On the High Performance Implementation of Quaternionic Matrix Operations

`wavefunction91.github.io`

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Problem Motivation

- Moving towards the end of Moore's law: Simply applying existing algorithms and data structures not sufficient.
- Quaternion symmetry is very common in many scientific and engineering disciplines, especially those whose target involves physical space.
- Much research has been afforded to real / complex linear algebra algorithms to exploit this symmetry (Dongerra, et al, 1984; Shiozaki, 2018)

The quaternion algebra is [...] somewhat complicated, and its computation cannot be easily mapped to highly optimized linear algebra libraries such as BLAS and LAPACK.

Problem Statement

How can we leverage techniques such as auto-tuning and microarchitechture optimization to provide optimized implementations of quaternion linear algebra software?

This talk will attempt to answer (discuss) three questions:

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- What are quaternions and why do we care?
- What possible use could I have for matrices of quaternions?
- What does all of this have to do with auto-tuning?

Quaternions: Formally

Quaternions are defined as the set $\mathbb{H}$ of all q such that

$$q = q^0 e_0 + q^1 e_1 + q^2 e_2 + q^3 e_3, \qquad q^0, q^1, q^2, q^3 \in \mathbb{R}$$

with

$$e_0 e_j = e_j e_0 = e_j, \qquad j \in \{0, 1, 2, 3\},$$

$$e_i e_j = -\delta_{ij} e_0 + \sum_{k=1}^{3} \varepsilon_{ij}^{k} e_k, \qquad i, j \in \{1, 2, 3\},$$

Quaternions: Formally

$$a, b, c \in \mathbb{R}, \quad c = ab, \qquad [a, b] = 0$$

$$w, v, z \in \mathbb{C}, \quad z = wv = w^0 v^0 - w^1 v^1 + (w^0 v^1 + w^1 v^0) i \quad [w, v] = 0$$

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$$p, q, r \in \mathbb{H}$$

$$r = pq = \left(p^0 q^0 - \sum_{i=1}^{3} p^i q^i \right) e_0 + \sum_{k=1}^{3} \left(p^0 q^k + p^k q^0 + \sum_{i,j=1}^{3} \varepsilon_{ij}^k p^i q^j \right) e_k,$$

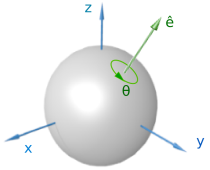
$$[p, q] = \sum_{i,j,k=1}^{3} \varepsilon_{ij}^k \left(p^i q^j - p^j q^i \right) e_k \neq 0.$$

Quaternion Applications: Spacial Rotations

Topologically, the set of unit quaternions (versors)

$$\mathbb{V} = \{v \in \mathbb{H} \text{ s.t. } ||v|| = 1\}$$

is S^3, and thus isomorphic to SU(2) which provides a double cover of SO(3) (rotations in $\mathbb{R}^3$).



We may describe spatial rotations in $\mathbb{R}^3$ via

$$\boldsymbol{r} \in \mathbb{R}^3 \mapsto r^H = r^1 e_1 + r^2 e_2 + r^3 e_3$$

$$\boldsymbol{R}(\hat{\boldsymbol{e}}, \theta) \in \mathrm{SO}(3) \mapsto \pm v = \pm \exp\left(\frac{\theta}{2}(\hat{e}^1 e_1 + \hat{e}^2 e_2 + \hat{e}^3 e_3)\right)$$

such that

$$\boldsymbol{r}' = \boldsymbol{R}(\hat{\boldsymbol{e}}, \theta)\, \boldsymbol{r} \quad \mapsto \quad r'^H = v r^H v^{-1}$$

Quaternion Applications: Spacial Rotations

The SO(3) cover has found extensive exploitation in computer graphics / vision

- (v^0, v^1, v^2, v^3) (4 real numbers) vs. $\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$ (9 real numbers)
- $v_1, v_2 \in \mathbb{H}$, $v_1 v_2$ (16 FLOPs) vs $\boldsymbol{R}_1, \boldsymbol{R}_2 \in \mathrm{SO}(3)$, $\boldsymbol{R}_1 \boldsymbol{R}_2$ (27 FLOPs)
- SLERP (**S**pherical **L**inear **Interp**olation)

Matrices of Quaternions

The algebra generated by $\{e_0, e_1, e_2, e_3\}$ is identical to the algebra generated by the Pauli matrices, thus $\mathbb{H} \cong \langle \mathrm{SU}(2) \rangle \subset \mathbb{M}_2(\mathbb{C})$,

$$e_0 \leftrightarrow \sigma_0, \quad e_1 \leftrightarrow i\sigma_3, \quad e_2 \leftrightarrow i\sigma_2, \quad e_3 \leftrightarrow i\sigma_1,$$

with

$$\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Such that

$$q \leftrightarrow q_{\mathbb{C}} = \begin{bmatrix} q^0 + q^1 i & q^2 + q^3 i \\ -q^2 + q^3 i & q^0 - q^1 i \end{bmatrix} = \begin{bmatrix} \underline{q}^0 & \underline{q}^1 \\ -\overline{\underline{q}}^1 & \overline{\underline{q}}^0 \end{bmatrix} \in \mathbb{M}_2(\mathbb{C})$$

Matrices of Quaternions

The set of quaternion matrices, $\mathbb{M}_N(\mathbb{H})$, is defined by

$$Q = Q^0 e_0 + Q^1 e_1 + Q^2 e_2 + Q^3 e_3, \quad Q^0, Q^1, Q^2, Q^3 \in \mathbb{M}_N(\mathbb{R}).$$

Examining the $\mathbb{M}_2(\mathbb{C})$ representation of a particular element

$$(Q_{\mu\nu})_{\mathbb{C}} = Q^0_{\mu\nu}\sigma_0 + iQ^1_{\mu\nu}\sigma_3 + iQ^2_{\mu\nu}\sigma_2 + iQ^3_{\mu\nu}\sigma_1.$$

which yields the Kronecker structure

$$\begin{aligned} Q_{\mathbb{C}} &= Q^0 \otimes \sigma_0 + Q^1 \otimes i\sigma_3 + Q^2 \otimes i\sigma_2 + Q^3 \otimes i\sigma_1 \\ &= \begin{bmatrix} \underline{Q}^0 & \underline{Q}^1 \\ -\overline{\underline{Q}}^1 & \overline{\underline{Q}}^0 \end{bmatrix} \in \mathbb{M}_{2N}(\mathbb{C}), \end{aligned}$$

Matrices of Quaternions

$$Q \in \mathbb{M}_N(\mathbb{H}) \leftrightarrow \begin{bmatrix} Q^0 & Q^1 \\ -\overline{Q}^1 & \overline{Q}^0 \end{bmatrix} \in \mathbb{M}_{2N}(\mathbb{C}),$$

- Ubiquitous in quantum chemistry / nuclear physics (time-reversal symmetry).
- Applications in image processing and machine learning (quaternion PCA, etc).

Formal theory for quaternion linear algebra has been developed

- QR Algorithm
- Diagonalization, SVD
- LU, Cholesky, LDLH Factorizations

Performance Considerations

Table: Real floating point operations (FLOPs) comparison for elementary arithmetic operations using $\mathbb{H}$ and $\mathbb{M}_2(\mathbb{C})$ data structures.

Operation	FLOPs in $\mathbb{H}$	FLOPs in $\mathbb{M}_2(\mathbb{C})$
Addition	4	8
Multiplication	16	32

$$
\begin{aligned}
p + q \quad &\longleftrightarrow \quad p_{\mathbb{C}} + q_{\mathbb{C}}, \\
pq \quad &\longleftrightarrow \quad p_{\mathbb{C}} q_{\mathbb{C}},
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Addition	$4N^2$	$8N^2$
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Performance Considerations

Quaternion arithmetic offers:

- 0.5x required FLOPs
- 0.5x memory footprint (4x / 8x floats)
- 2x arithmetic intensity (FLOPs / byte)

We should be using quaternion arithmetic!

$\mathbb{H}$AXX

- `gh/wavefunction91/HAXX`
- Optimized C++14 library for quaternion arithmetic
- $\mathbb{H}$BLAS: Optimized quaternionic BLAS functionality
- $\mathbb{H}$LAPACK: Optimized quaternionic LAPACK functionality (in progress)
- Intrinsics + Assembly kernels

Quaternion Matrix Multiplication

The most fundamental linear algebra operation is the general matrix multiply (GEMM).

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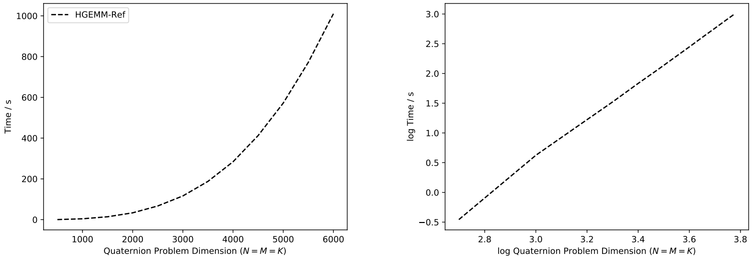
Great! Quaternion GEMM $\Longrightarrow$ HP Quaternion Linear Algebra, Right?



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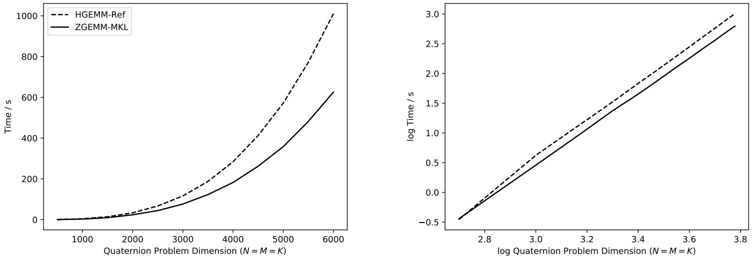

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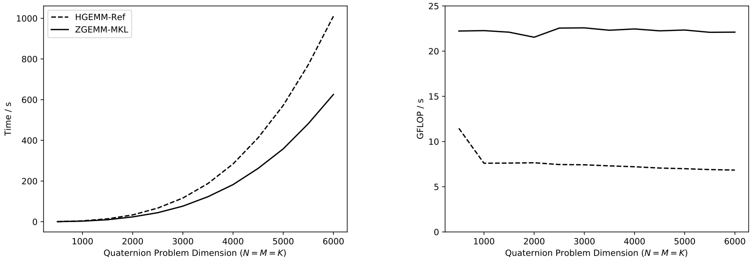


Reference GEMM

Algorithm 0: Reference GEMM

Input : $A \in \mathbb{M}_{m,k}(\mathbb{F})$, $B \in \mathbb{M}_{k,n}(\mathbb{F})$,
$C \in \mathbb{M}_{m,n}(\mathbb{F})$,
Scalars $\alpha, \beta \in \mathbb{F}$

Output: $C = \alpha AB + \beta C$

```
for j = 1 : n do
    Load C_j = C(:,j)
    C_j = βC_j
    for l = 1 : k do
        Load A_l = A(:,l)
        C_j = C_j + αA_l B_lj
    end
    Store C_j
end
```

Pros:

- ✓ Able to implement in an afternoon
- ✓ Architecture agnostic

Cons:

- ✗ No caching of B
- ✗ Reloads all of A for each C_j
- ✗ For large m, k, A load boots C_j from cache
- ✗ Relies on optimizing compiler for SIMD, FMA, etc
- ✗ (Scalable) parallelism is non-trivial
- ✗ **Not tunable**

High-Performance Matrix-Matrix Multiplication

A layered (Goto-style) algorithm significantly improves performance

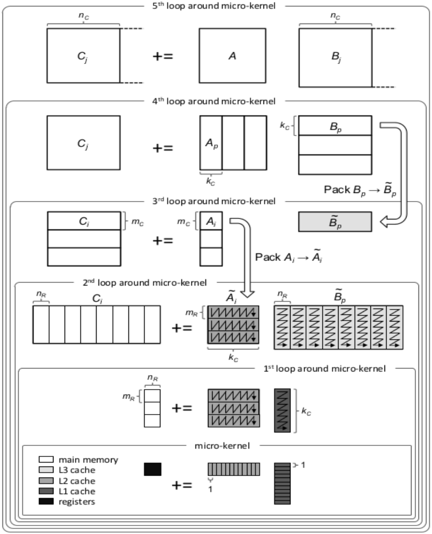
Pros:

- ✓ Caches parts of A, B for maximum resuability
- ✓ Factors architecture specific μ-ops into single micro-kernel
- ✓ Obvious avenue for SMP
- ✓ **Tunable!**

Cons:

- ✗ Significantly more complicated than naive algorithm
- ✗ Requires allocation of auxiliary memory
- ✗ Micro-kernel must be written for each architecture

Van Zee, F.G., *et al* **2017**, *ACM TOMS* 7:1-7:36.



High-Performance Quaternionic GEMM (HGEMM)

The optimized implementation of GEMM in $\mathbb{H}$BLAS utilizes the Goto algorithm. In essence, Goto's original algorithm may be extended to $\mathbb{H}$ by specialization of two sets routines:

- Micro-kernels which perform the $\mathbb{H}$ rank-1 update (assembly / intrinsics)
- Efficient matrix packing routines (intrinsics)

and optimization of 3 caching parameters, m_c, n_c and k_c for the architecture of interest.

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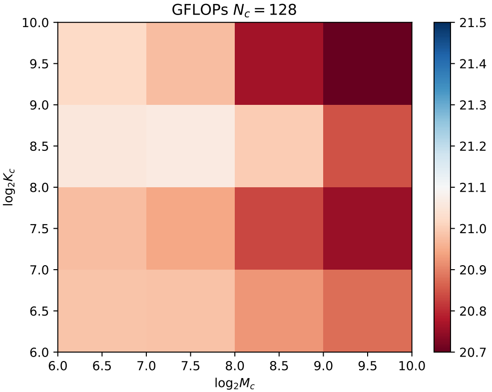
Optimization of Cache Parameters

- OpenTuner: An open source Python framework for auto-tuning
- Register blocks fixed (on AVX / AVX2), $n_r = m_r = 2$.
- Integer discretize $m_c, k_c \in \{2^n\}_{n=3}^{12}$, $n_c \in \{2^n\}_{n=5}^{16}$
- Find $\{m_c, n_c, k_c\}$ which minimizes run time (maximizes GFLOP/s)
  - Average over 5 cold (cache invalidated) runs on select matrix sizes (500,1k,2k,4k)

Possible to brute force otimimize, but not convienient!

Optimization of Cache Parameters



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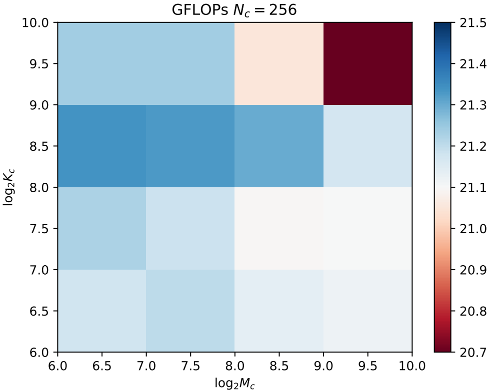

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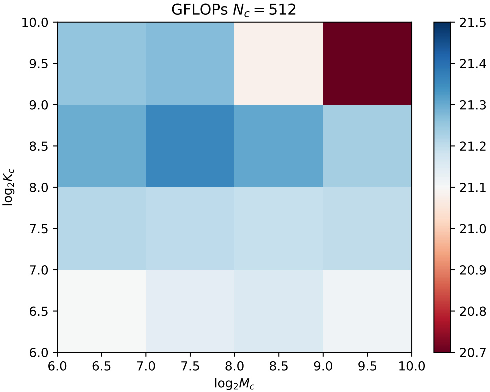

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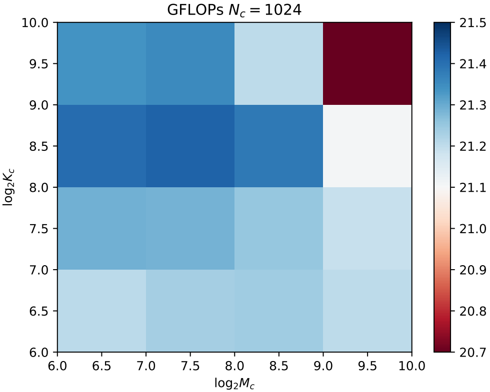

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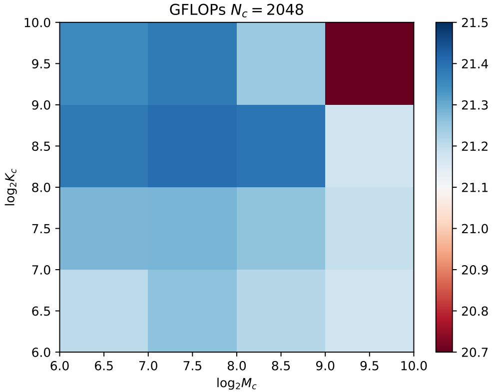

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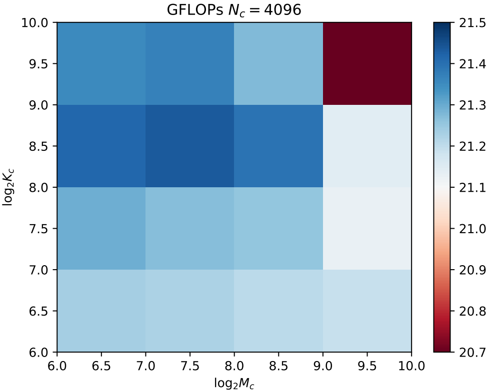
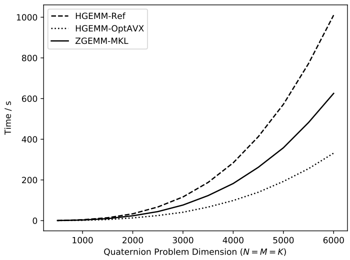


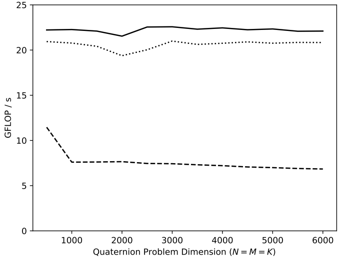
AVX Optimized HGEMM Implementation

Intel Sandy Bridge (L1d: 32k, L1i: 32k, L2: 256k, L3: 20480k)

OpenTuner results:

- 10 tests x 10 runs (˜1 hour vs 10 hours brute force)
- $m_c = k_c = 64$
- $n_c = 1024$





Conclusions

- With instruction sets newer than AVX, high-performance quaternionic linear algebra is possible and a viable alternative to complex linear algebra for appropriate problems.
- Goto's algorithm + auto-tuning drastically improves performance
  - Impractical with reference implementations.

Future Work

- Fill out $\mathbb{H}$BLAS and $\mathbb{H}$LAPACK coverage of the BLAS and LAPACK standards.
- Package autotuner and tuning methodology to automate optimization of caching parameters (+...) on new architectures.
- Address parallelism (SMP + MPI)

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