How to Write Fast Numerical Code

Spring 2017

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

Instructor: Markus Püschel

TA: Alen Stojanov, Georg Ofenbeck, Gagandeep Singh

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Overview

- **Linear algebra software: history, 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 most of the numerical computation across disciplines (sciences, computer science, engineering)**
- **Efficient software is extremely relevant**

The Path to Fast Libraries

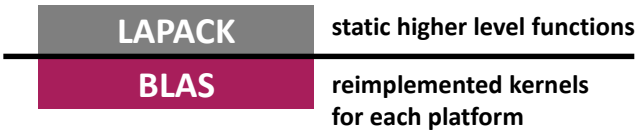
- **EISPACK and LINPACK (early 70s)**
  - Libraries for linear algebra algorithms
  - Jack Dongarra, Jim Bunch, Cleve Moler, Gilbert Stewart
  - LINPACK still the name of the benchmark for the TOP500 (Wiki) list of most powerful supercomputers
- **Problem:**
  - Implementation vector-based = low operational intensity *(e.g., MMM as double loop over scalar products of vectors)*
  - Low performance on computers with deep memory hierarchy (in the 80s)
- **Solution: LAPACK**
  - Reimplement all algorithms "block-based," i.e., with locality
  - Developed late 1980s, early 1990s
  - Jim Demmel, Jack Dongarra et al.

Matlab

- **Invented in the late 70s by Cleve Moler**
- **Commercialized (MathWorks) in 84**
- **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)

LAPACK and BLAS

- **Basic Idea:**



- **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 implemented on top of BLAS**
  - Using BLAS 3 as much as possible

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

cache size

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):** $I(n) =$

$O(1)$

$O(\sqrt{C})$

Overview

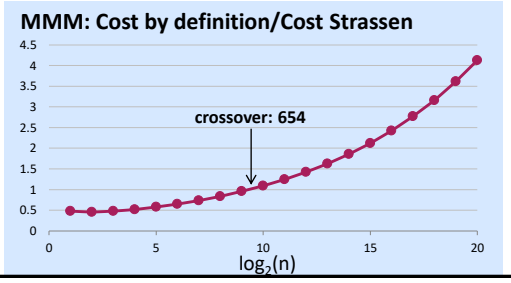
- Linear algebra software: history, LAPACK and BLAS
- Blocking (BLAS 3): key to performance
- **Fast MMM**
  - Algorithms
  - ATLAS
  - model-based ATLAS

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

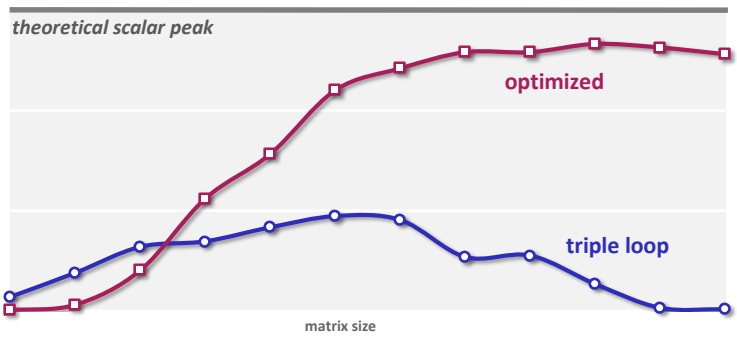
- Coppersmith, D. and Winograd, S.: **"Matrix Multiplication via Arithmetic Programming,"** *J. Symb. Comput.* 9, 251-280, 1990
- **MMM is $O(n^{2.376})$**
- **But no practical algorithm**

- **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

MMM: Memory Hierarchy Optimization

MMM (square real double) Core 2 Duo 3Ghz



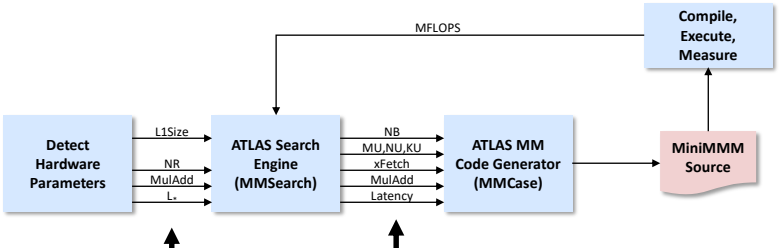
- **Huge performance difference for large sizes**
- **Great case study to learn memory hierarchy optimization**

ATLAS

- BLAS program generator and library (web, successor of PhiPAC)
- Idea: automatic porting

- People can also contribute handwritten code
- The generator uses empirical search over implementation alternatives to find the fastest implementation
  no vectorization or parallelization: so not really used anymore
- We focus on BLAS 3 MMM
- Search only over cost $2n^3$ algorithms
  (cost equal to triple loop)

ATLAS Architecture

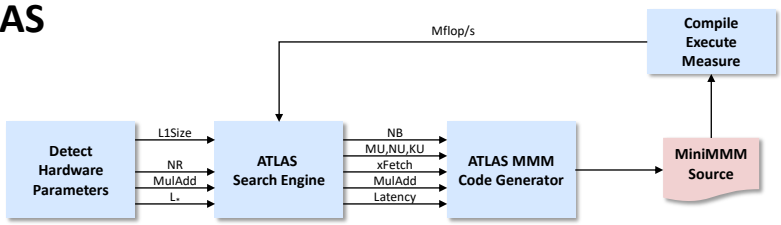


Search parameters:
- for example blocking sizes
- span search space
- specify code
- found by orthogonal line search

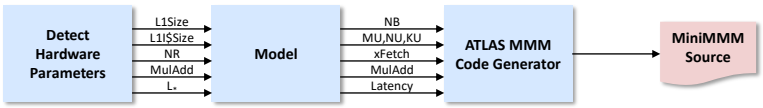
Hardware parameters:
- L1Size: size of L1 data cache
- NR: number of registers
- MulAdd: fused multiply-add available?
- L_* : latency of FP multiplication

source: Pingali, Yotov, Cornell U.

ATLAS



Model-Based ATLAS



- Search for parameters replaced by model to compute them
- More hardware parameters needed

source: Pingali, Yotov, Cornell U.

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  r1 = r3 + r4
R  r2 = 2r1
```

nothing can be done
no ILP

- Write after read (WAR) or antidependency

```
R  r1 = r2 + r3
W  r2 = r4 + r5
```

dependency only by name → rename

```
r1 = r2 + r3
r  = r4 + r5
```

now ILP

- Write after write (WAW) or output dependency

```
W  r1 = r2 + r3
   …
W  r1 = r4 + r5
```

dependency only by name → rename

```
r1 = r2 + r3
…
r  = r4 + r5
```

now ILP

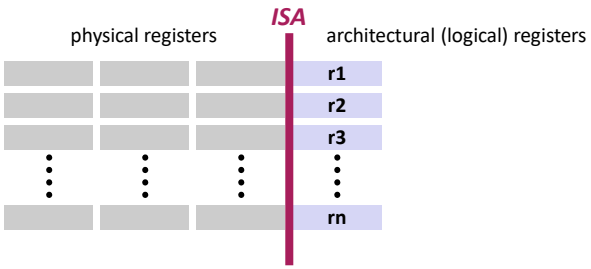
Resolving WAR by Renaming

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

now ILP

- **Compiler: Use a different register, r = r_6**
- **Hardware (if supported): register renaming**
  - Requires a separation of architectural and physical registers
  - Requires more physical than architectural registers

Register Renaming



- **Hardware manages mapping architectural → physical registers**
- **More physical than logical registers**
- **Hence: more instances of each r_i can be created**
- **Used in superscalar architectures (e.g., Intel Core) to increase ILP by resolving WAR dependencies**

Scalar Replacement Again

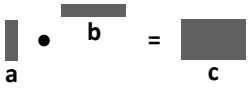
- **How to avoid WAR and WAW in your basic block source code**
- **Solution: Single static assignment (SSA) code:**
  - Each variable is assigned exactly once

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>
```


Micro-MMM Standard Model

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

- MU = 1, NU = NR – 2 = 14

reuse in c

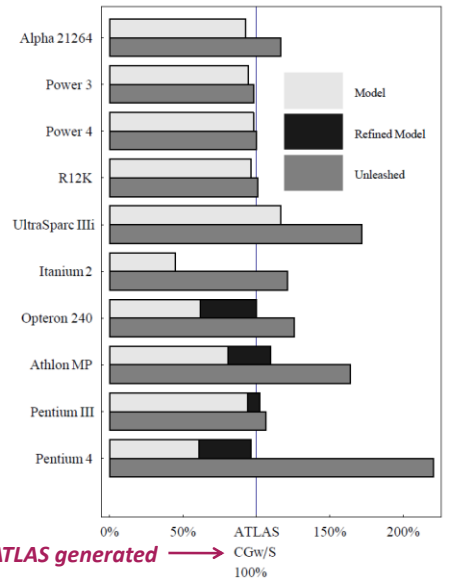
- Code sketch (KU = 1)

```
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: renaming resolves it)
  rb = rb*a
  rc2 = rc2 + rb
  …
}
c[0] = rc1, …, c[13
```

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

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