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

Kenjiro Taura

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- Introduction
- 2 Analyzing data access complexity of serial programs
 - Overview
 - Model of a machine
 - An analysis methodology
- 3 Applying the methodology to matrix multiply
- 1 Tools to measure cache/memory traffic
 - perf command
 - PAPI library
- 6 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

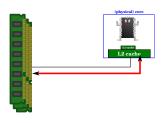
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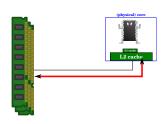
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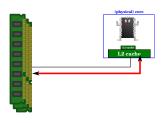
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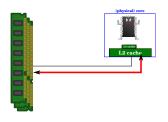
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- in practical terms, this is a proxy of *cache misses*
- the analysis assumes a simple two level memory hierarchy

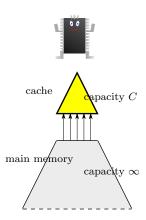


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Model (of a single processor machine)

- a machine consists of
 - a processor,
 - a fixed size cache (C words), and
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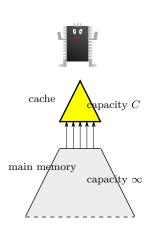


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 - a processor,
 - a fixed size cache (C words), and
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- the cache holds the most recently accessed C words; \approx
 - line size = single word (whatever is convenient)
 - fully associative
 - LRU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

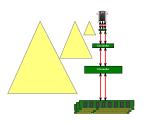
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Gaps between our model and real machines

• hierarchical caches:

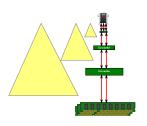
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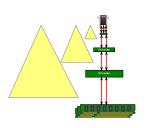
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- the model only counts the amount of data transferred
- in practice the cost heavily depends on how many concurrent accesses you have
- this model cannot capture the difference between link list traversal and random array access

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- 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

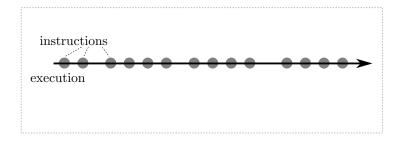
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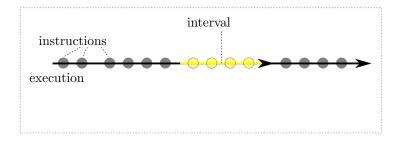
• an *execution* of a program is the sequence of instructions



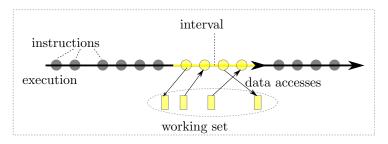
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- an *interval* in an execution is a consecutive sequence of instructions in the execution
- the working set of an interval is the number of distinct words accessed by the interval

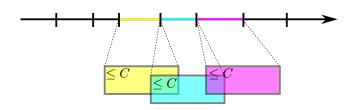


A basic methodology

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) (*)



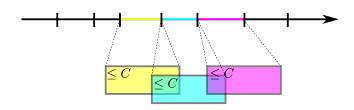
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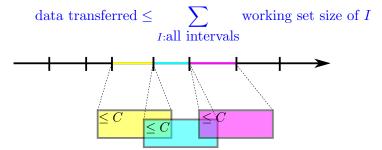
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- therefore,



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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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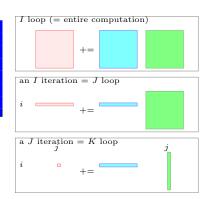
Applying the methodology

- 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>
```

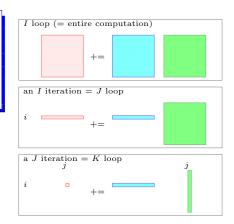
• key question: which iteration fits the cache?



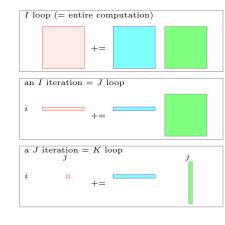
Working sets

```
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

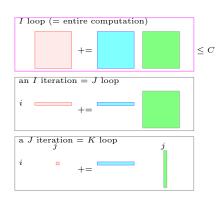


Cases to consider



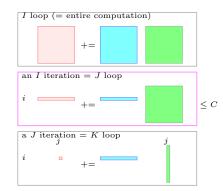
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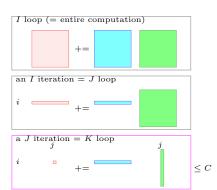
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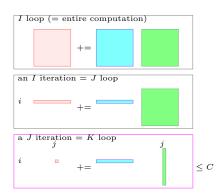
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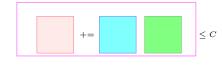
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- Case 4: none of the above (1+2n>C)



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

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

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



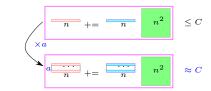
interpretation: each element of A, B, and C are reused n times

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 $\leq C$ words, so



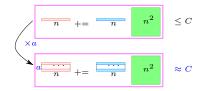
$$R(n) \le \frac{n}{a}C = \frac{n}{a}(n^2 + 2an) = \left(\frac{1}{a} + \frac{2}{n}\right)n^3$$

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, they all stay in the cache
- so

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

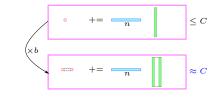


Case $3 (1 + 2n \le C)$

• 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 $\leq C$ 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

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



Summary

• summarize $R(n)/n^3$, the number of misses per multiply-add $(0 \sim 3)$

$R(n)/n^3$	range
$\frac{3}{n}$	~ 0
$\frac{1}{a} + \frac{2}{n}$	$0 \sim 1$
$\frac{1}{b} + 1 + \frac{1}{n}$	$1 \sim 2$
$2 + \frac{1}{c}$	$2 \sim 3$
	$R(n)/n^3$ $\frac{3}{n}$ $\frac{1}{a} + \frac{2}{n}$ $\frac{1}{b} + 1 + \frac{1}{n}$ $2 + \frac{1}{c}$

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 - compute/data ratio,
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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)

The straightforward loop in light of compute intensity

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

- the outermost loop has an O(n) compute intensity
- yet each iteration of which has only an O(1) compute intensity

- for matrix multiplication, let l be the maximum number that satisfies $3l^2 \leq C$ (i.e., $l \approx \sqrt{C/3}$) and form a subcomputation that performs a $(l \times l)$ matrix multiplication
- ignoring remainder iterations, it looks like:

```
1 = \sqrt{C/3};
for (ii = 0; ii < n; ii += 1)
  for (jj = 0; jj < n; jj += 1)
  for (kk = 0; kk < n; kk += 1)
    /* working set fits in the cache below */
  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);</pre>
```

```
+= -
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 - performs $2l^3$ flops and
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• or, the traffic is

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

```
\frac{2l^3}{3l^2} = \frac{2}{3}l \approx \frac{2}{3}\sqrt{\frac{C}{3}} 
\frac{1}{3}\sqrt{\frac{C}{3}}
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```

Effect of cache blocking

condition	$R(n)/n^3$	range
$3n^2 \le C$	$\frac{3}{n}$	~ 0
$2n + n^2 \le C$	$\frac{1}{a} + \frac{2}{n}$	$0 \sim 1$
$1 + 2n \le C$	$\frac{1}{b} + 1 + \frac{1}{n}$	$1 \sim 2$
$\boxed{1 + 2n > C}$	$2+\frac{1}{c}$	$2 \sim 3$
blocking	$\frac{3\sqrt{3}}{\sqrt{C}}$	below

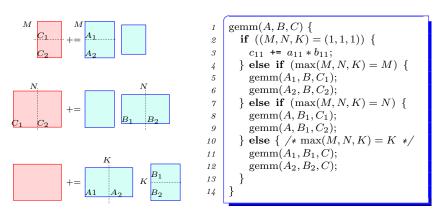
• assume a word = 4 bytes (float)

bytes	C	l	$R(n)/n^3$
32K	8K	52	0.72
256K	64K	147	0.43
3MB	768K	886	0.0059

Recursive blocking

- the tiling technique just mentioned targets a cache of a particular size (= level)
- need 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(M, N, K) be the number of words transferred between cache and memory when multiplying $M \times K$ and $K \times N$ matrices (the cache is initially empty)
- 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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$$R(w) \equiv \max_{MK + KN + MN < w} R(M, N, K)$$

we want to bound R(w) from the above

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

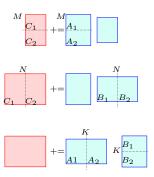
$$\max(M, N, K) \le 2\min(M, N, K)$$

The largest subproblem that fits in the cache

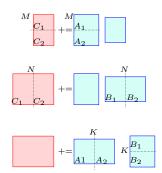
- the working set of gemm(A,B,C) is (MK+KN+MN) (words)
- it fits in the cache if this is $\leq C$
- thus we have:

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

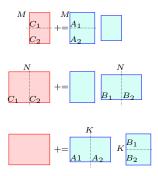
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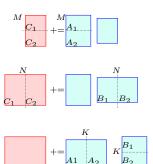


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- in the "nearly square" assumption, the working set becomes $\leq 1/4$ when we divide 3 times
- to make math simpler, we take it that the working set becomes $\leq \frac{1}{\sqrt[3]{4}} (= 2^{-2/3})$ of the original size on each recursion. i.e.,



- when MK + KN + MN > C, the interval doing gemm(A,B,C) is two subintervals, each of which does gemm for slightly smaller matrices
- in the "nearly square" assumption, the working set becomes ≤ 1/4 when we divide 3 times
- to make math simpler, we take it that the working set becomes $\leq \frac{1}{\sqrt[3]{4}} (=2^{-2/3})$ of the original size on each recursion. i.e.,

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



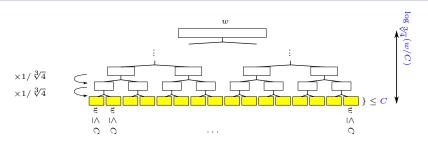
Combined

• 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);
           \operatorname{gemm}(A, B_1, C_2);
10
        } else { /* \max(M, N, K) = K */
11
           \operatorname{gemm}(A_1, B_1, C);
12
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13
14
15
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- in practice we stop recursion when the matrices become "small enough"
- but how small is small enough?

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- when the threshold \leq level x cache, the analysis holds for all levels x and lower

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• on the other hand, we like to make it large, to reduce control overhead

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Tools to measure cache/memory traffic

- analyzing data access performance is harder than analyzing computational efficiency (ignoring caches)
 - the code reflects how much computation you do
 - you can experimentally confirm your understanding by counting cycles (or wall-clock time)
- caches are complex and subtle
 - the same data access expression (e.g., a[i]) may or may not count as the traffic
 - gaps are larger between our model and the real machines (associativity, prefetches, local variables and stacks we often ignore, etc.)
- we like to have a tool to measure what happened on the machine → performance counters

Performance counters

- recent CPUs equip with *performance counters*, which count the number of times various events happen in the processor
- OS exposes it to users (e.g., Linux perf_event_open system call)
- there are tools to access them more conveniently
 - command: Linux perf (man perf)
 - library: PAPI http://icl.cs.utk.edu/papi/
 - GUI: hpctoolkit http://hpctoolkit.org/, VTunes, ...

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perf command

• perf command is particularly easy to use

```
will show you cycles, instructions, and some other info
```

• to access performance counters of your interest (e.g., cache misses), specify them with -e

```
perf stat -e counter -e counter ... command line
```

• to know the list of available counters

```
1 perf list
```

perf command

Event	\	Umask		
Num.	Event Mask Mnemonic	Value	Description	Comment
3CH	UnHalted Core Cycles	00H	Unhalted core cycles	
3CH	UnHalted Reference Cycles	01H	Unhalted reference cycles	Measures bus cycle ¹
COH	Instruction Retired	00H	Instruction retired	
2EH	LLC Reference	4FH	Longest latency cache references	
ZEH	LLC Misses	41H	Longest latency cache misses	
C4H	Branch Instruction Retired	00H	Branch instruction at retirement	
C5H	Branch Misses Retired	00H	Mispredicted Branch Instruction at retirement	

- many interesting counters are not listed by perf list
- we often need to resort to "raw" events (defined on each CPU model)
- consult intel document ¹
- if the table says Event Num = 2EH, Umask Value = 41H, then you can access it via perf by -e r412e (umask; event num)

¹Intel 64 and IA-32 Architectures Developer's Manual: Volume 3B: System Programming Guide, Part 2. Chapter 19 "Performance Monitoring Events" http://www.intel.com/content/www/us/en/architecture-and-technology/64-ia-32-architectures-software-developer-vol-3b-part-2-manual.html

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PAPI library

- library for accessing performance counters
- http://icl.cs.utk.edu/papi/index.html
- basic concepts
 - create an empty "event set"
 - add events of interest to the event set
 - start counting
 - do whatever you want to measure
 - stop counting
- visit http://icl.cs.utk.edu/papi/docs/index.html and see "Low Level Functions"

PAPI minimum example (single thread)

• A minimum example with a single thread and no error checks

```
#include <papi.h>
int main() {

do_whatever(); }

freturn 0;
}
```

PAPI minimum example (single thread)

• A minimum example with a single thread and no error checks

```
#include <papi.h>
    int main() {
      PAPI_library_init(PAPI_VER_CURRENT);
      int es = PAPI_NULL;
      PAPI_create_eventset(&es):
5
      PAPI_add_named_event(es, "ix86arch::LLC_MISSES");
6
      PAPI_start(es):
      long long values[1];
8
      { do_whatever(); }
      PAPI_stop(es, values);
10
      printf("%lld\n", values[0]);
11
      return 0;
12
13
```

Compiling and running PAPI programs

• compile and run

```
$ gcc ex.c -lpapi
$ ./a.out
3
```

- papi_avail and papi_native_avail list available event names (to pass to PAPI_add_named_event)
 - perf_raw::rnnnn for raw counters (same as perf command)

Error checks

- be prepared to handle errors (never assume you know what works)!
- many routines return PAPI_OK on success and a return code on error, which can then be passed to PAPI_strerror(return_code) to convert it into an error message
- encapsulate such function calls with this

```
void check_(int ret, const char * fun) {
   if (ret != PAPI_OK) {
     fprintf(stderr, "%s failed (%s)\n", fun, PAPI_strerror(ret));
     exit(1);
   }
}

#define check(call) check_(call, #call)
```

A complete example with error checks

```
#include <stdio.h>
     #include <stdlib h>
     #include <papi.h>
4
 5
     void check (int ret, const char * fun) {
       if (ret != PAPI_OK) {
 7
         fprintf(stderr, "%s failed (%s)\n", fun, PAPI_strerror(ret));
 8
         exit(1):
10
11
     #define check(f) check (f, #f)
12
13
     int main() {
14
       int ver = PAPI_library_init(PAPI_VER_CURRENT);
1.5
       if (ver != PAPI VER CURRENT) {
16
         fprintf(stderr, "PAPI_library_init(%d) failed (returned %d)\n",
17
                 PAPI_VER_CURRENT, ver);
18
         exit(1):
19
20
       int es = PAPI_NULL;
       check(PAPI create eventset(&es));
21
22
       check(PAPI add named event(es, "ix86arch::LLC MISSES"));
23
       check(PAPT start(es)):
24
       { do_whatever(); }
25
       long long values[1];
26
       check(PAPI_stop(es, values));
27
       printf("%lld\n", values[0]);
28
       return 0:
29
```

Multithreaded programs

- must call PAPI_thread_init(id_fun) in addition to PAPI_library_init(PAPI_VER_CURRENT)
 - *id_fun* is a function that returns identity of a thread (e.g., pthread_self, omp_get_thread_num)
- each thread must call PAPI_register_thread
- event set is private to a thread (each thread must call PAPI_create_eventset(), PAPI_start(), PAPI_stop())

Multithreaded example

```
#include <stdio.h>
    #include <stdlib.h>
   #include <omp.h>
   #include <papi.h>
    /* check_ and check omitted (same as single thread) */
5
    int main() {
6
      /* error check for PAPI_library_init omitted (same as single thread) */
      PAPI_library_init(PAPI_VER_CURRENT);
8
      check(PAPI_thread_init((unsigned long(*)()) omp_get_thread_num));
    #pragma omp parallel
10
11
        check(PAPI_register_thread()); /* each thread must do this */
12
        int es = PAPI NULL:
13
        check(PAPI_create_eventset(&es)); /* each thread must create its own set */
14
        check(PAPI_add_named_event(es, "ix86arch::LLC_MISSES"));
1.5
16
        check(PAPI start(es)):
        { do_whatever(); }
17
18
        long long values[1];
        check(PAPI_stop(es, values));
19
        printf("thread %d: %lld\n", omp_get_thread_num(), values[0]);
20
21
      return 0;
22
23
```

Several ways to obtain counter values

- PAPI_stop(es, values): get current values and stop counting
- PAPI_read(es, values): get current values and continue counting
- PAPI_accum(es, values): accumulate current values, reset counters, and continue counting

Useful PAPI commands

- papi_avail, papi_native_avail: list event counter names
- papi_mem_info: report information about caches and TLB (size, line size, associativity, etc.)

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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);
                                           1.5
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++;
```

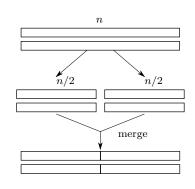
note: as always, actually switch to serial sort below a threshold (not shown in the code above)

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

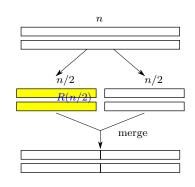
$$\therefore R(n) \le 2n \quad (2n \le C)$$

```
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);
```



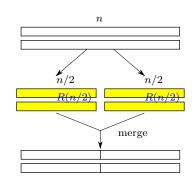
$$\therefore R(n) \le 2R(n/2) + 2n \quad (n > C/2)$$

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2 /* sort 1st half */
3 ms(a, c, t, 1 - dest);
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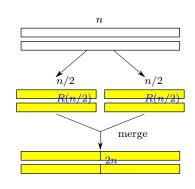
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```



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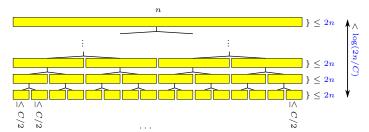
Combined

• 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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Improving merge sort

• so what can we do to improve this?

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

- 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 $(\log \frac{2n}{C}) \Rightarrow multi-way\ merge$

• understanding and assessing data access performance (e.g., cache misses) is important



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- 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



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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



Next step

- our next goal is to understand data access performance of parallel algorithms
- we are particularly interested in performance of dynamically scheduled task parallel algorithms
- to this end, we first describe schedulers of task parallel systems