Advanced Systems Lab

Spring 2023

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

Instructor: Markus Püschel, Ce Zhang

TA: Joao Rivera, several more

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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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*

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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, data science and machine learning, engineering)

Efficient software is extremely relevant

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The Path to Fast Libraries

EISPACK and LINPACK (early 1970s)

- *Focus on dense matrices*
- *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 (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)

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*
- *Jack Dongarra (Turing award 2021), Jim Demmel et al.*

Two-layer architecture

LAPACK	static higher-level functions
BLAS	kernel functions implemented for each computer

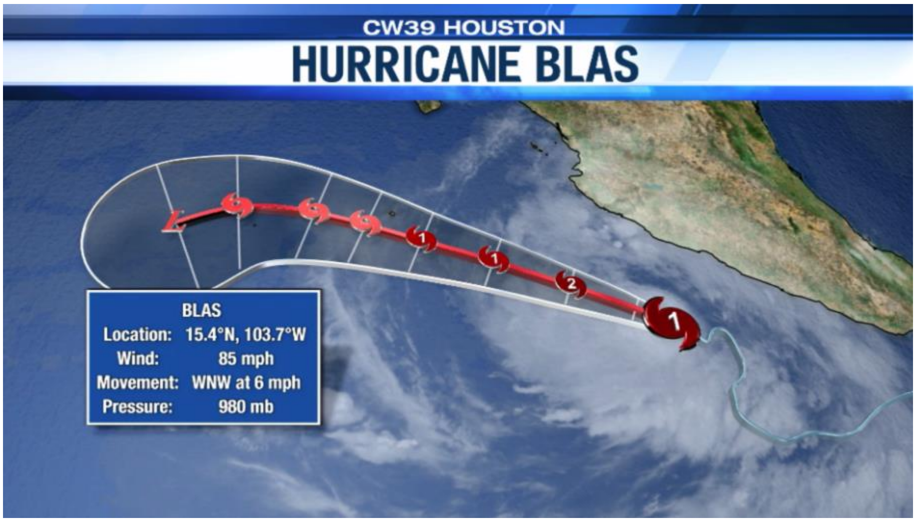
Basic Linear Algebra Subroutines (BLAS)

	$I(n) =$
BLAS 1: vector-vector operations (e.g., vector sum)	$O(1)$
BLAS 2: matrix-vector operations (e.g., matrix-vector product)	$O(1)$
BLAS 3: matrix-matrix operations (e.g., MMM)	$O(\sqrt{C})$

↑ cache size

LAPACK uses BLAS 3 as much as possible

Fast MMM → fast BLAS3 (since all MMM related)

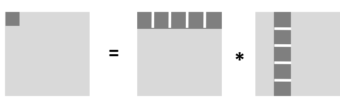


Reminder: Why is BLAS3 so important?

Using BLAS 3 (instead of BLAS 1 or 2) in LAPACK
= blocking
= high operational intensity I
= high performance

Remember (blocking MMM): $I(n) =$

$O(1)$



$O(\sqrt{C})$

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?

Strassen's Algorithm

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

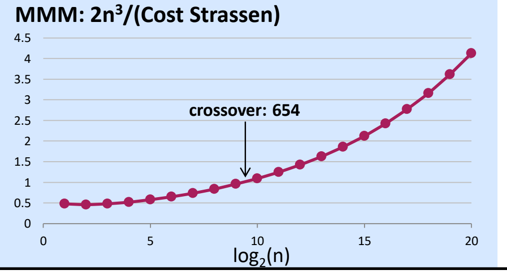
Until then, MMM was thought to be $\Theta(n^3)$

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 → 15/4*

Fewer ops from n = 654, but …

- *Structure more complex → 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 $O(n^{2.376...})$

Current best (Oct. 2022): $O(n^{2.37188...})$ Previous best: $O(n^{2.3728596...})$

But unpractical (a galactic algorithm)

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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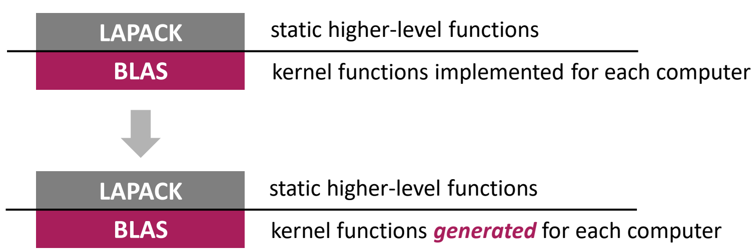
The Path to Fast Libraries (continued)



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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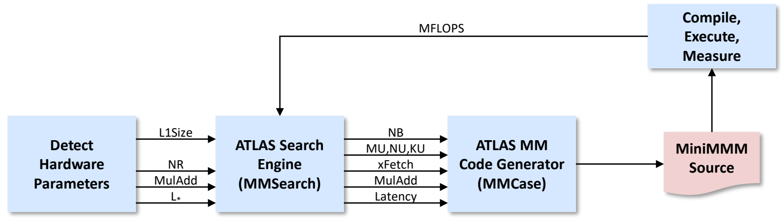
ATLAS Architecture



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

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

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

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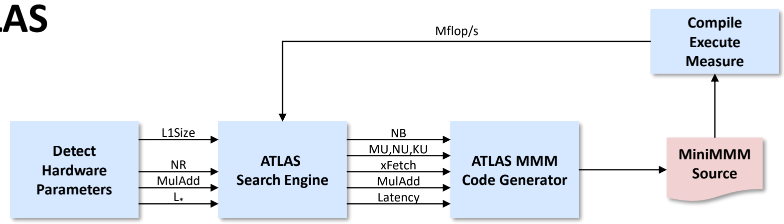
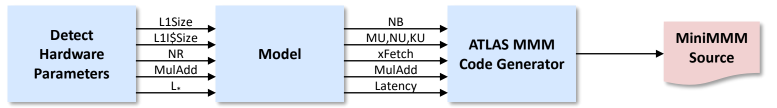
ATLAS



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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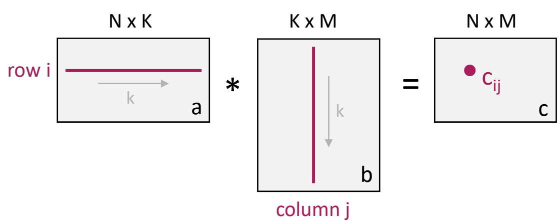
0: Starting Point

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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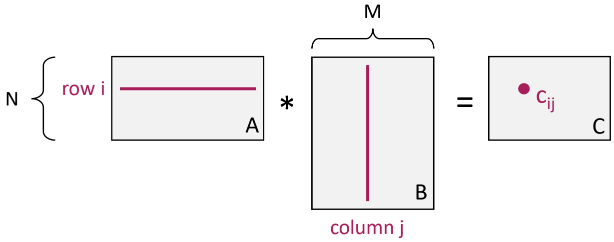
1: Loop Order

```
// 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!

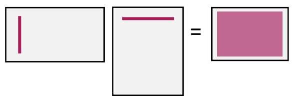


i-j-k: B is reused, good if M < N (B is smaller than A)

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

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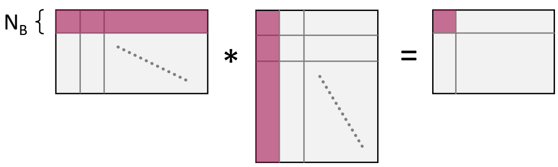
2: Blocking for Cache



Like multiplying matrices consisting of size N_B x 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 $N_B^2 \leq \min(C, 80^2)$ (C = measured cache size)
Model: explained next, uses C_1 = measured L1 cache size

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2: Blocking for Cache

a) Idea: Working set has to fit into cache
Easy estimate: |working set| = $3 N_B^2$
Model: $3 N_B^2 \le C_1$

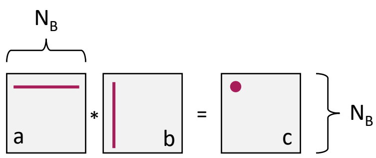
b) Closer analysis of working set:

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

(N_B^2: all of b; N_B: row of a; 1: element of c)

c) Take into account cache block size B_1:

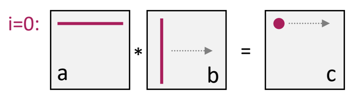
$$\left\lceil \frac{N_B^2}{B_1} \right\rceil + \left\lceil \frac{N_B}{B_1} \right\rceil + 1 \le \frac{C_1}{B_1}$$



a mini-MMM

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

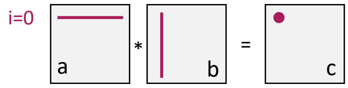
Corresponding history:

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

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

2: Blocking for Cache

d) Take into account LRU replacement



History (i = 0):

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

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: $2n^2$ operations
- n^2 independent mults
- n^2 independent adds

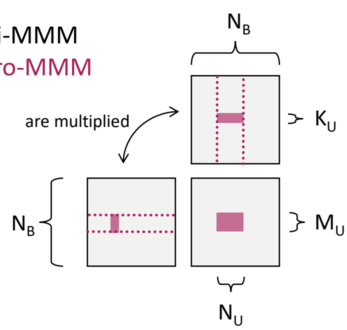
} Better ILP (but larger working set)

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

3: Blocking for Registers

```
for i = 0:N_B:N-1
  for j = 0:N_B:M-1
    for k = 0:N_B:K-1
      for i' = i:M_U:i+N_B-1                       mini-MMM
        for j' = j:N_U:j+N_B-1
          for k' = k:K_U:k+N_B-1
            for k" = k':k'+K_U-1                   micro-MMM
       X {    for i" = i':i'+M_U-1
                for j" = j':j'+N_U-1
                  c_i"j" = c_i"j" + a_i"k"*b_k"j"
```

mini-MMM
micro-MMM



How to find the best M_U, N_U, K_U?
ATLAS: uses search with bound

$$\underbrace{M_U + N_U + M_U N_U}_{\text{size of working set in } X} \leq N_R \quad \text{number of registers}$$

size of working set in X
(all the red parts on the left)

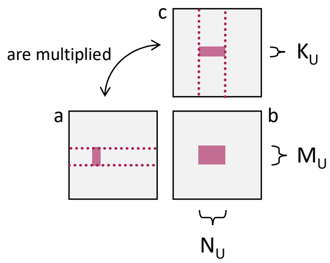
Model: Use largest M_U, N_U that satisfy this equation and $M_U \approx N_U$

4: Basic Block Optimizations

```
for i = 0:N_B:N-1
  for j = 0:N_B:M-1
    for k = 0:N_B:K-1
      for i' = i:M_U:i+N_B-1                         (1)   mini-MMM
        for j' = j:N_U:j+N_B-1
          for k' = k:K_U:k+N_B-1                     (2)
            for k" = k':k'+K_U-1                           micro-MMM
              for i" = i':i'+M_U-1
                for j" = j':j'+N_U-1
                  c_i"j" = c_i"j" + a_i"k"*b_k"j"
```

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
(all the red parts on the right)

Example of ATLAS-generated code



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5: Other optimizations (see paper)

Skewing: separate dependent add-mults for better ILP

Software pipelining: move load from one iteration to previous iteration to hide 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 → 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*
	…	*name → rename*	…	
W	$r_1 = r_4 + r_5$		$r = r_4 + r_5$	

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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:

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

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>
```

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:

1. C source code (= you rename)

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

3. Hardware (if supported): dynamic register renaming
   - *Requires a separation of architectural and physical registers*
   - *Requires more physical than architectural registers*

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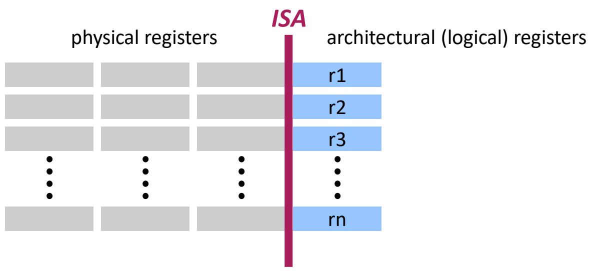
Register Renaming



Each logical register has several associated physical registers

Hardware manages mapping architectural → 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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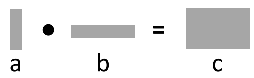
Micro-MMM Standard Model

$M_U*N_U + M_U + N_U \le N_R - \text{ceil}((L_x+1)/2)$

this parameter I did not explain, see paper

Core ($N_R = 16$): $M_U = 2$, $N_U = 3$



reuse in a, b, c

Code sketch ($K_U = 1$)

```
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
```

But on x86 that's not what ATLAS' search found

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Extended Model (x86)

Set $M_U = 1$, $N_U = N_R - 2 = 14$

reuse in c only

Code sketch ($K_U = 1$)

```
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)
 {rb = b[2]      // reuse register (WAR: register renaming resolves it)
 {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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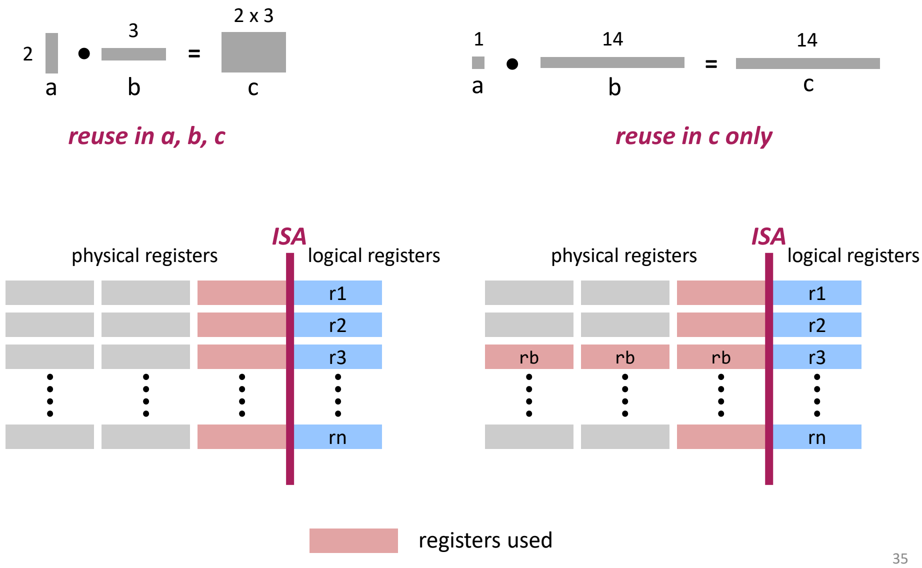
Visualization of What Seems to Happen



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Experiments

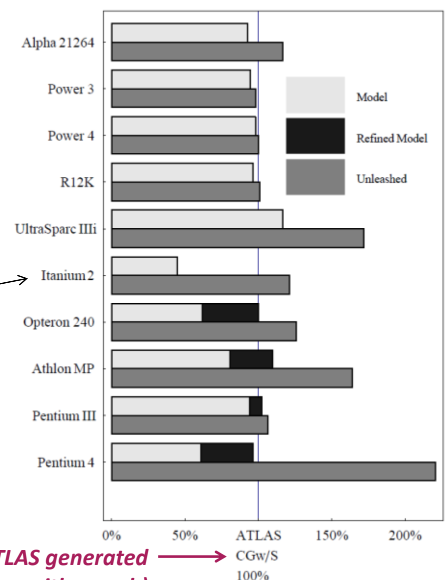
Unleashed: Not generated = hand-written contributed mini-MMM code

Refined model for computing register tiles on x86

Blocking by model is for L1 cache

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

Search optimized for L2 cache (without knowing), the model blocks for L1 cache which here cannot store floats



ATLAS generated (Code generation with search) is the baseline

graph: Pingali, Yotov, Cornell U.

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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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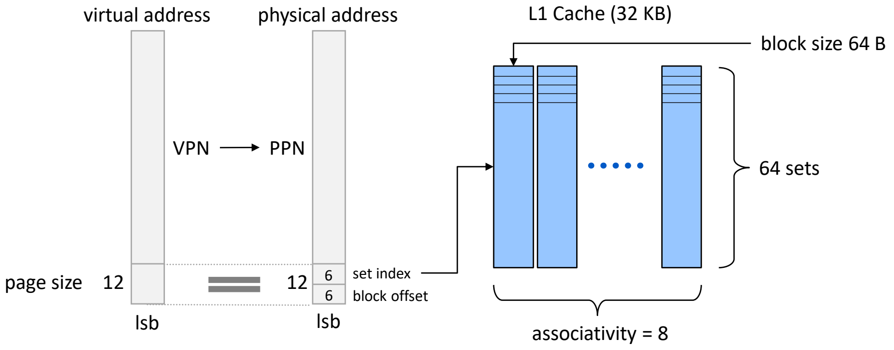
Virtual/Physical Addresses

Processor: virtual addresses
Caches: physical addresses
Page size = 4 KB

VPN: virtual page number
PPN: physical page number



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)

Skylake:

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

Level 2 Shared (STLB): 1536 entries

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 Skylake: STLB = 1536

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 B = 128 KB (fits into L2 cache)

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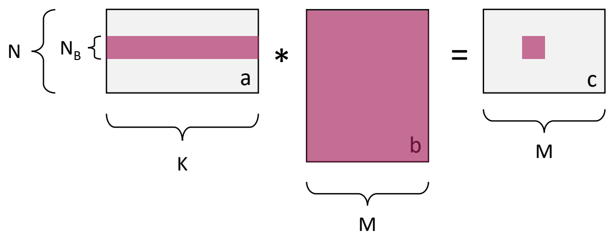
Example MMM



Working set at highest level

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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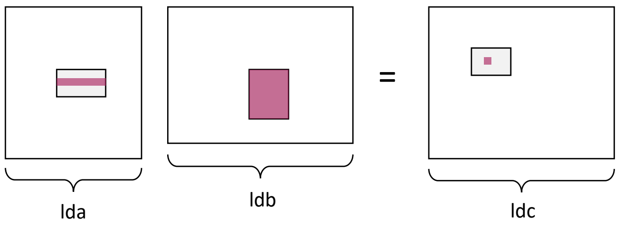
Example MMM, contd.

Interface BLAS function: `dgemm(a, b, c, N, K, M, lda, ldb, ldc)`

matrices (a, b, c) — sizes (N, K, M) — leading dimensions (lda, ldb, ldc)

Leading dimensions: Enable use on matrices inside matrices



Assume lda, ldb, ldc > 512:

- *Block row of a: spread over ≥ N_B pages*
- *All of b: spread over ≥ K pages*
- *Block of c: Spread over ≥ N_B pages*

So copying to contiguous memory may pay off

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Example MMM, contd.

Resulting code (sketch):

```
// all of b reused: possible copy to contiguous memory
for i = 0:N_B:N-1
  // block row of a reused: possibly copy
  for j = 0:N_B:M-1
    // block of c reused: possibly copy
    for k = 0:N_B:K-1
      ……
```

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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)

Path to Fast Libraries

LAPACK	static higher level functions
BLAS	kernel functions ***generated*** for each computer

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)

Small scale linear algebra requires quite different optimizations
(see program generator SLinGen/LGen)

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