

Advanced Systems Lab

Spring 2021

Lecture: Dense linear algebra, LAPACK/BLAS, ATLAS, fast MMM

Instructor: Markus Püschel, Ce Zhang

TA: Joao Rivera, several more

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Overview

Linear algebra software: the path to fast libraries, LAPACK and BLAS

Blocking (BLAS 3): key to performance

Fast MMM

- *Algorithms*
- *ATLAS*
- *model-based ATLAS*

Linear Algebra Algorithms: Examples

Solving systems of linear equations

Eigenvalue problems

Singular value decomposition

LU/Cholesky/QR/... decompositions

... and many others

Make up much of the numerical computation across disciplines (sciences, computer science, engineering)

Efficient software is extremely relevant

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The Path to Fast Libraries

[EISPACK](#) and [LINPACK](#) (early 1970s)

- *Jack Dongarra, Jim Bunch, Cleve Moler, Gilbert Stewart*
- *LINPACK still the name of the benchmark for the [TOP500 \(Wiki\)](#) list of most powerful supercomputers*

Matlab: Invented in the late 1970s by Cleve Moler

Commercialized (MathWorks) in 1984

Motivation: Make LINPACK, EISPACK easy to use

Matlab uses linear algebra libraries but can only call it *if you operate with matrices and vectors and do not write your own loops*

- *$A*B$ (calls MMM routine)*
- *$A\b b$ (calls linear system solver)*

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The Path to Fast Libraries

EISPACK/LINPACK Problem:

- Implementation vector-based = low operational intensity (e.g., MMM as double loop over scalar products of vectors)
- Low performance on computers with deep memory hierarchy (became apparent in the 80s)

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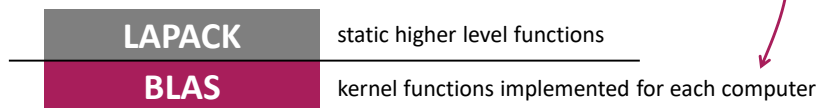
The Path to Fast Libraries

Now there is implementation effort for each processor!

LAPACK (late 1980s, early 1990s)

- Redesign all algorithms to be "block-based" to increase locality
- Jim Demmel, Jack Dongarra et al.

Two-layer architecture



Basic Linear Algebra Subroutines (BLAS)

- BLAS 1: vector-vector operations (e.g., vector sum)
- BLAS 2: matrix-vector operations (e.g., matrix-vector product)
- BLAS 3: matrix-matrix operations (e.g., MMM)

LAPACK uses BLAS 3 as much as possible

$$I(n) = \begin{matrix} O(1) \\ O(1) \\ O(\sqrt{C}) \end{matrix}$$

↑
cache size

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Reminder: Why is BLAS3 so important?

Using BLAS 3 (instead of BLAS 1 or 2) in LAPACK

= *blocking*

= *high operational intensity I*

= *high performance*

Remember (blocking MMM):

$I(n) =$



$O(1)$



$O(\sqrt{C})$

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Small Detour: MMM Complexity?

Usually computed as $C = AB + C$

Cost as computed before

- n^3 multiplications + n^3 additions = $2n^3$ floating point operations
- = $O(n^3)$ runtime

Blocking

- Increases locality
- Does not decrease cost

Can we reduce the op count?

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Strassen's Algorithm

Strassen, V. "Gaussian Elimination is Not Optimal," *Numerische Mathematik* 13, 354-356, 1969

Until then, MMM was thought to be $O(n^3)$

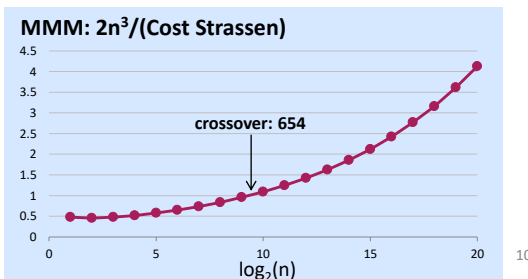
Recurrence for flops:

- $T(n) = 7T(n/2) + 9/2 n^2 = 7n^{\log_2(7)} - 6n^2 = O(n^{2.808})$
- Later improved: $9/2 \rightarrow 15/4$

Fewer ops from $n = 654$, but ...

- Structure more complex \rightarrow runtime crossover much later
- Numerical stability inferior

Can we reduce more?



MMM Complexity: What is known

Coppersmith, D. and Winograd, S.: "Matrix Multiplication via Arithmetic Programming," *J. Symb. Comput.* 9, 251-280, 1990

Makes MMM $O(n^{2.376\dots})$

Current best (Oct. 2020): $O(n^{2.3728596\dots})$ Previous best: $O(n^{2.3728639\dots})$

But unpractical

MMM is obviously $\Omega(n^2)$

It could well be close to $\Theta(n^2)$

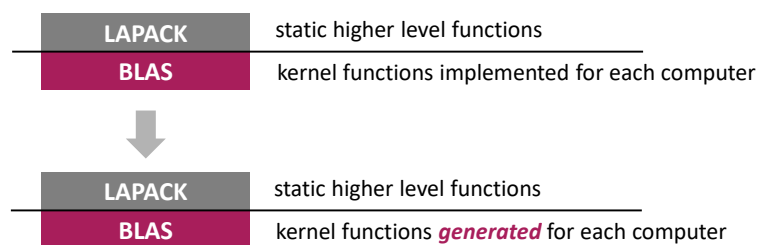
Practically all code out there uses $2n^3$ flops

Compare this to matrix-vector multiplication:

- Known to be $\Theta(n^2)$ (Winograd), i.e., boring

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The Path to Fast Libraries (continued)



ATLAS (late 1990s, inspired by PhiPAC): BLAS generator

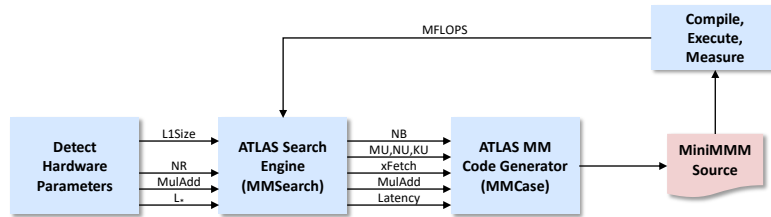
Enumerates many implementation variants (blocking etc.) and picks the fastest (example): advent of so-called autotuning

Enables automatic performance porting

Most important: BLAS3 MMM generator

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ATLAS Architecture



Hardware parameters:

- L1Size: size of L1 data cache
- NR: number of registers
- MulAdd: fused multiply-add available?
- L* : latency of FP multiplication

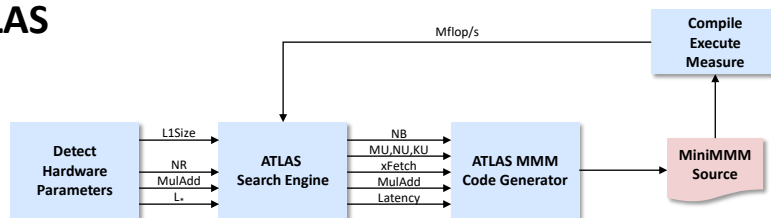
Search parameters:

- for example blocking sizes
- span search space
- specify code
- found by orthogonal line search

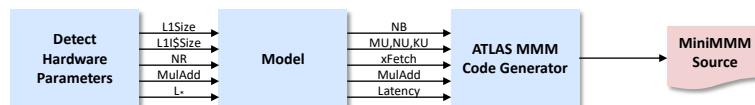
source: Pingali, Yotov, et al., Cornell U.

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ATLAS



Model-Based ATLAS (2005)



- Search for parameters replaced by model to compute them
- Much faster + provides understanding of what parameters are found

source: Pingali, Yotov, et al., Cornell U.

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Optimizing MMM



References:

R. Clint Whaley, Antoine Petitet and Jack Dongarra, *Automated Empirical Optimization of Software and the ATLAS project*, *Parallel Computing*, 27(1-2):3-35, 2001

K. Goto and R. van de Geijn, *Anatomy of high-performance matrix multiplication*, *ACM Transactions on mathematical software (TOMS)*, 34(23), 2008

K. Yotov, X. Li, G. Ren, M. Garzaran, D. Padua, K. Pingali, P. Stodghill, *Is Search Really Necessary to Generate High-Performance BLAS?*, *Proceedings of the IEEE*, 93(2), pp. 358–386, 2005.

Our presentation is based on this paper

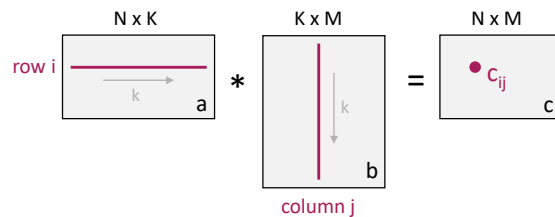
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0: Starting Point

Standard triple loop

```
// Computes c = c + ab
for i = 0:N-1
  for j = 0:M-1
    for k = 0:K-1
      c_ij = c_ij + a_ik*b_kj
```

Matlab-style
code notation



Most important in practice (based on usage in LAPACK)

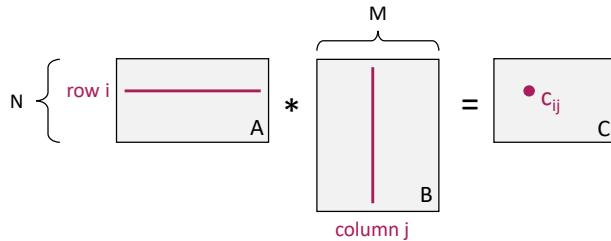
- Two out of N , M , K are small
- One out of N , M , K is small
- None is small (e.g., square matrices)

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1: Loop Order

```
// Computes C = C + AB
for i = 0:N-1
  for j = 0:M-1
    for k = 0:K-1
      c_ij = c_ij + a_ik*b_kj
```

i,j,k loops can be permuted in any order!

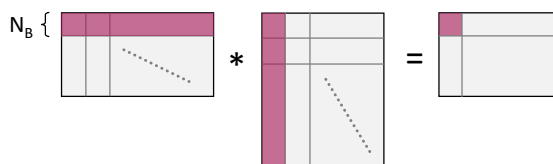


i-j-k: B is reused, good if $M < N$ (B is smaller than A)
 j-i-k: A is reused, good if $N < M$

} ATLAS does versioning (code for both variants)

Other options are inferior, e.g., k-i-j: Poor temporal locality w.r.t. C

2: Blocking for Cache



Like multiplying matrices consisting of size $N_B \times N_B$ entries
 Assume $N_B | M, N, K$

Results in six-fold loop
 Formally obtained through loop-tiling and loop exchange

```
for i = 0:N_B:N-1
  for j = 0:N_B:M-1
    for k = 0:N_B:K-1
      for i' = i:i+N_B-1
        for j' = j:j+N_B-1
          for k' = k:k+N_B-1
            c_i'j' = c_i'j' + a_i'k'*b_k'j'
```

} mini-MMMs

How to find the best N_B ?

ATLAS: uses search over all $N_B^2 \leq C_1$ (cache size)

Model: explained next

2: Blocking for Cache

a) Idea: Working set has to fit into cache

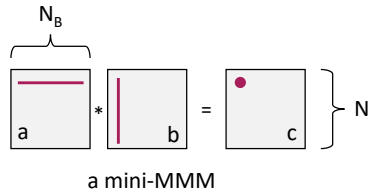
Easy estimate: | working set | = $3 N_B^2$

Model: $3 N_B^2 \leq C_1$

b) Closer analysis of working set:

$$N_B^2 + N_B + 1 \leq C_1$$

\uparrow all of b \uparrow row of a \uparrow element of c



c) Take into account cache block size B_1 :

$$\left\lceil \frac{N_B^2}{B_1} \right\rceil + \left\lceil \frac{N_B}{B_1} \right\rceil + 1 \leq \frac{C_1}{B_1}$$

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2: Blocking for Cache

d) Take into account LRU replacement

Build a history of accessed elements



$i=0$: $a_{0,0} b_{0,0} a_{0,1} b_{1,0} \dots a_{0,N_B-1} b_{N_B-1,0} c_{0,0}$ ($j=0$)

$a_{0,0} b_{0,1} a_{0,1} b_{1,1} \dots a_{0,N_B-1} b_{N_B-1,1} c_{0,1}$ ($j=1$)

...

$a_{0,0} b_{0,N_B-1} a_{0,1} b_{1,N_B-1} \dots a_{0,N_B-1} b_{N_B-1,N_B-1} c_{0,N_B-1}$ ($j=N_B-1$)

Corresponding history:

$b_{0,0} b_{1,0} \dots b_{N_B-1,0} c_{0,0}$

$b_{0,1} b_{1,1} \dots b_{N_B-1,1} c_{0,1}$

...

$a_{0,0} b_{0,N_B-1} a_{0,1} b_{1,N_B-1} \dots a_{0,N_B-1} b_{N_B-1,N_B-1} c_{0,N_B-1}$

Observations:

- All of b has to fit for next iteration ($i = 1$)
- When $i = 1$, row 1 of a will not cleanly replace row 0 of a
- When $i = 1$, elements of c will not cleanly replace previous elements of c

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2: Blocking for Cache

d) Take into account LRU replacement



History ($i = 0$):

$$b_{0,0} b_{1,0} \dots b_{N_B-1,0} c_{0,0}$$

$$b_{0,1} b_{1,1} \dots b_{N_B-1,1} c_{0,1}$$

...

$$a_{0,0} b_{0,N_B-1} a_{0,1} b_{1,N_B-1} \dots a_{0,N_B-1} b_{N_B-1,N_B-1} c_{0,N_B-1}$$

Observations:

- All of b has to fit for next iteration ($i = 1$)
- When $i = 1$, row 1 of a will not cleanly replace row 0 of a
- When $i = 1$, elements of c will not cleanly replace previous elements of c

This has to fit:

- Entire b
- 2 rows of a
- 1 row of c
- 1 element of c

$$\left\lceil \frac{N_B^2}{B_1} \right\rceil + 3 \left\lceil \frac{N_B}{B_1} \right\rceil + 1 \leq \frac{C_1}{B_1}$$

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2: Blocking for Cache


e) Take into account blocking for registers (next optimization)

$$\left\lceil \frac{N_B^2}{B_1} \right\rceil + 3 \left\lceil \frac{N_B M_U}{B_1} \right\rceil + \left\lceil \frac{M_U N_U}{B_1} \right\rceil \leq \frac{C_1}{B_1}$$


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3: Blocking for Registers

Blocking mini-MMMs into micro-MMMs for registers revisits the question of loop order:

i-j-k:  For fixed i,j: 2n operations

- n independent mults
- n dependent adds

k-i-j:  For fixed k: 2n² operations

- n² independent mults
- n² independent adds

} Better ILP (but larger working set)

Result: k-i-j loop order for micro-MMMs

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3: Blocking for Registers

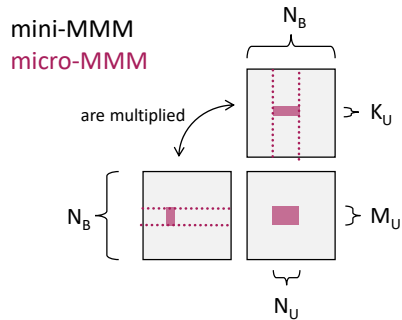
```

for i = 0:NB:N-1
  for j = 0:NB:M-1
    for k = 0:NB:K-1
      for i' = i:MU:i+NB-1
        for j' = j:NU:j+NB-1
          for k' = k:KU:k+NB-1
            for i'' = i':i'+MU-1
              for j'' = j':j'+NU-1
                c_i''j'' = c_i''j'' + a_i''k''*b_k''j''
          
```

mini-MMM (lines 4-6)

micro-MMM (lines 7-9)

X { lines 8-9



How to find the best M_U, N_U, K_U ?

ATLAS: uses search with bound

$$M_U + N_U + M_U N_U \leq N_R \quad \text{number of registers}$$

size of working set in X

Model: Use largest M_U, N_U that satisfy this equation and $M_U \approx N_U$

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4: Basic Block Optimizations

```
for i = 0:Nb:N-1
  for j = 0:Nb:M-1
    for k = 0:Nb:K-1
      for i' = i:MU:i+Nb-1
        for j' = j:NU:j+Nb-1
          for k' = k:KU:k+Nb-1
            for i'' = i':i'+MU-1
              for j'' = j':j'+NU-1
                c_i''j'' = c_i''j'' + a_i''k''*b_k''j''
```

mini-MMM

micro-MMM

Unroll micro-MMMs

Scalar replacement

Loads from c ($M_U N_U$ many) at ①

Loads from a and b ($M_U + N_U$ many) at ②

Requires $M_U + N_U + M_U N_U$ scalar variables

[Example of ATLAS-generated code](#)

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5: Other optimizations

Skewing: separate dependent add-mults for better ILP

Software pipelining: move load from one iteration to previous iteration to high load latency (a form of prefetching)

Buffering to avoid TLB misses (later)

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Remaining Details

Register renaming and the refined model for x86

TLB-related optimizations

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Dependencies

Read-after-write (RAW) or true dependency

W $r_1 = r_3 + r_4$ *nothing can be done*
R $r_2 = 2r_1$ *no ILP*

Write after read (WAR) or antidependency

R $r_1 = r_2 + r_3$ *dependency only by* $r_1 = r_2 + r_3$ *now ILP*
W $r_2 = r_4 + r_5$ *name \rightarrow rename* $r = r_4 + r_5$

Write after write (WAW) or output dependency

W $r_1 = r_2 + r_3$ *dependency only by* $r_1 = r_2 + r_3$ *now ILP*
...
W $r_1 = r_4 + r_5$ *name \rightarrow rename* $r = r_4 + r_5$

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Resolving WAR by Renaming

R $r_1 = r_2 + r_3$ *dependency only by* $r_1 = r_2 + r_3$ *now ILP*
W $r_2 = r_4 + r_5$ *name → rename* $r = r_4 + r_5$

Renaming can be done at three levels:

C source code (= you rename): use SSA style (next slide)

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Scalar Replacement + SSA

How to avoid WAR and WAW in your basic block source code

Solution: Single static assignment (SSA) code:

- Each variable is assigned exactly once

no duplicates

```
<more>
s266 = (t287 - t285);
s267 = (t282 + t286);
s268 = (t282 - t286);
s269 = (t284 + t288);
s270 = (t284 - t288);
s271 = (0.5*(t271 + t280));
s272 = (0.5*(t271 - t280));
s273 = (0.5*((t281 + t283) - (t285 + t287)));
s274 = (0.5*(s265 - s266));
t289 = ((9.0*s272) + (5.4*s273));
t290 = ((5.4*s272) + (12.6*s273));
t291 = ((1.8*s271) + (1.2*s274));
t292 = ((1.2*s271) + (2.4*s274));
a122 = (1.8*(t269 - t278));
a123 = (1.8*s267);
a124 = (1.8*s269);
t293 = ((a122 - a123) + a124);
a125 = (1.8*(t267 - t276));
t294 = (a125 + a123 + a124);
t295 = ((a125 - a122) + (3.6*s267));
t296 = (a122 + a125 + (3.6*s269));
<more>
```

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Resolving WAR by Renaming

R $r_1 = r_2 + r_3$ *dependency only by* $r_1 = r_2 + r_3$ *now ILP*
W $r_2 = r_4 + r_5$ *name \rightarrow rename* $r = r_4 + r_5$

Renaming can be done at three levels:

C source code (= you rename)

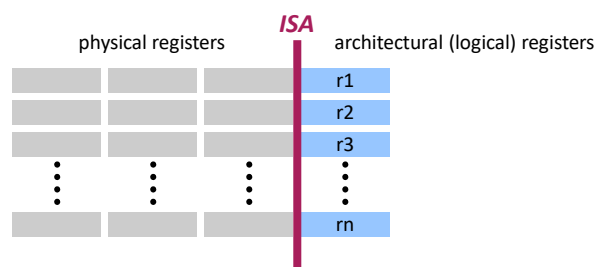
Compiler: Uses a different register upon register allocation, $r = r_6$

Hardware (if supported): dynamic register renaming

- Requires a separation of architectural and physical registers
- Requires more physical than architectural registers

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Register Renaming



Hardware manages mapping architectural \rightarrow physical registers

Each logical register has several associated physical registers

Hence: more instances of each r_i can be created

Used in superscalar architectures (e.g., Intel Core) to increase ILP by dynamically resolving WAR/WAW dependencies

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Micro-MMM Standard Model

$$MU * NU + MU + NU \leq NR - \text{ceil}((Lx+1)/2)$$

this parameter I did not explain, see paper

Core (NR = 16): MU = 2, NU = 3



Code sketch (KU = 1)

```
rc1 = c[0,0], ..., rc6 = c[1,2] // 6 registers
loop over k {
  load a // 2 registers
  load b // 3 registers
  compute // 6 independent mults, 6 independent adds, reuse a and b
}
c[0,0] = rc1, ..., c[1,2] = rc6
```

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Extended Model (x86)

Set MU = 1, NU = NR - 2 = 14



Code sketch (KU = 1)

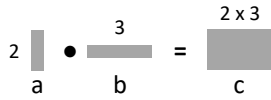
```
rc1 = c[0], ..., rc14 = c[13] // 14 registers
loop over k {
  load a // 1 register
  { rb = b[1] // 1 register
    rb = rb*a // mult (two-operand)
    rc1 = rc1 + rb // add (two-operand)
  } // reuse register (WAR: register renaming resolves it)
  { rb = b[2]
    rb = rb*a
    rc2 = rc2 + rb
  }
  ...
}
c[0] = rc1, ..., c[13] = rc14
```

Summary:

- no reuse in a and b
- + larger tile size available for c since for b only one register is used

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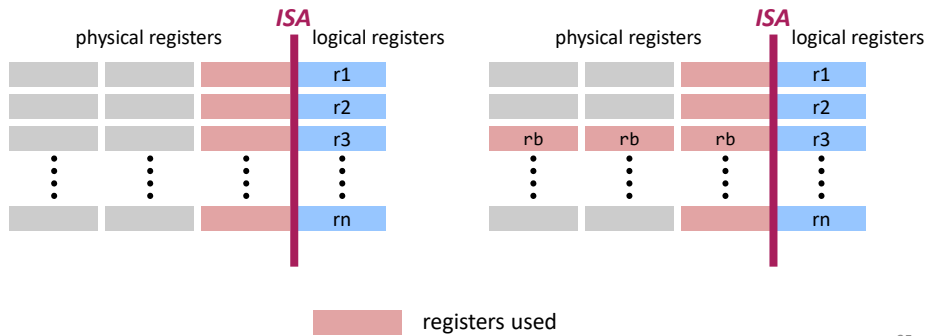
Visualization of What Seems to Happen



reuse in a, b, c



reuse in c



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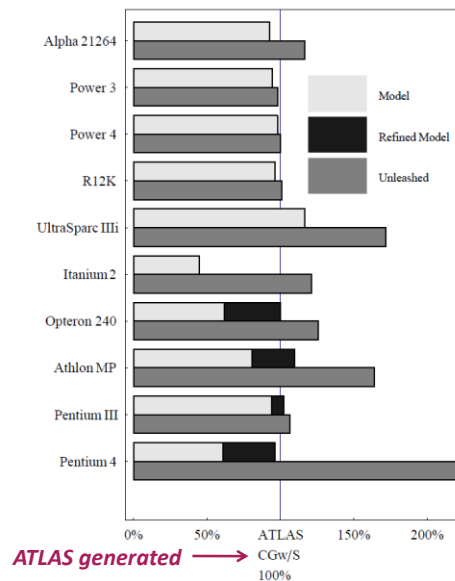
Experiments

Unleashed: Not generated = hand-written contributed code

Refined model for computing register tiles on x86

Blocking is for L1 cache

Result: Model-based is comparable to search-based (except Itanium)



graph: Pingali, Yotov, Cornell U. 36

Remaining Details

Register renaming and the refined model for x86

TLB-related optimizations

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Virtual Memory System (Core Family)

The processor works with *virtual addresses*

All caches work with *physical addresses*

Both address spaces are organized in pages

Page size: 4 KB (can be changed to 2 MB and even 1 GB in OS settings)

Address translation: virtual address → physical address

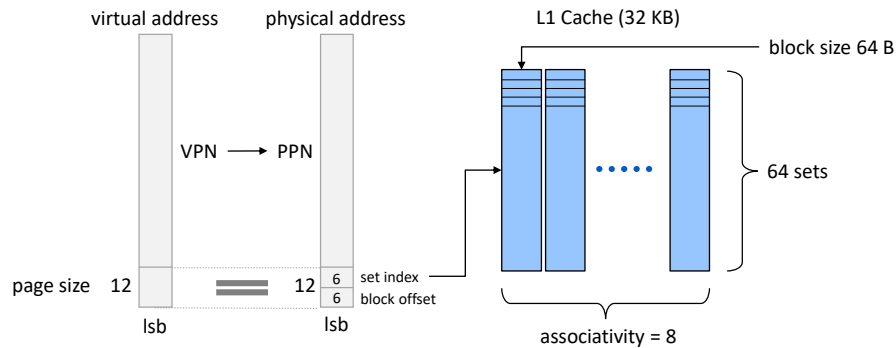
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Virtual/Physical Addresses

Processor: virtual addresses

Caches: physical addresses

Page size = 4 KB



L1 cache lookup can start concurrently with address translation!

How would Intel (likely) increase the L1 cache size?

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Address Translation

Uses a cache called translation lookaside buffer (TLB)

Haswell/Skylake:

Level 1 ITLB (instructions): 128 entries
DTLB (data): 64 entries

Level 2 Shared (STLB): 1024/1536 entries (Haswell/Skylake)

Miss Penalties:

- DTLB hit: no penalty
- DTLB miss, STLB hit: few cycles penalty
- STLB miss: can be very expensive

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Impact on Performance

Repeatedly accessing a working set spread over too many pages yields TLB misses and can result in a significant slowdown.

Example Haswell: STLB = 1024

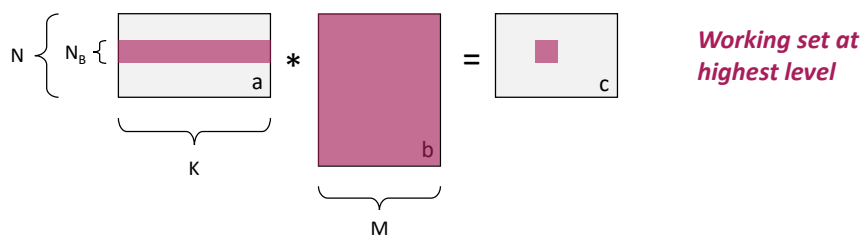
A computation that repeatedly accesses a working set of 2048 doubles spread over 2048 pages will cause STLB misses.

How much space will this working set occupy in cache (assume no conflicts)?

$2048 * 64 \text{ B} = 128 \text{ KB}$ (fits into L2 cache)

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Example MMM



We are looking for parts in the working set that are spread out in memory:

- Block row of a : contiguous
- All of b : contiguous
- Block of c : if $M > 512$, then spread over N_B pages

Typically, N_B is in the 10s, so no problem

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Fast MMM: Principles

Optimization for memory hierarchy

- *Blocking for cache*
- *Blocking for registers*

Basic block optimizations

- *Loop order for ILP*
- *Unrolling + scalar replacement*
- *Scheduling & software pipelining*

Optimizations for virtual memory

- *Buffering (copying spread-out data into contiguous memory)*

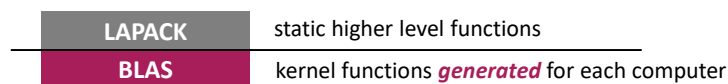
Autotuning

- *Search over parameters (ATLAS)*
- *Model to estimate parameters (Model-based ATLAS)*

*All high performance MMM libraries do some of these
(but possibly in slightly different ways)*

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Path to Fast Libraries



The advent of SIMD vector instructions (SSE, 1999) made ATLAS obsolete

The advent of multicore systems (ca. 2005) required a redesign of LAPACK (just parallelizing BLAS is suboptimal)

Recently, BLAS interface needs to be extended to handle higher-order tensor operations (used in machine learning)

Automatic generation of blocked algorithms, alternatives to LAPACK ([FLAME](#))

Program generator for small linear algebra operations ([SLinGen/LGen](#))

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Lessons Learned

Implementing even a relatively simple function with optimal performance can be highly nontrivial

Autotuning can find solutions that a human would not think of implementing

Understanding which choices lead to the fastest code can be very difficult

MMM is a great case study, touches on many performance-relevant issues

Most domains are not studied as carefully as dense linear algebra

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