GEMM3: Constant-Workspace High-Performance Multiplication of Three Matrices for Matrix Chaining

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Matrix chaining problem

- Problem: compute $A_1 A_2 \cdots A_n$ efficiently
- $O(n \log n)$ algorithm, also $O(n^3)$ with dynamic programming
- Fewer flops $\rightarrow$ more performance?

Generalized matrix chaining

- In reality — transposes, inverses, properties
- Ensemble Kalman filter $X_i^b S_i (Y_i^b)^T R_i^{-1}$
  Tridiagonalization $\tau_u \tau_v v v^T A u u^T$
  Two-sided triangular solve $L^{-1} A L^{-H}$ (L lower triangular)
- Performance with BLAS/LAPACK – must be expert
- Less performance with Matlab, numpy, etc. (left-to-right)
- Linnea: expression $\rightarrow$ BLAS calls automagically

GEMM3 — Why bother?

-
  - $\boldsymbol{X_i^b S_i (Y_i^b)^T} R_i^{-1}$
  - $\tau_u \tau_v \boldsymbol{v v^T A u u^T}$
  - $\boldsymbol{L}^{-1}\boldsymbol{A}(\boldsymbol{L}^{-1})^{\boldsymbol{H}}$ (L lower triangular)
- All multiply three matrices as a subproblem
- (Notation: $G \mathrel{+}= DEF$ and GEMM3)
- Not everything divides well this way

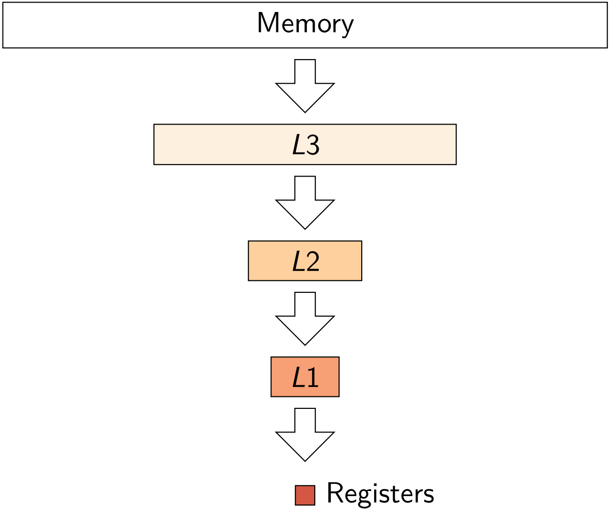
GEMM3 — Why a new algorithm?

- Current approach: parentheses, multiply twice, store temporary T
- T often eats memory (& perf)
- We can do better!
- Use how GEMM works to nest computations
- $O(1)$ extra memory, maybe more performance

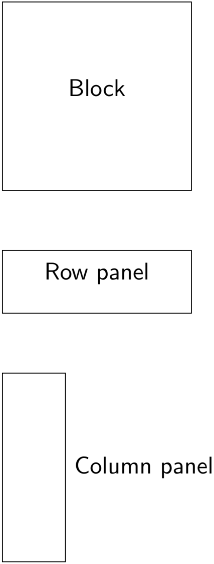
Section 2

High-Performance GEMM

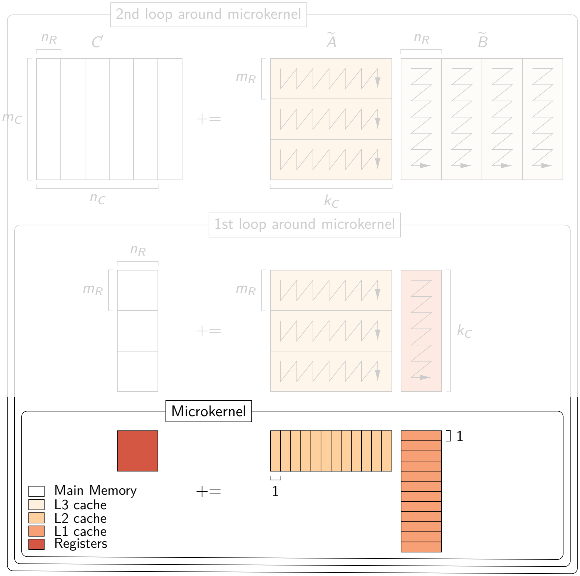
Memory hierarchy



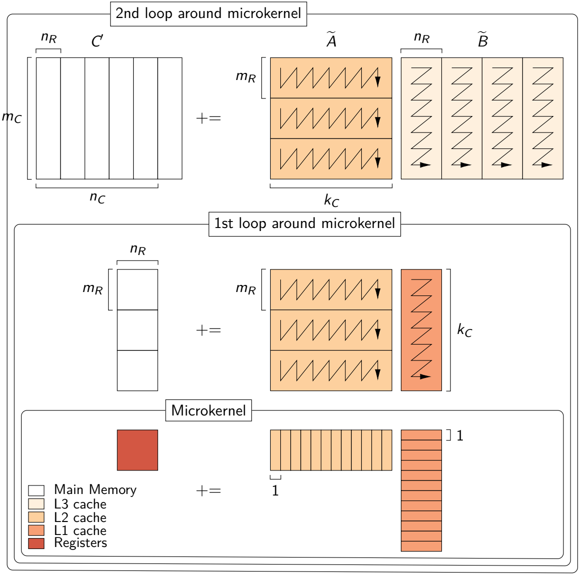
Important matrix shapes



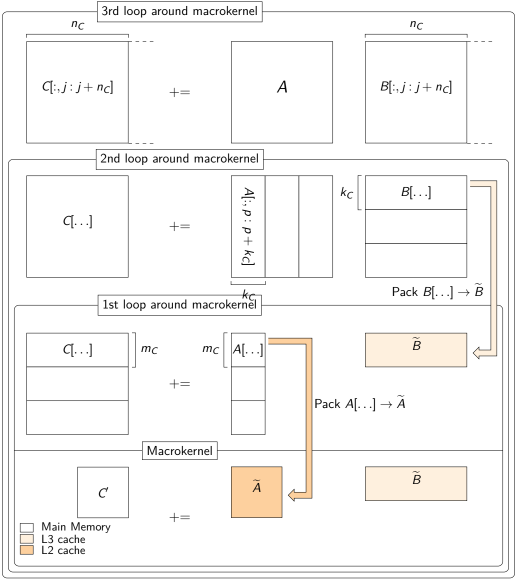
GEMM: The kernels



GEMM: The kernels



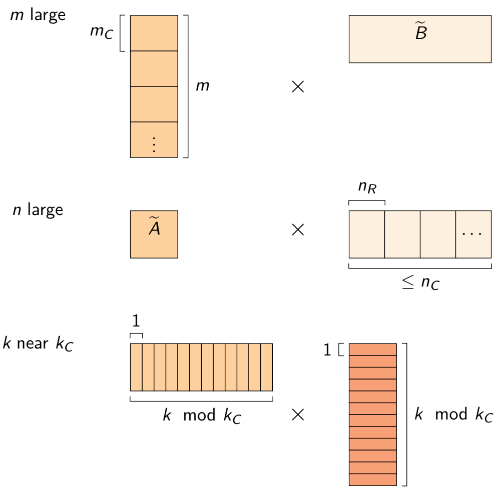
GEMM: The algorithm



Data reuse

- Every loop reads *something* repeatedly

Want:



Section 3

The GEMM3 algorithm

Key concept of the algorithm

- We want $G += DEF$, (dimensions: m, k, l, n in order)
- EF first needed in packing step
- Compute a row panel then

Deriving GEMM3: Partitionings

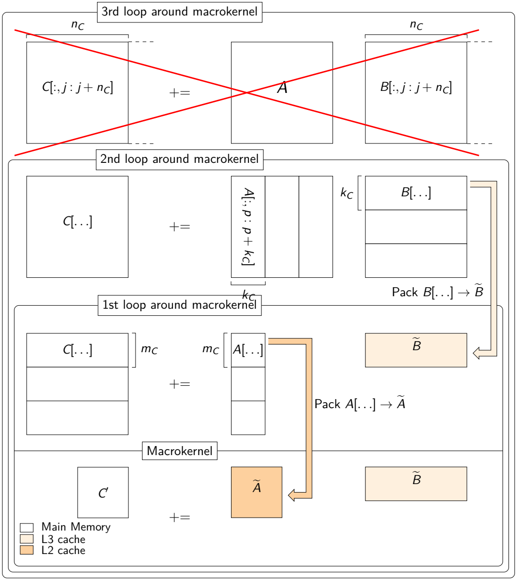
	G	$+=$	D	$[(EF)$	$\leftrightarrow$	E	$F]$
1.	$m \times n$	$+=$	$m \times k$	$k \times n$	$\leftrightarrow$	$k \times l$	$l \times n$
2.	$m \times n_C$	$+=$	$m \times k$	$k \times n_C$	$\leftrightarrow$	$k \times l$	$l \times n_C$
3.	$m \times n_C$	$+=$	$m \times k_C$	$k_C \times n_C$	$\leftrightarrow$	$k_C \times l$	$l \times n_C$

Deriving GEMM3: Inner algorithm

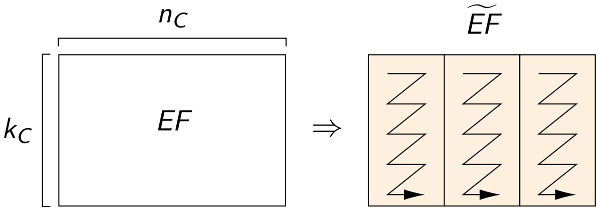
$$EF\colon k_C \times n_C \quad = \quad E\colon k_C \times l \quad F\colon l \times n_C$$

- Only point to compute EF in constant memory
- GEMM algorithm needs tweaks

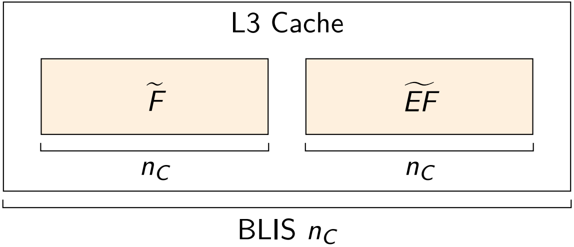
Inner algorithm tweaks: Removing the outer loop



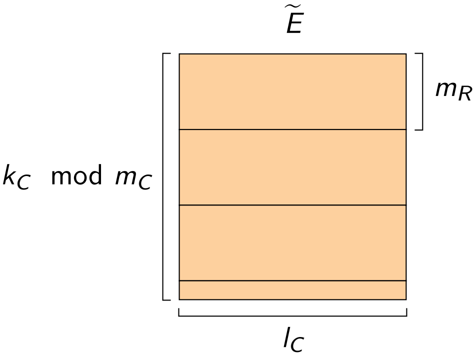
Inner alg. tweaks: Microkernel packed writes



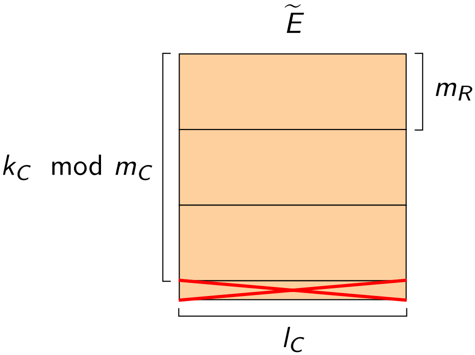
Inner alg. tweaks: Halving n_C



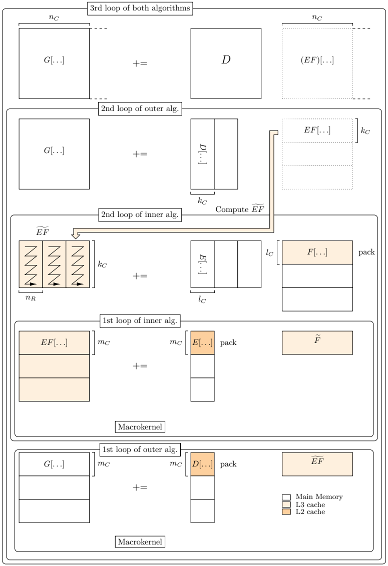
Inner algtweaks: Small k_C reduction



Inner algtweaks: Small k_C reduction



The algorithm

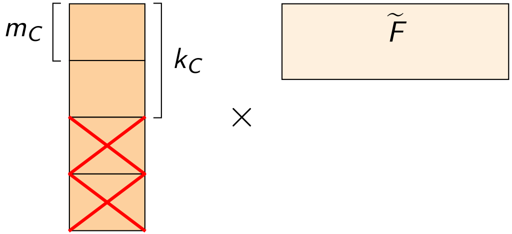


The small drawback

Problem shape:

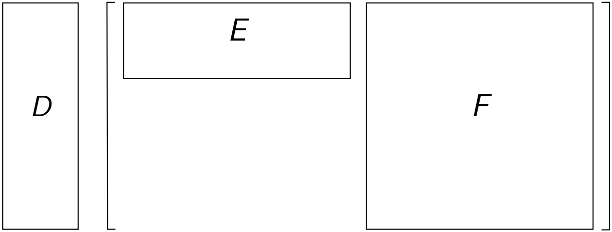
$$\widetilde{EF}\colon k_C \times n_C \quad = \quad E\colon k_C \times l \quad F\colon l \times n_C$$

Reuse problem: m small



$G \mathrel{+}= (DE)F$

Ex: Don't



- Putting parentheses there sometimes better
- Deriving directly doesn't work — bad shape
- However, $G \mathrel{+}= (DE)F \Leftrightarrow G^T \mathrel{+}= F^T(E^T D^T)$

Section 4

Experiments and Results

Implementation details

- Multilevel Optimization of Matrix Multiply Sandbox (MOMMS)
- Extended to support three matrices
- Implement both GEMM3 and BLIS algorithm
- BLIS algorithm port performs like BLIS
- Machine: 3.5 GHz (one core used), 15 GB RAM, 32 KB $L1$ cache, 256 KB $L2$, 8 MB $L3$. Peak perf 56 GFLOPS/s.

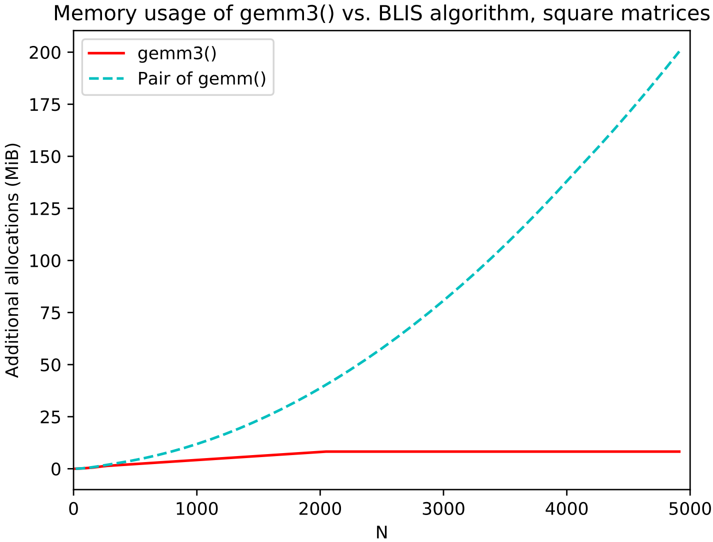
	GEMM3	BLIS algorithm
m_R	6	6
n_R	8	8
m_C	72	72
k_C	252	256
l_C	256	
n_C	2040	4080

Table: Parameters for Haswell CPUs

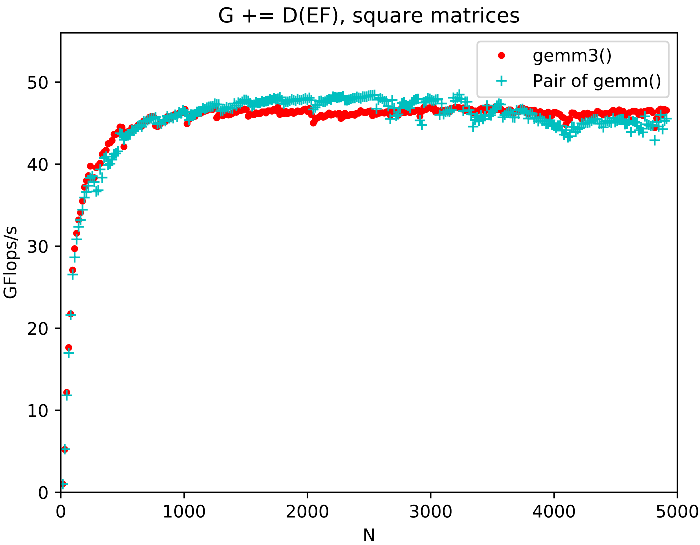
Experiments

1. $G \mathrel{+}= D(EF)$, square matrices
   - Inputs column-major, outputs row-major for fairness
2. $G^T \mathrel{+}= F^T(E^T D^T)$, square matrices
   - After transpose, all row major
3. $G \mathrel{+}= D(EF)$, rectangles (one dimension small)

Workspace usage, square matrices



$G += D(EF)$, square matrices



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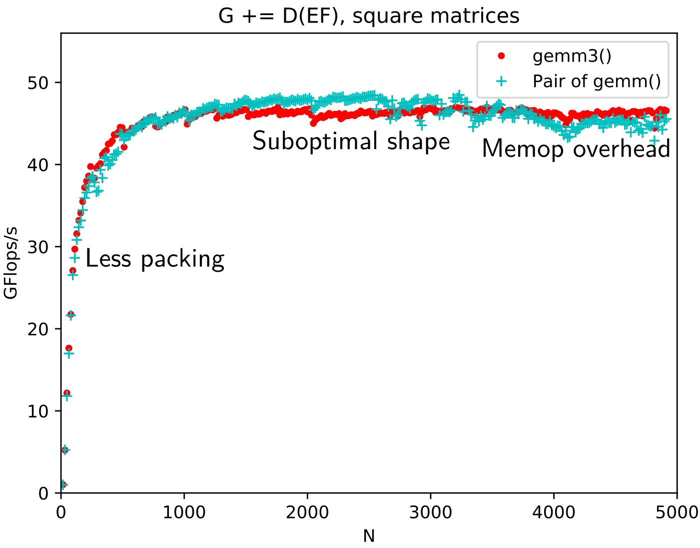
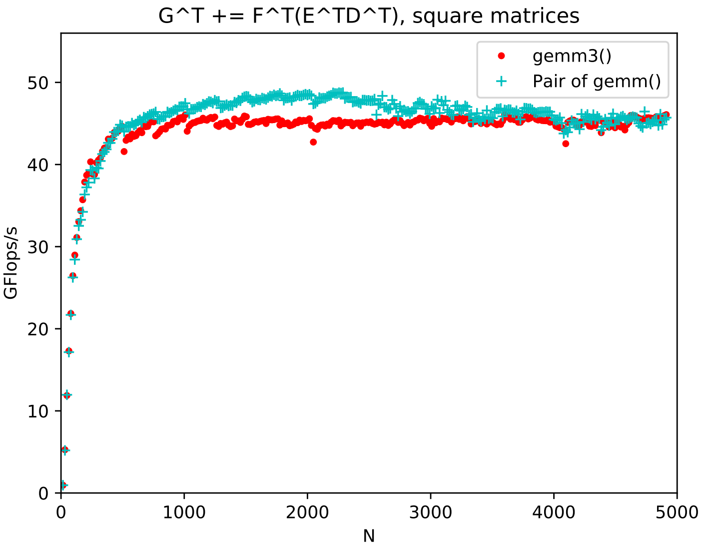
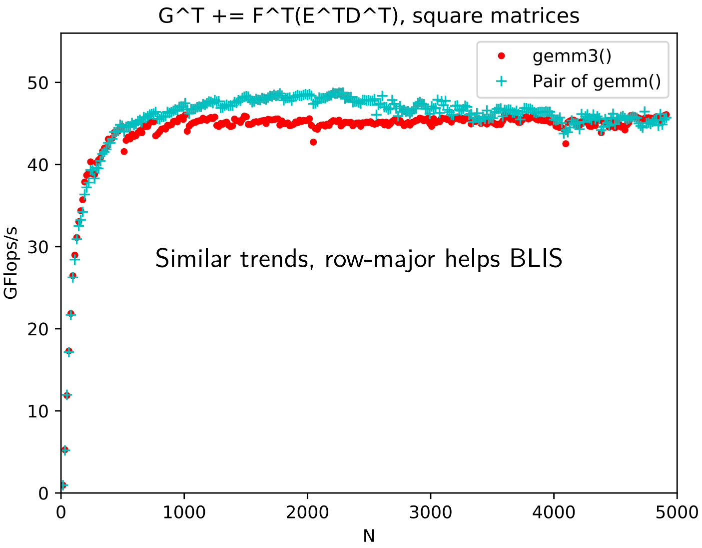


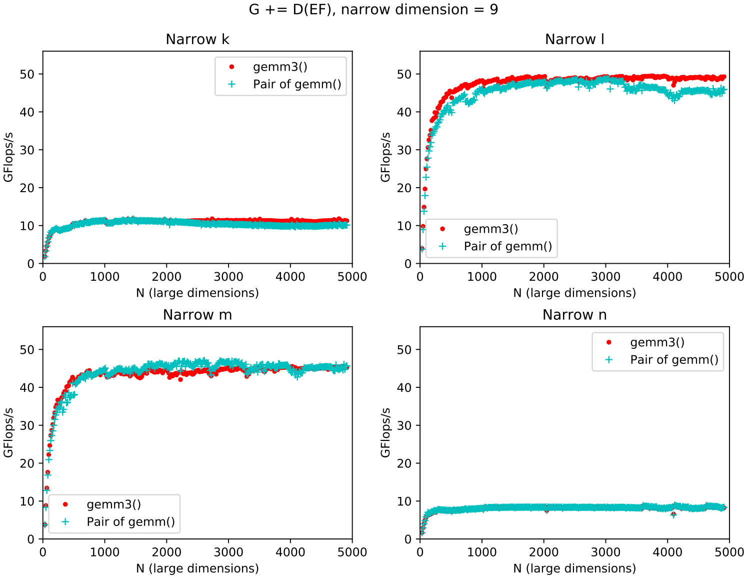
$G += (DE)F$, square matrices



$G \mathrel{+}= (DE)F$, square matrices



$G += D(EF)$, rectangular matrices



Conclusions

- GEMM structure lets us make GEMM3
- Constant memory
- Comprable performance
- Cleaner API

Future Work

- Parallel case
- More architectures

Acknowledgments

- Prof. Robert van de Geijn — advising and providing inspiration
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Questions?

Picking parameters: m_R, n_R

- Determine microkernel
- Based on microarchitecture — register width, FMA properties
- We're reusing BLIS's work
- Can swap m_R and n_R

Picking parameters: k_C

Placing memory in cache: [tag][set #][offset in line]

$$m_r k_c S_{elem} = C_A C_{L1} N_{L1} \qquad n_r k_C S_{elem} = C_B C_{L1} N_{L1}$$

L1
Cache:

$$\begin{matrix} A & A & B & B \\ A & B & B & C \end{matrix} \quad \cdots$$

$$C_A + C_B + 1 \leq W_{L1}$$

Maximizing k_C improves performance

$$\begin{aligned} C_B &= \left\lceil \frac{n_R k_C S_{elem}}{N_{L1} C_{L1}} \right\rceil \\ &= \left\lceil \frac{n_R}{m_R} C_A \right\rceil \\ C_A &\leq \left\lfloor \frac{W_{L1} - 1}{1 + \frac{n_R}{m_R}} \right\rfloor \end{aligned}$$

Picking parameters: m_C and n_C

- For m_C: reserve ways for B and C
- Then take all you can
- n_C, leave out what architecture requires, then divide
- L3 is very big, tuning is much less needed