Analyzing Data Access of Algorithms and How to Make Them Cache-Friendly?

Kenjiro Taura

Contents

- Introduction
- 2 Analyzing data access complexity of serial programs
 - Overview
 - Model of a machine
 - An analysis methodology
- 3 Applying the methodology to matrix multiply
- 4 Analyzing merge sort

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- it is thus clearly important to analyze how "good" your algorithm is, in terms of data access performance
- we routinely analyze computational complexity of algorithms to predict or explain algorithm performance, but it ignores the differing costs of accessing memory hierarchy (all memory accesses are O(1))
- we like to do something analogous for data access

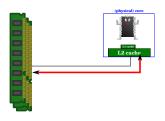
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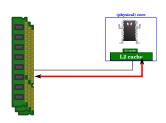
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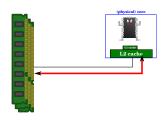
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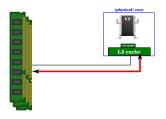
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- in practical terms, this is a proxy of *cache misses*
- the analysis assumes a simple two level memory hierarchy

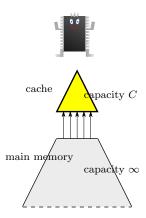


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Model (of a single processor machine)

- a machine consists of
 - a processor,
 - a fixed size cache (C words), and
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 - accessing a word not in the cache mandates transferring the word into the cache

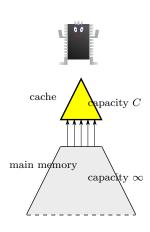


For now, we assume a single processor machine.

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 - a processor,
 - a fixed size cache (C words), and
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- the cache holds the most recently accessed C words; \approx
 - line size = single word (whatever is convenient)
 - fully associative
 - LRU replacement

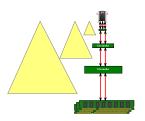
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Gaps between our model and real machines

• hierarchical caches:

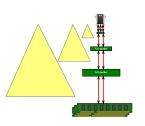
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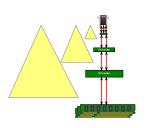
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- in practice the cost heavily depends on how many concurrent accesses you have
- this model cannot capture the difference between link list traversal and random array access

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• concurrent accesses:

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- in practice the cost heavily depends on how many concurrent accesses you have
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• prefetch:

• similarly, this model cannot capture the difference between sequential accesses that can take advantages of the hardware prefetcher and random accesses that cannot

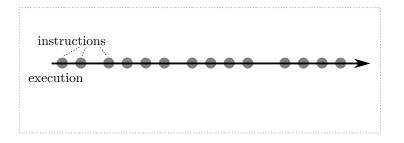
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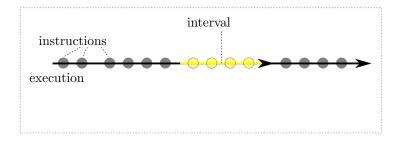
• an *execution* of a program is the sequence of instructions



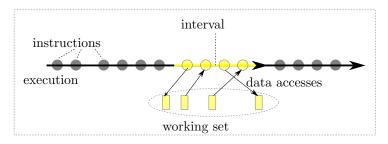
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- an *interval* in an execution is a consecutive sequence of instructions in the execution



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- an *interval* in an execution is a consecutive sequence of instructions in the execution
- the working set of an interval is the number of distinct words accessed by the interval

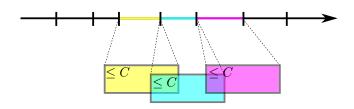


A basic methodology

to calculate the amount of data transferred in an execution,

• split an execution into intervals each of which fits in the cache; i.e.,

working set size of an interval $\leq C$ (cache size) (*)



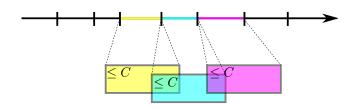
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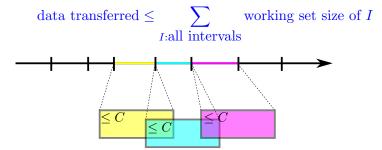
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- therefore,



Remarks

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- each word in an interval misses at most only once, because
 - the cache is LRU, and
 - the condition (*) guarantees that each word is never evicted within the interval
- in practical terms, an essential step to analyze data transfer is to identify the largest intervals that fits in the cache

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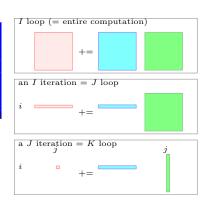
Applying the methodology

- we will apply the methodology to some of the algorithms we have studied so far
- the key is to find subproblems (intervals) that fit in the cache

Analyzing the triply nested loop

```
for (i = 0; i < n; i++) {
  for (j = 0; j < n; j++) {
  for (k = 0; k < n; k++) {
      C(i,j) += A(i,k) * B(k,j);
   }
}
</pre>
```

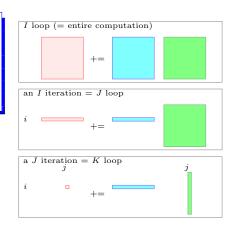
• key question: which iteration fits in the cache?



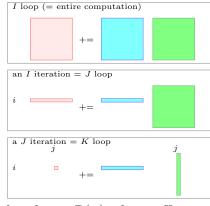
Working sets

```
for (i = 0; i < n; i++) {
  for (j = 0; j < n; j++) {
    for (k = 0; k < n; k++) {
        C(i,j) += A(i,k) * B(k,j);
    }
}</pre>
```

level	working set size
I loop	$3n^2$
J loop	$2n + n^2$
K loop	1+2n
K iteration	3



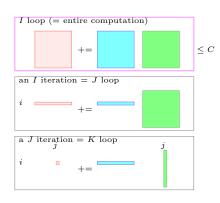
Cases to consider



Goal: for each case, bound from the above R(n), the traffic between memory and cache for $n \times n$ matrix-multiply

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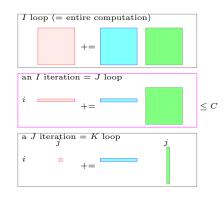
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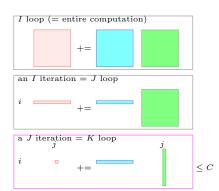
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- Case 2: a single *i* iteration (\approx a matrix) fits in the cache ($2n + n^2 < C$)



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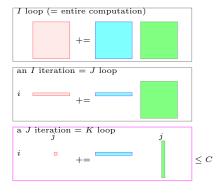
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- Case 1: the three matrices all fit in the cache $(3n^2 \le C)$
- Case 2: a single *i* iteration $(\approx \text{a matrix})$ fits in the cache $(2n + n^2 \le C)$
- Case 3: a single j iteration (\approx two vectors) fits in the cache $(1 + 2n \le C)$
- Case 4: none of the above (1+2n>C)

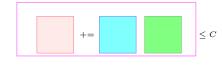


Goal: for each case, bound from the above R(n), the traffic between memory and cache for $n \times n$ matrix-multiply

Case 1 $(3n^2 \le C)$

• trivially, each element misses the cache only once. thus,

$$R(n) \le 3n^2 = \frac{3}{n} \cdot n^3$$



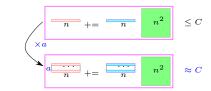
interpretation: each element of A, B, and C are reused n times

Case 2 $(2n + n^2 \le C)$

• the maximum number of *i*-iterations that fit in the cache is:

$$a \approx \frac{C - n^2}{2n}$$

• each such set of iterations transfer < C words, so



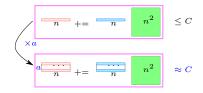
$$R(n) \le \frac{n}{a}C = \frac{n}{a}(n^2 + 2an) = \left(\frac{1}{a} + \frac{2}{n}\right)n^3$$

interpretation: each element of B is reused a times in the cache; each element in A or C many $(\propto n)$ times

A Remark

- for a particular access pattern of the matrix multiplication, a better bound can be obtained
- as we know all elements of B are accessed in each i-iteration, B stays in the cache for any number of a iterations
- so, in this case too,

$$R(n) \le 3n^2 = \frac{3}{n} \cdot n^3$$

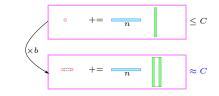


Case $3 (1 + 2n \le C)$

• the maximum number of *j*-iterations that fit in the cache is:

$$b \approx \frac{C - n}{n + 1}$$

• each such set of iterations transfer < C words, so



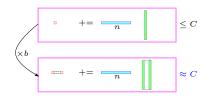
$$R(n) \le \frac{n^2}{b}C = \frac{n^2}{b}(n+b(n+1)) = \left(\frac{1}{b}+1+\frac{1}{n}\right)n^3$$

interpretation: each element in B is never reused; each element in A b times; each element in C many $(\propto n)$ times

A Remark

- a similar argument shows that an entire row of A stays in the cache for any number of b iterations
- therefore

$$R(n) \le (2n+n^2)n = n^3 + 2n^2$$



Case 4 (1 + 2n > C)

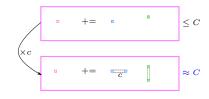
• the maximum number of k-iterations that fit in the cache is:

$$c \approx \frac{C - 1}{2}$$

• each such set of iterations transfer $\leq C$ words, so

$$R(n) \le \frac{n^3}{c}C = \left(2 + \frac{1}{c}\right)n^3$$

interpretation: each element of B or A never reused; each element of C reused c times



A Remark

- similarly, the element of *C* stays in the cache for any number of *c* iterations
- SO

$$R(n) \le (2n+1)n^2 = 2n^3 + n^2$$
 interpretation: each element of B or A never reused; each element of C reused n times



Summary

• $n^3/R(n)$ or the number of FMAs per memory accesses (cache miss)

condition	R(n)	$n^3/R(n)$
$2n + n^2 \le C$	$3n^2$	n/3
$1 + 2n \le C$	$2n^2 + n^3$	≈ 1
1 + 2n > C	$n^2 + 2n^3$	$\approx 1/2$

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- to reduce the traffic, you arrange the computation (order subcomputations) so that you do a lot of computation on the same amount of data

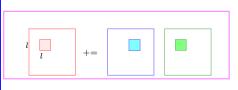
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 - compute/data ratio,
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 - compute intensity, or
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- the notion is so important that it is variously called
 - compute/data ratio,
 - flops/byte,
 - compute intensity, or
 - arithmetic intensity
- the key is to identify the unit of computation (task) whose compute intensity is high (compute-intensive task)

Cache blocking (tiling)

- for matrix multiplication, let l be the maximum number that satisfies $2l + l^2 \leq C$ (i.e., $l \approx \sqrt{C}$) and form a subcomputation that performs a $(l \times l)$ matrix multiplication
- ignoring remainder iterations, it looks like:

```
 1 = \sqrt{C} - \text{small constant}; 
for (ii = 0; ii < n; ii += 1)
for (jj = 0; jj < n; jj += 1)
for (kk = 0; kk < n; kk += 1)
/* block below misses each */
/* element at most once */
for (i = ii; i < ii + 1; i++)
for (j = jj; j < jj + 1; j++)
for (k = kk; k < kk + 1; k++)
 A(i,j) += B(i,k) * C(k,j);
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Cache blocking (tiling)

- each block:
 - performs l^3 FMAs and
 - touches $3l^2$ distinct words,

```
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5 /* block below misses each */

6 /* element at most once */

7 for (i = ii; i < ii + 1; i++)

8 for (j = jj; j < jj + 1; j++)

9 for (k = kk; k < kk + 1; k++)

10 A(i,j) += B(i,k) * C(k,j);
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Cache blocking (tiling)

- each block:
 - performs l^3 FMAs and
 - touches $3l^2$ distinct words,
- so, the traffic of the entire computation

$$\leq 3l^2 \cdot \left(\frac{n}{l}\right)^3 = \frac{3}{l}n^3 = \frac{3}{\sqrt{C}}n^{3^{l0}}$$

```
 \begin{aligned} 1 &= \sqrt{C} - \text{small constant;} \\ \text{for (ii = 0; ii < n; ii += 1)} \\ \text{for (jj = 0; jj < n; jj += 1)} \\ \text{for (kk = 0; kk < n; kk += 1)} \\ &/* block below misses each */ \\ &/* element at most once */ \\ \text{for (i = ii; i < ii + 1; i++)} \\ \text{for (j = jj; j < jj + 1; j++)} \\ \text{for (k = kk; k < kk + 1; k++)} \\ &A(i,j) &+= B(i,k) * C(k,j); \end{aligned}
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Effect of cache blocking

condition	R(n)	$n^3/R(n)$
$2n + n^2 \le C$	$3n^2$	n/3
$1 + 2n \le C$	$2n^2 + n^3$	~ 1
1 + 2n > C	$n^2 + 2n^3$	$\sim 1/2$
blocking	$\frac{3}{\sqrt{C}}n^3$	$\frac{\sqrt{C}}{3}$

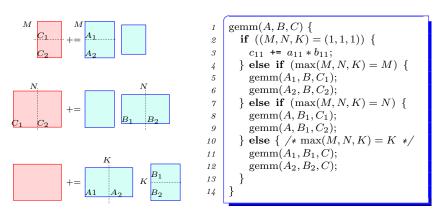
• assume a word = 4 bytes (float)

bytes	C	l	$n^3/R(n)$
32K	8K	≈ 90.50	30.16
256K	64K	≈ 256	85.33
3MB	768K	≈ 886	295.60

Recursive blocking

- ullet the tiling technique just mentioned needs to determine l for a particular size (= level)
- it may have to do this at all levels (12 deep nested loop)?
- we also (for the sake of simplicity) assumed all matrices are square
- for generality, portability, simplicity, recursive blocking may apply

Recursively blocked matrix multiply



- it divides flops into two
- it divides two of the three matrices, along the longest axis

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- let R(w) be the maximum number of words transferred for any matrix multiply of up to w words in total:

$$R(w) \equiv \max_{MK+KN+MN \le w} R(M, N, K)$$

we want to bound R(w) from the above

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we want to bound R(w) from the above

• to avoid making analysis tedious, assume all matrices are "nearly square"

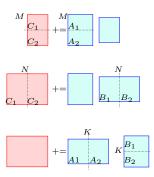
$$\max(M, N, K) \le 2\min(M, N, K)$$

The largest subproblem that fits in the cache

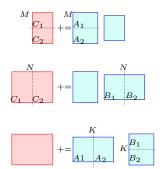
- the working set of gemm(A,B,C) is (MK+KN+MN) (words)
- it fits in the cache if this is $\leq C$
- thus we have:

$$R(w) \leq C \quad (w \leq C)$$

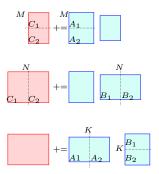
 when MK + KN + MN > C, the interval doing gemm(A,B,C) is two subintervals, each of which does gemm for slightly smaller matrices



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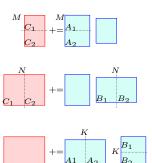


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$$\therefore R(w) \le 2R(w/\sqrt[3]{4}) \quad (w > C)$$



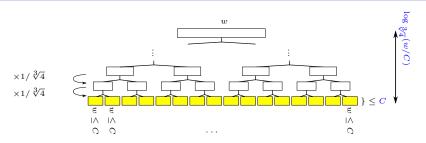
Combined

• we have:

$$R(w) \le \begin{cases} w & (w \le C) \\ 2R(w/\sqrt[3]{4}) & (w > C) \end{cases}$$

- when w > C, it takes up to $d \approx \log_{\sqrt[3]{4}}(w/C)$ recursion steps until the working set becomes $\leq C$
- the whole computation is essentially 2^d consecutive intervals, each transferring $\leq C$ words

Illustration



$$\therefore R(w) < 2^{d} \cdot C$$

$$= 2^{\log \sqrt[3]{4}(w/C)} \cdot C$$

$$= C\left(\frac{w}{C}\right)^{\frac{1}{\log \sqrt[3]{4}}}$$

$$= \frac{1}{\sqrt{C}}w^{3/2}$$

Result

• we have:

$$R(w) \le \frac{1}{\sqrt{C}} w^{3/2}$$

• for square $(n \times n)$ matrices $(w = 3n^2)$,

$$\therefore R(n) = R(3n^2) = \frac{3\sqrt{3}}{\sqrt{C}}n^3$$

• the same as the blocking we have seen before (not surprising), but we achieved this for all cache levels

A practical remark

• in practice we stop recursion when the matrices become "small enough"

```
gemm(A, B, C) {
        if (A, B, C \text{ together fit in the cache}) {
           for (i, j, k) \in [0..M] \times [0..N] \times [0..K]
             c_{ij} += a_{ik} * b_{kj};
        } else if (\max(M, N, K) = M) {
           gemm(A_1, B, C_1);
           \operatorname{gemm}(A_2, B, C_2);
        } else if (\max(M, N, K) = N) {
           \operatorname{gemm}(A, B_1, C_1);
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10
        } else { /* \max(M, N, K) = K */
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12
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13
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• on the other hand, we like to make it large, to reduce control overhead

Contents

- Introduction
- 2 Analyzing data access complexity of serial programs
 - Overview
 - Model of a machine
 - An analysis methodology
- 3 Applying the methodology to matrix multiply
- 4 Analyzing merge sort

Review: (serial) merge sort

```
/* sort a..a_end and put the result into
       (i) a (if dest = 0)
       (ii) t (if dest = 1) */
    void ms(elem * a, elem * a_end,
            elem * t, int dest) {
      long n = a_end - a;
      if (n == 1) {
        if (dest) t[0] = a[0]:
      } else {
        /* split the array into two */
10
11
        long nh = n / 2:
        elem * c = a + nh:
12
        /* sort 1st half */
13
                             1 - dest);
        ms(a, c, t,
14
        /* sort 2nd half */
1.5
        ms(c, a_end, t + nh, 1 - dest);
16
        elem * s = (dest ? a : t):
17
        elem * d = (dest ? t : a);
18
        /* merge them */
19
        merge(s, s + nh,
20
             s + nh, s + n, d);
21
22
23
```

```
/* merge a_beg ... a_end
        and b\_beg ... b\_end
       into c */
   void
   merge(elem * a, elem * a_end,
          elem * b, elem * b_end,
          elem * c) {
     elem * p = a, * q = b, * r = c;
     while (p < a_end && q < b_end) {
        if (*p < *q) { *r++ = *p++; }
       else { *r++ = *q++; }
     while (p < a_{end}) *r++ = *p++;
     while (q < b_end) *r++ = *q++;
1.5
```

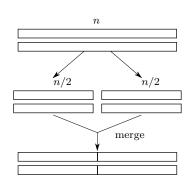
note: as always, actually switch to serial sort below a threshold (not shown in the code above)

Memory \leftrightarrow cache transfer in merge sort (1) base case

- merge sorting n elements takes two arrays of n elements each, and touch all elements of them \Rightarrow the working set is 2n words
- thus, it fits in the cache when 2n < C

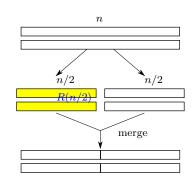
$$\therefore R(n) \le 2n \quad (2n \le C)$$

```
1 long nh = n / 2;
2 /* sort 1st half */
3 ms(a, c, t, 1 - dest);
4 /* sort 2nd half */
5 ms(c, a_end, t + nh, 1 - dest);
6 ...
7 /* merge them */
8 merge(s, s + nh,
9 s + nh, s + n, d);
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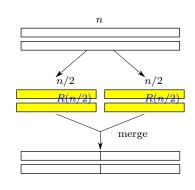
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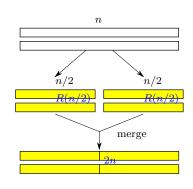
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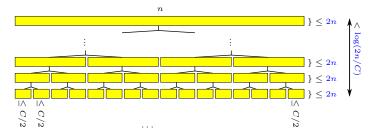
Combined

• so far we have:

$$R(n) \le \begin{cases} 2n & (n \le C/2) \\ 2R(n/2) + 2n & (n > C/2) \end{cases}$$

- for n > C/2, it takes at most $d \approx \log \frac{2n}{C}$ divide steps until it becomes $\leq C/2$
- thus,

$$R(n) \le 2n \cdot d = 2n \log \frac{2n}{C}$$



Improving merge sort

• so what can we do to improve this?

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- there are not much we can do to improve a single merge (:: each element of arrays is accessed only once)
- so the hope is to reduce the number of steps $(\log \frac{2n}{C}) \Rightarrow multi-way\ merge$

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- I hope I have taught that it's a subject of a rigid analysis, not a black art
- the key for the assessment/analysis is to identify a unit of computation that fits in the cache, not to microscopically follow the state of the cache
- the key to achieve good cache performance is to keep *the compute intensity of cache-fitting computation* high

