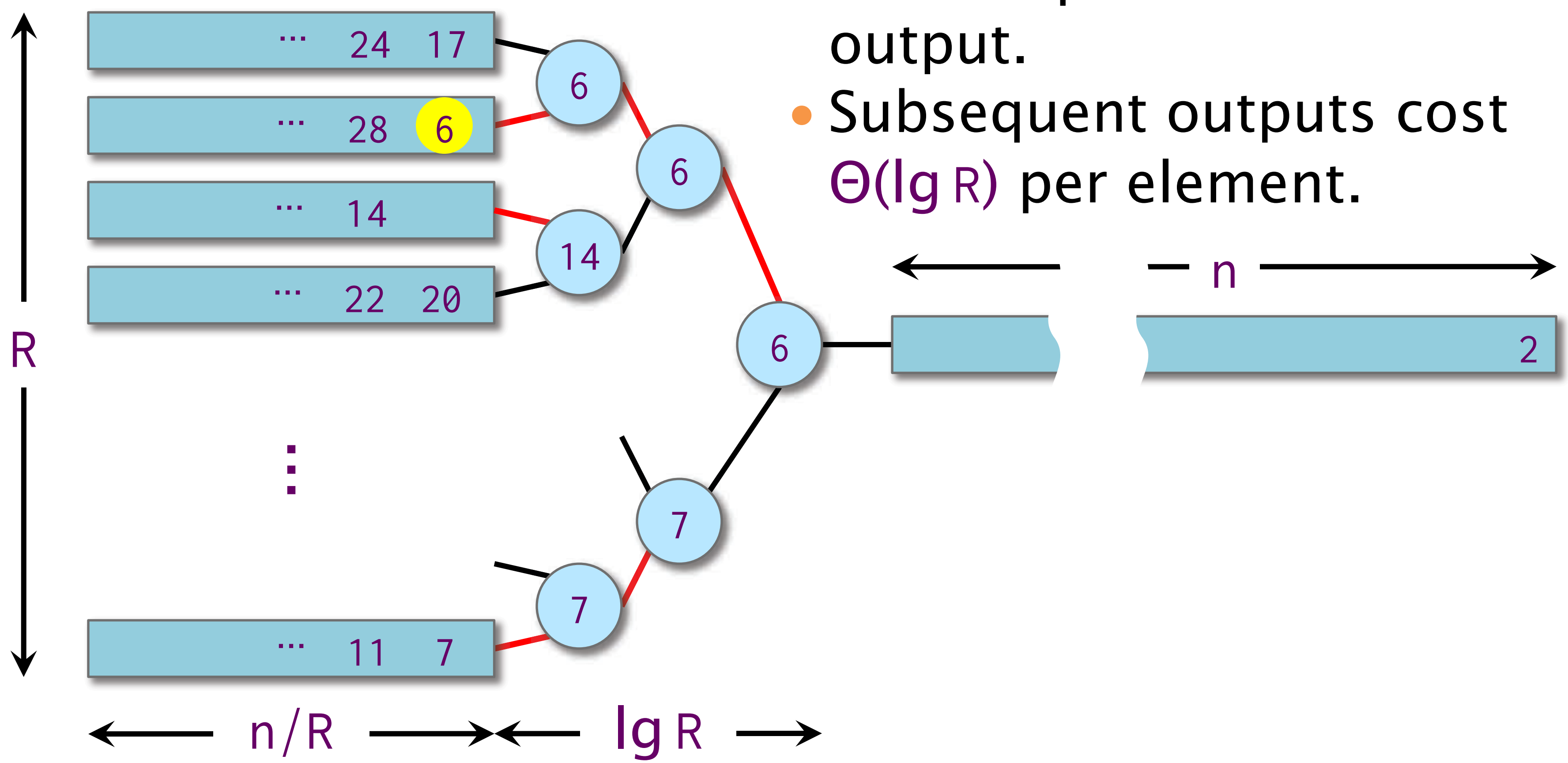
IDEA: Merge $R < n$ subarrays with a tournament.



- Tournament takes $\Theta(R)$ work to produce the first output.
- Subsequent outputs cost $\Theta(\lg R)$ per element.

Multiway Merging

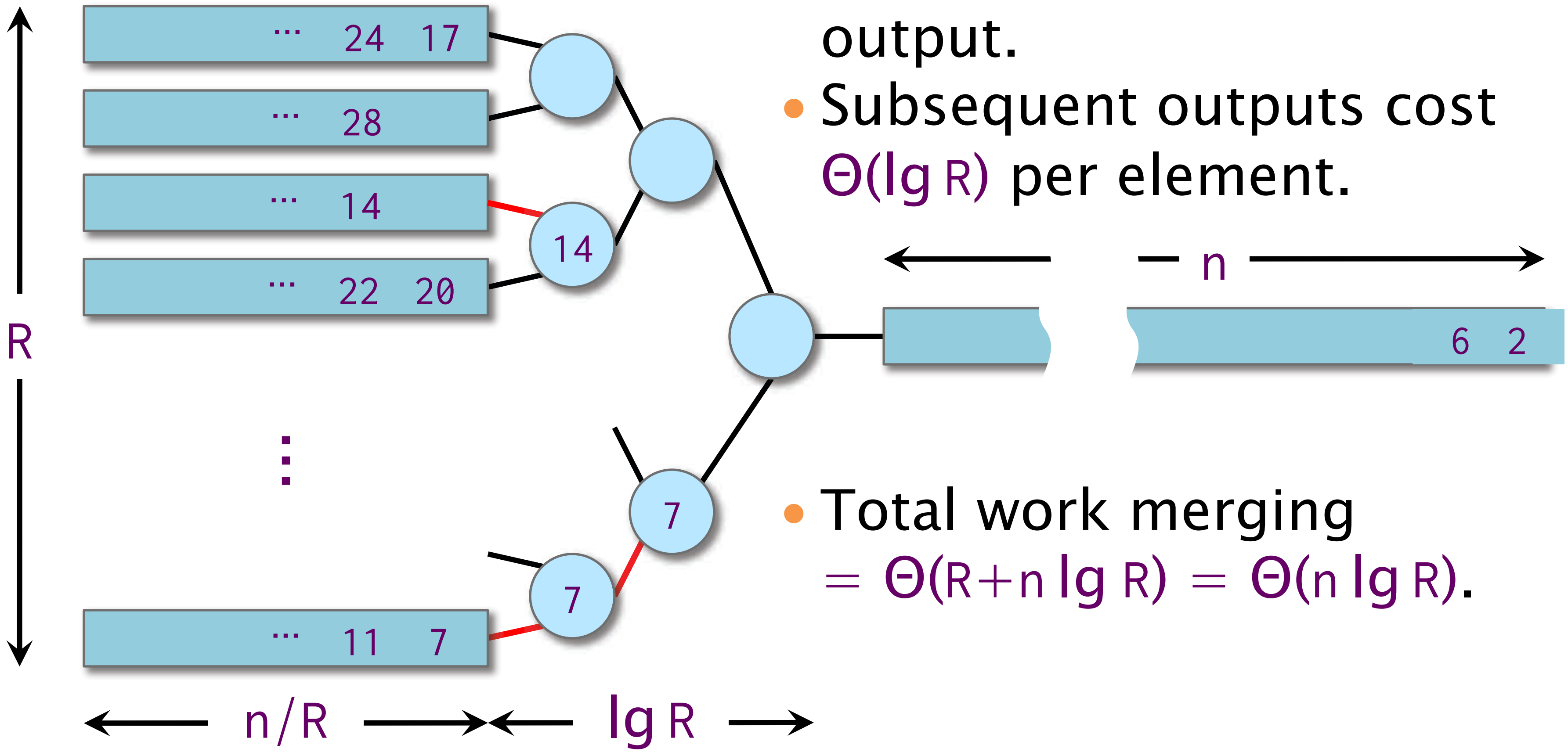
IDEA: Merge R < n subarrays with a tournament.



- Tournament takes Θ(R) work to produce the first output.
- Subsequent outputs cost Θ(lg R) per element.

Multiway Merging

IDEA: Merge $R < n$ subarrays with a tournament.

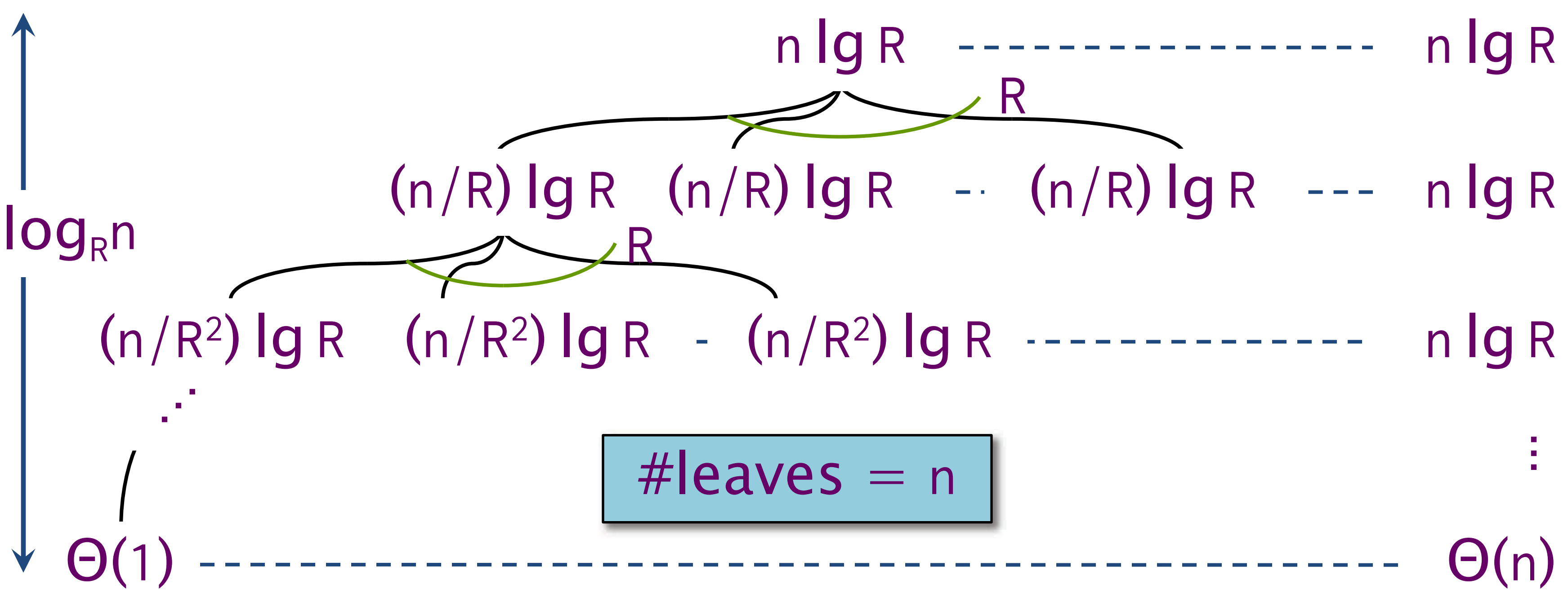


- Tournament takes $\Theta(R)$ work to produce the first output.
- Subsequent outputs cost $\Theta(\lg R)$ per element.
- Total work merging $= \Theta(R + n \lg R) = \Theta(n \lg R)$.

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



$$\begin{aligned} W(n) &= \Theta((n \lg R) \log_R n + n) \\ &= \Theta((n \lg R)(\lg n)/\lg R + n) \\ &= \Theta(n \lg n) \end{aligned}$$

Same as binary merge sort.

Caching Recurrence

Assume that we have $R < c\mathcal{M}/\mathcal{B}$ for a sufficiently small constant $c \leq 1$.

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

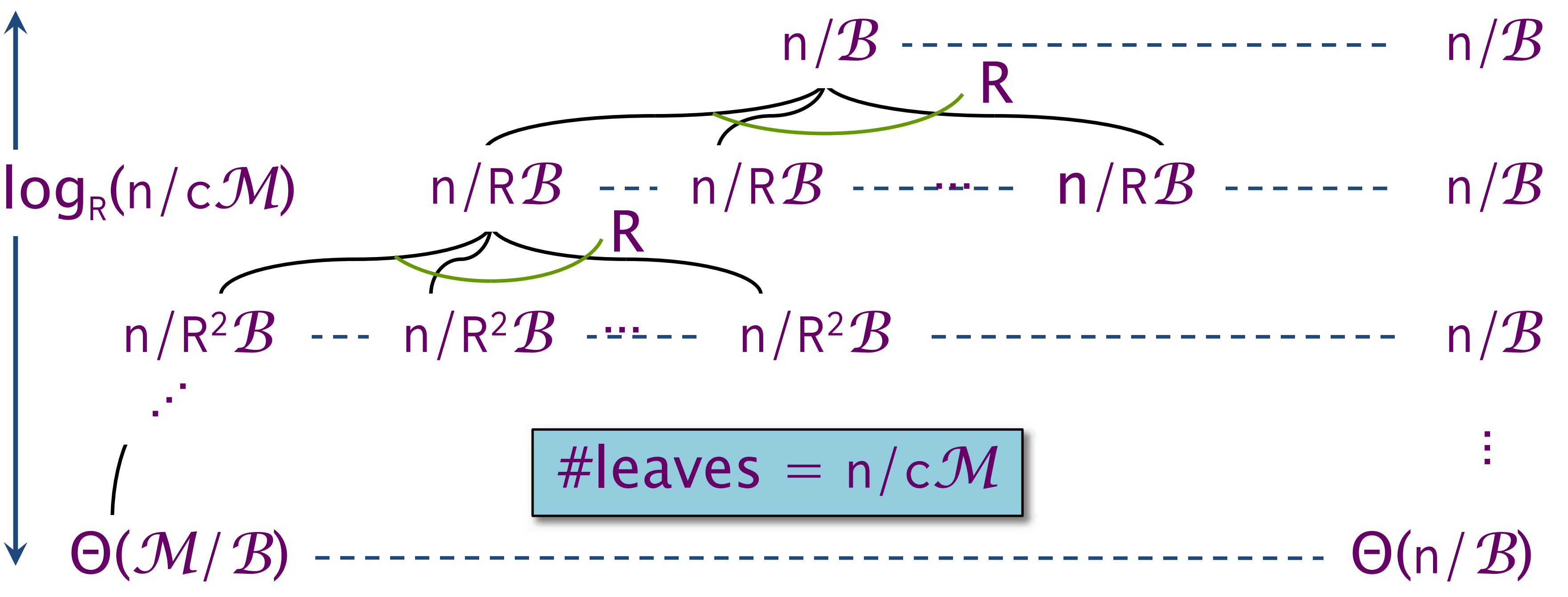
R–way merge sort

$$Q(n) \leq \begin{cases} \Theta(n/\mathcal{B}) & \text{if } n < c\mathcal{M}; \\ R \cdot Q(n/R) + \Theta(n/\mathcal{B}) & \text{otherwise.} \end{cases}$$

Cache Analysis

$$Q(n) \le \begin{cases} \Theta(n/\mathcal{B}) & \text{if } n < c\mathcal{M}; \\ R \cdot Q(n/R) + \Theta(n/\mathcal{B}) & \text{otherwise} \end{cases}$$

Recursion tree



$$Q(n) = \Theta((n/\mathcal{B}) \log_R(n/\mathcal{M}))$$

Tuning the Voodoo Parameter

We have

$$Q(n) = \Theta((n/\mathcal{B}) \log_R(n/\mathcal{M})) \ ,$$

which decreases as $R \le c\mathcal{M}/\mathcal{B}$ increases. Choosing R as big as possible yields

$$R = \Theta(\mathcal{M}/\mathcal{B}) \ .$$

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

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

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

Multiway versus Binary Merge Sort

We have

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

versus

$$\begin{aligned} Q_{\text{binary}}(n) &= \Theta((n/\mathcal{B}) \lg(n/\mathcal{M})) \\ &= \Theta((n \lg n)/\mathcal{B}) , \end{aligned}$$

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: $\mathcal{M} = 2^{15} \Rightarrow 15\times$ savings.
- L2-cache: $\mathcal{M} = 2^{18} \Rightarrow 18\times$ savings.
- L3-cache: $\mathcal{M} = 2^{23} \Rightarrow 23\times$ 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 k^3 items in k sorted lists, incurring at most

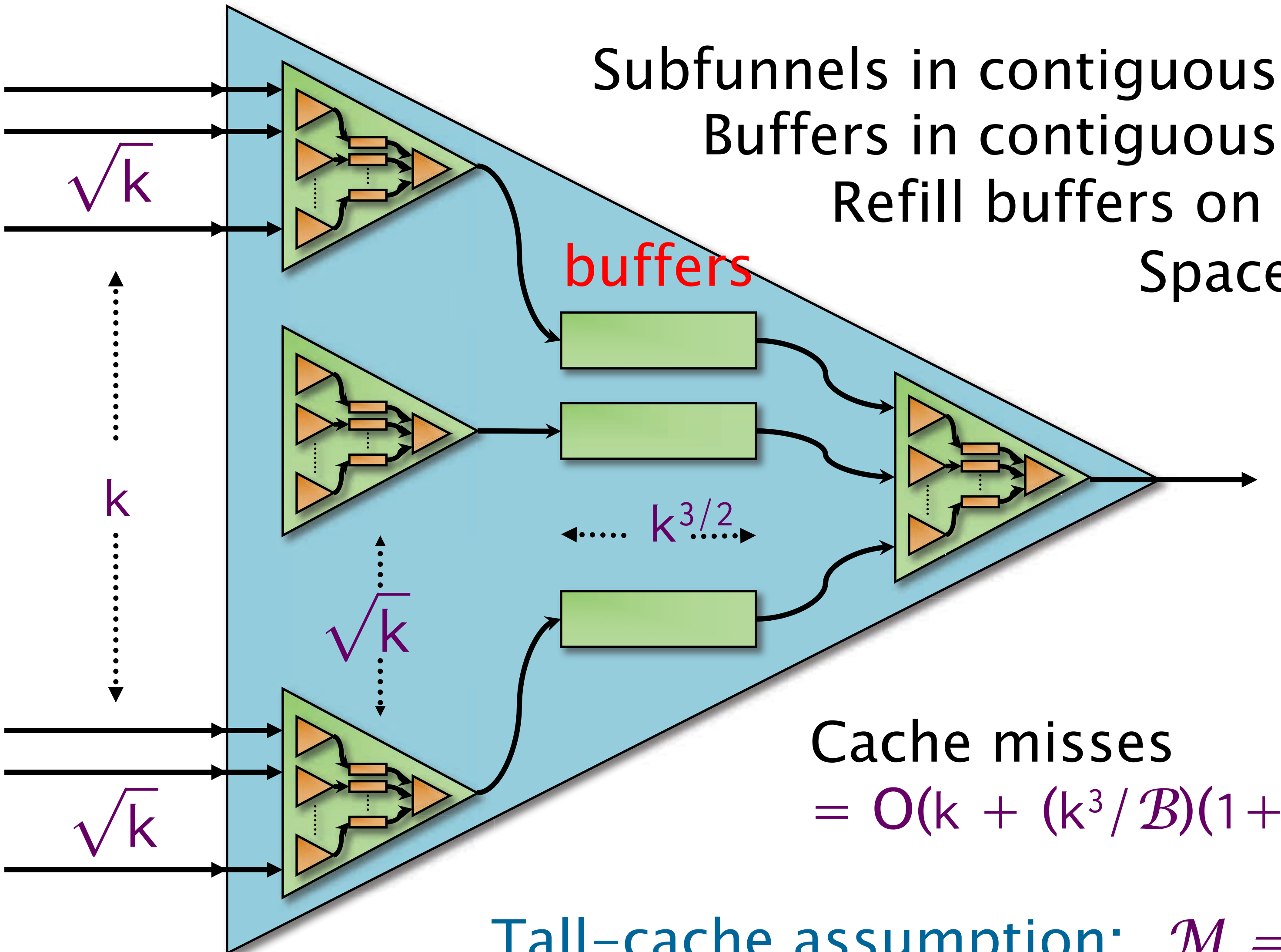
$$\Theta(k + (k^3/\mathcal{B})(1 + \log_{\mathcal{M}} k))$$

cache misses. Thus, funnelsort incurs

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

cache misses, which is asymptotically optimal [AV88].

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: $\mathcal{M} = \Omega(\mathcal{B}^2)$.

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 or 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.