

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 automatically

GEMM3 — Why bother?

- ▶ ▶ $\mathbf{X}_i^b \mathbf{S}_i (\mathbf{Y}_i^b)^T \mathbf{R}_i^{-1}$
- ▶ $\tau_u \tau_v \mathbf{v} \mathbf{v}^T \mathbf{A} \mathbf{u} \mathbf{u}^T$
- ▶ $\mathbf{L}^{-1} \mathbf{A} (\mathbf{L}^{-1})^H$ (\mathbf{L} lower triangular)
- ▶ All multiply three matrices as a subproblem
- ▶ (Notation: $G \mathrel{+}= DEF$ and GEMM3)

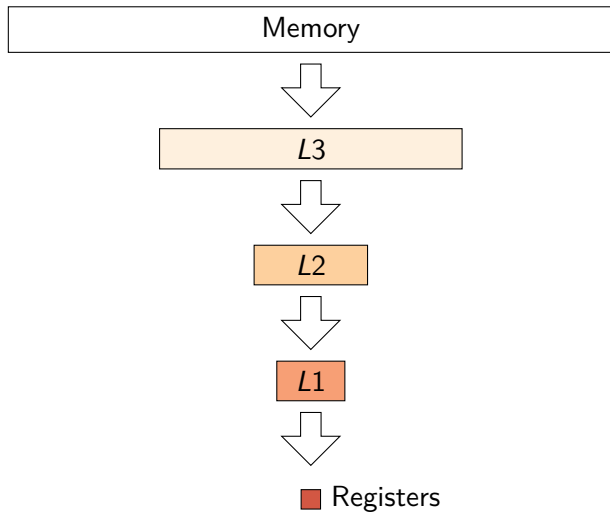
GEMM3 — Why a new algorithm?

- ▶ 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

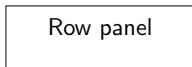
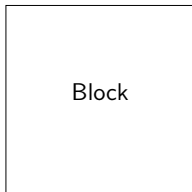
Section 2

High-Performance GEMM

Memory hierarchy

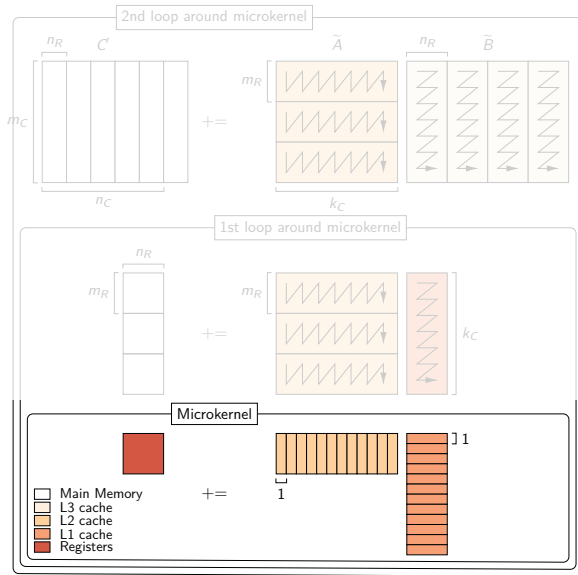


Important matrix shapes

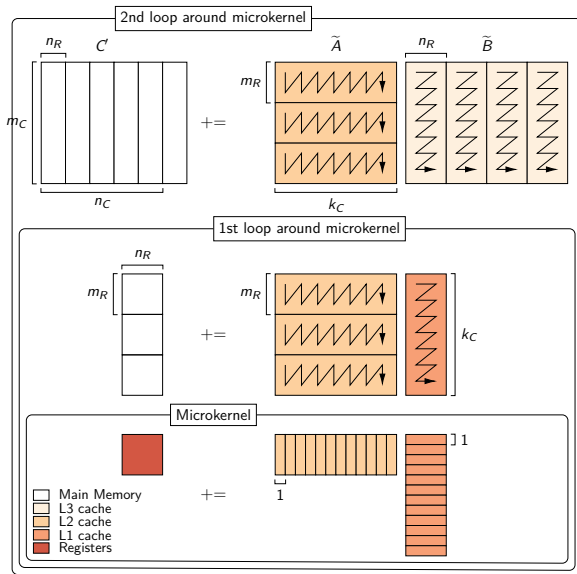


Column panel

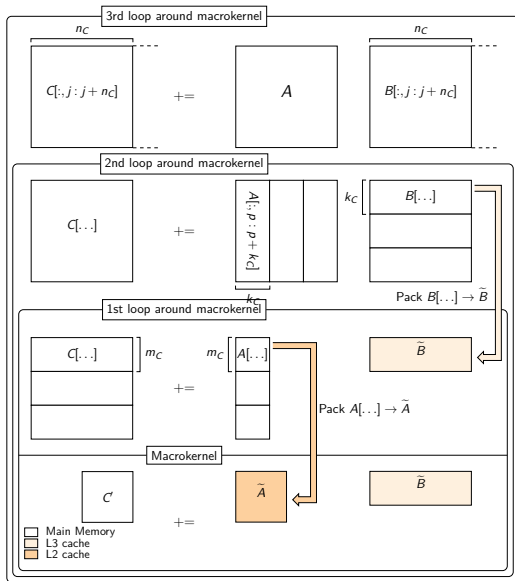
GEMM: The kernels



GEMM: The kernels



GEMM: The algorithm



Data reuse

- ▶ Every loop reads *something* repeatedly
- ▶ Relevant things: packed regions — making them takes time
- ▶ Packed region reuse when:
 - ▶ m large — many blocks of A per \tilde{B}
 - ▶ n large — many column panels in \tilde{B}
 - ▶ k not tiny — more time in microkernel

Section 3

The GEMM3 algorithm

Key concept of the algorithm

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

Deriving GEMM3: Partitionings

$$G \quad += \quad D \quad [(EF) \quad \leftrightarrow \quad E \quad F]$$

1. $m \times n \quad += \quad m \times k \quad \left[\begin{array}{c} k \times n \end{array} \right] \leftrightarrow \begin{array}{cc} k \times l & l \times n \end{array}$

2. $m \times n_C \quad += \quad m \times k \quad \left[\begin{array}{c} k \times n_C \end{array} \right] \leftrightarrow \begin{array}{cc} k \times l & l \times n_C \end{array}$

3. $m \times n_C \quad += \quad \begin{array}{c} m \times \\ k_C \end{array} \quad \left[\begin{array}{c} k_C \times n_C \end{array} \right] \leftrightarrow \begin{array}{cc} k_C \times l & l \times n_C \end{array}$

Deriving GEMM3: Inner algorithm

$$\boxed{\widetilde{EF}: k_C \times n_C} = \boxed{E: k_C \times l} \boxed{F: l \times n_C}$$

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

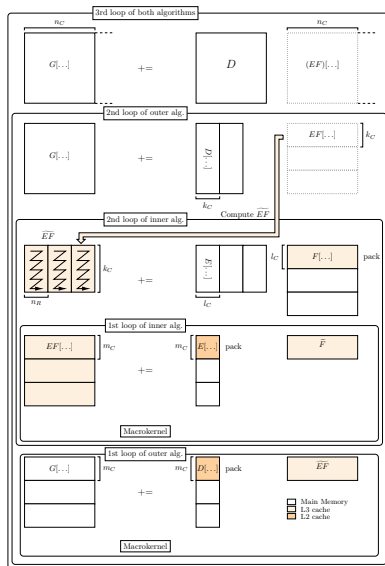
Deriving GEMM3: The tricky bits

Change	Why?
Remove outermost loop	Redundant ($n \leq n_C$)
Microkernel writes packed format	Save space/time
Halve n_C	\widetilde{EF} fights \widetilde{F} for L3
Lower k_C so $m_R \mid k_C$	Avoid fringe performance issues

Table: Tweaks needed to make GEMM fusion work

- ▶ Low \widetilde{F} reuse remains a problem
 - ▶ Low impact in practice

The algorithm



$$G += (DE)F$$

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

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

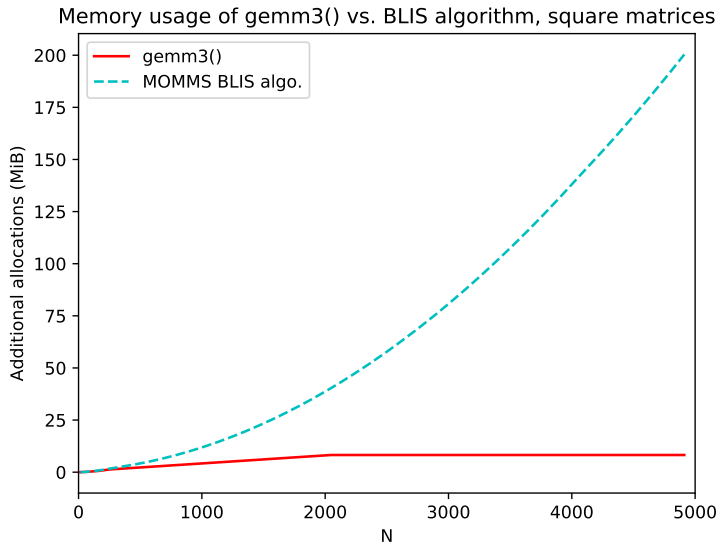
	GEMM3	BLIS algorithm
m_R	6	6
n_R	8	8
m_C	72	72
k_C	252	256
l_C	256	
n_C	2040	4080

Table: Parameters for Haswell CPUs

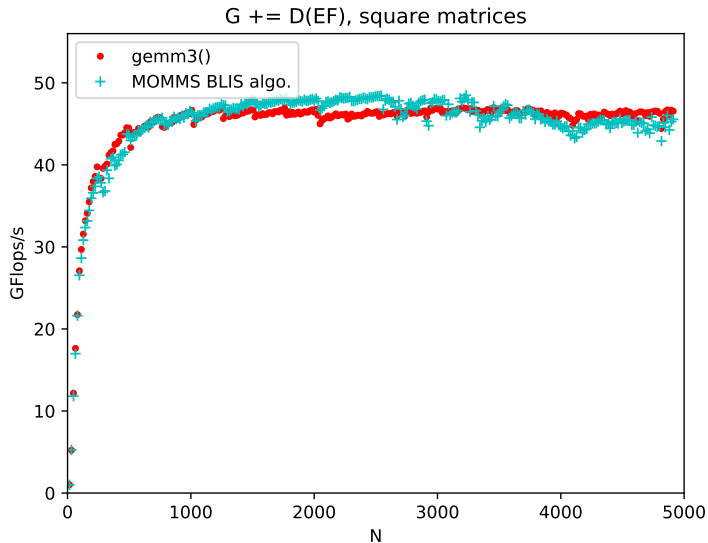
Experiments

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

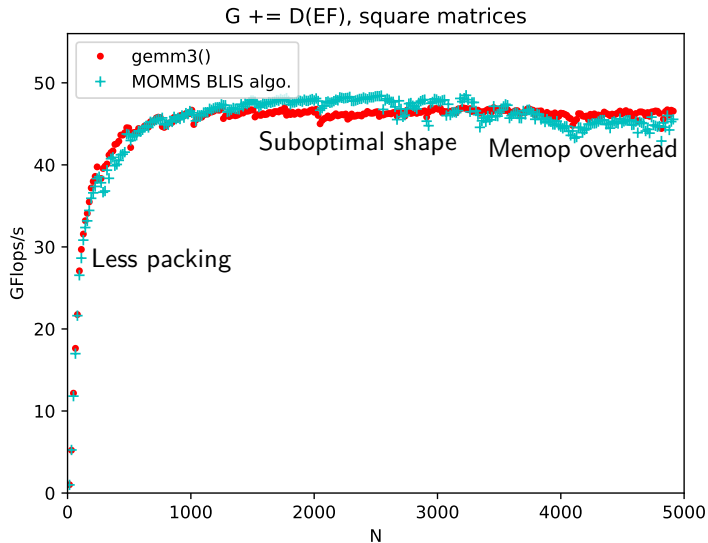
Workspace usage, square matrices



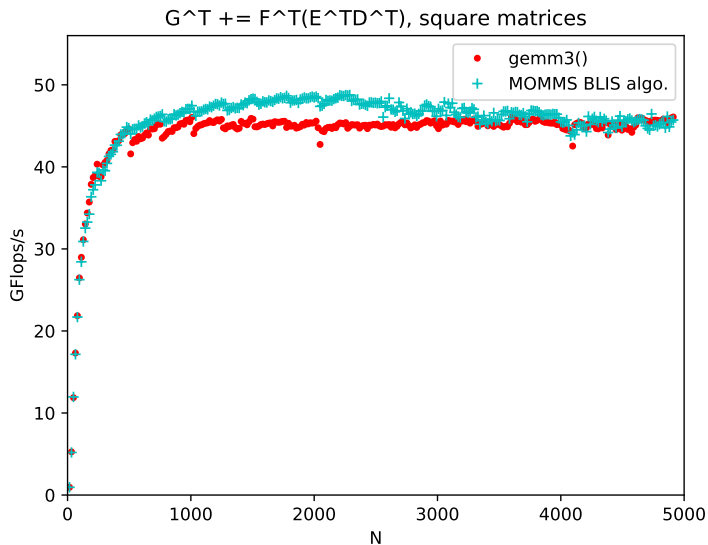
$G += D(EF)$, square matrices



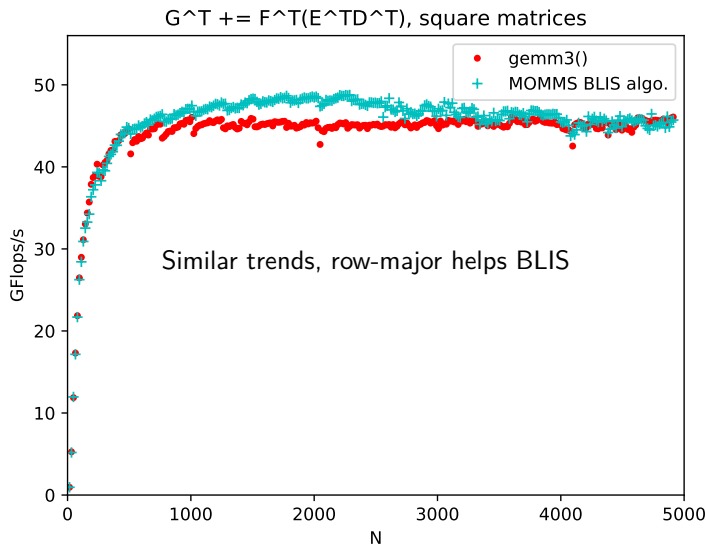
$G += D(EF)$, square matrices



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

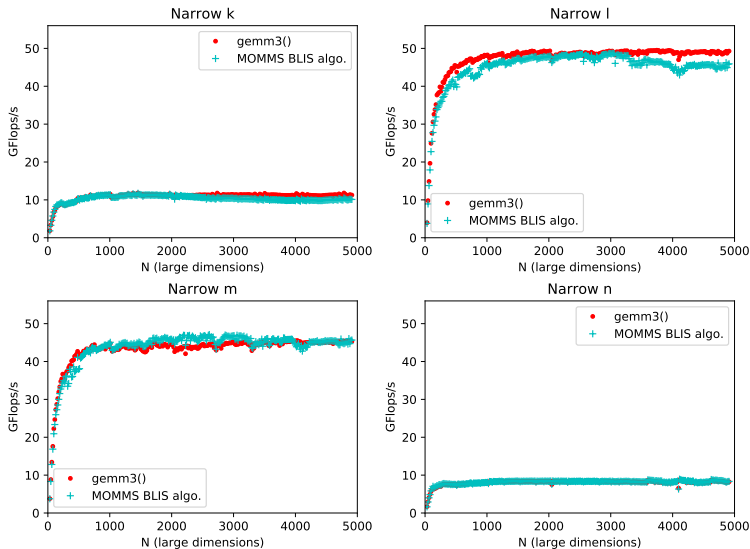


$G += (DE)F$, square matrices



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

$G += D(EF)$, narrow dimension = 9



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
- ▶ Dr. Tyler Smith — writing MOMMS and algorithm design
- ▶ Prof. Tze Meng Low — performance fixes
- ▶ NSF grant **TODO NNNNNNNN** — funding

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

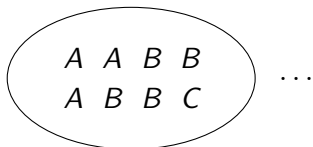
Placing memory in cache: [tag][set #][offset in line]

$$m_r k_C S_{elem} = C_A C_{L1} N_{L1}$$

$$n_r k_C S_{elem} = C_B C_{L1} N_{L1}$$

L1

Cache:



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

Maximizing k_C improves performance

$$C_B = \left\lceil \frac{n_R k_C S_{elem}}{N_{L1} C_{L1}} \right\rceil$$

$$= \left\lceil \frac{n_R}{m_R} C_A \right\rceil$$

$$C_A \leq \left\lfloor \frac{W_{L1} - 1}{1 + \frac{n_R}{m_R}} \right\rfloor$$

GEMM3

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