How to Write Fast Numerical Code

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

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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

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**

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
- **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
  - Jim Demmel, Jack Dongarra et al.
- **Requires a two layer architecture**

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

- **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**

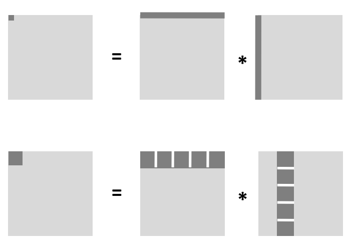
$I(n) =$
$O(1)$
$O(1)$
$O(\sqrt{C})$

cache size

5

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):** $I(n) =$



$O(1)$

$O(\sqrt{C})$

6

The Path to Fast Libraries

- **Before we continue a little detour**

Matlab

- **Invented in the late 1970s by Cleve Moler**
- **Commercialized (MathWorks) in 1984**
- **Motivation: Make LINPACK, EISPACK easy to use**
- **Matlab uses LAPACK and other 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)

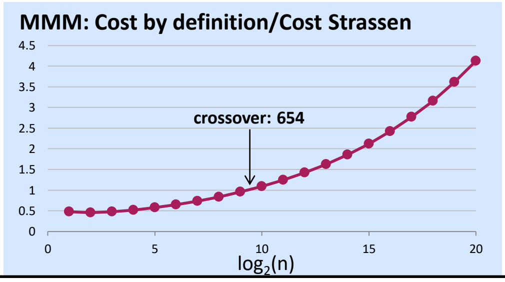
MMM: Complexity?

- **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?**

9

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?**



10

MMM Complexity: What is known

- Coppersmith, D. and Winograd, S.: **"Matrix Multiplication via Arithmetic Programming,"** *J. Symb. Comput.* 9, 251-280, 1990
- **Makes MMM is O($n^{2.376}$)**
- **Current best: O($n^{2.373}$)**
- **But unpractical**

- **MMM is obviously Ω(n^2)**
- **It could well be close to Θ(n^2)**
- **Practically all code out there uses $2n^3$ flops**

- **Compare this to matrix-vector multiplication:**
  - Known to be Θ(n^2) (Winograd), i.e., boring

11

The Path to Fast Libraries (continued)

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

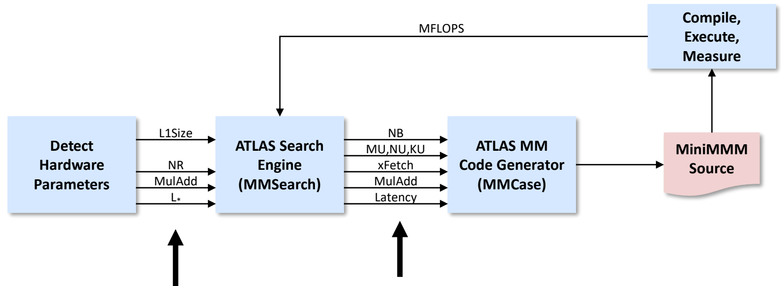
⇓

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

- **ATLAS (late 1990s, inspired by PhiPAC): BLAS generator**
- **Enumerates many implementation variants (blocking etc.) and picks the fastest (example)**
- **Enables automatic performance porting**
- **Most important: BLAS3 MMM generator**

12

ATLAS Architecture

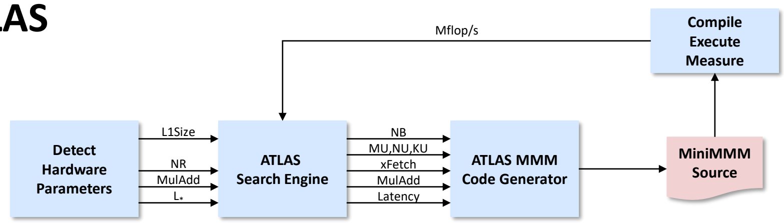


Search parameters:
- for example blocking sizes
- span search space
- specify code
- found by orthogonal line search

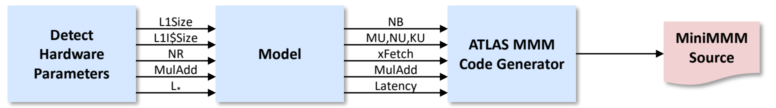
Hardware parameters:
- L1Size: size of L1 data cache
- NR: number of registers
- MulAdd: fused multiply-add available?
- L_* : latency of FP multiplication

source: Pingali, Yotov, Cornell U.

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, Cornell U.

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Optimizing MMM

- **Blackboard**
- **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

Remaining Details

- **Register renaming and the refined model for x86**
- **TLB effects**

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

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)**

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>
```

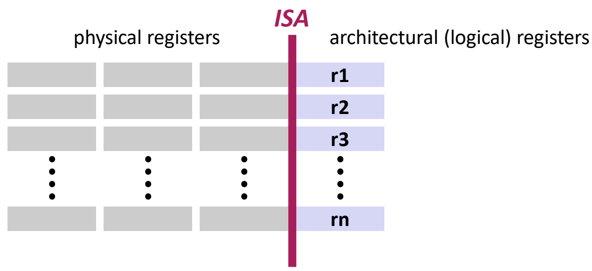

Resolving WAR by Renaming

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:

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

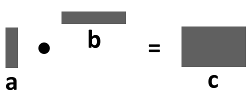
Register Renaming



- Hardware manages mapping architectural → 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

Micro-MMM Standard Model

- MU*NU + MU + NU ≤ NR – ceil((Lx+1)/2)
- Core (NR = 16): MU = 2, NU = 3



reuse in a, b, c

- 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 indep. mults, 6 indep. adds, reuse a and b
}
c[0,0] = rc1, …, c[1,2] = rc6
```

Extended Model (x86)

- Set MU = 1, NU = NR – 2 = 14

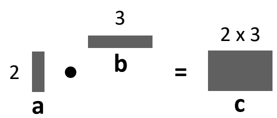
reuse in c

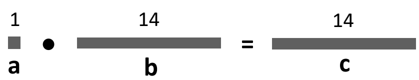
- Code sketch (KU = 1)

```
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)
  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

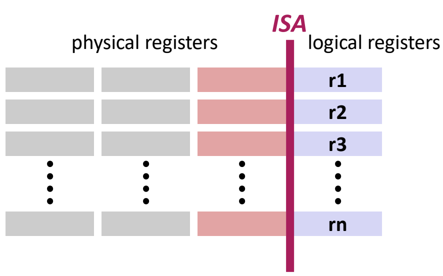
Visualization of What Seems to Happen

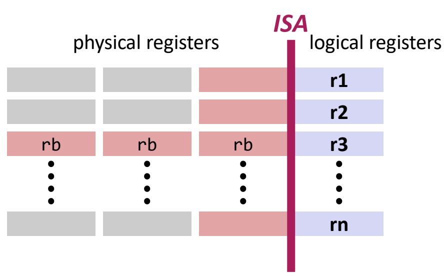




reuse in a, b, c

reuse in c





register used

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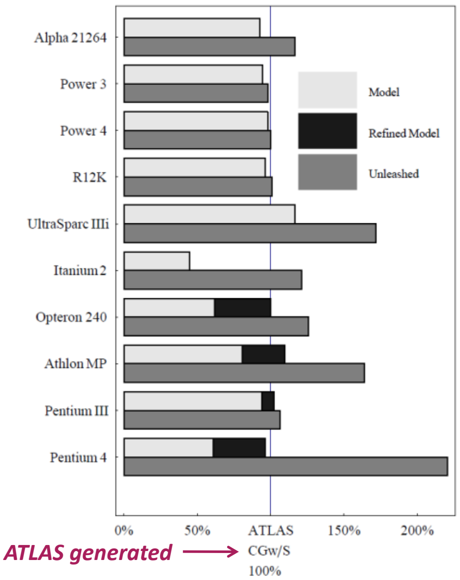
Experiments

- *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.

Remaining Details

- Register renaming and the refined model for x86
- TLB effects
  - Blackboard

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)**
- **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)**