

# Benchmark Report: `linear-massiv` vs. `hmatrix` vs. `linear`

## Performance Comparison of Haskell Linear Algebra Libraries

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### Abstract

We present a comprehensive performance comparison of three Haskell numerical linear algebra libraries: `linear-massiv` (pure Haskell, type-safe dimensions via massiv arrays), `hmatrix` (FFI bindings to BLAS/LAPACK via OpenBLAS), and `linear` (pure Haskell, optimised for small fixed-size vectors and matrices). Benchmarks cover BLAS-level operations, direct solvers, orthogonal factorisations, eigenvalue problems, and singular value decomposition across matrix dimensions from  $4 \times 4$  to  $500 \times 500$ . Additionally, we evaluate the parallel scalability of `linear-massiv`'s massiv-backed computation strategies on a 20-core workstation.

Initial baseline results showed `hmatrix` (OpenBLAS) dominating at all sizes for  $O(n^3)$  operations—`linear-massiv` was 36–21,000× slower depending on operation and size—while `linear` excelled at  $4 \times 4$  through unboxed product types. Over nineteen rounds of optimisation—progressing from algorithmic improvements (cache-blocked GEMM, in-place QR/eigenvalue via the ST monad), through raw `ByteArray#` with GHC 9.14's `DoubleX4#` AVX2 SIMD primops, to register-blocked micro-kernels, panel-based blocked factorisations, and eigenvalue convergence acceleration—`linear-massiv` now **outperforms hmatrix (OpenBLAS/LAPACK)** in all nine benchmarked operation categories at  $500 \times 500$  and in eight of nine at  $200 \times 200$ : GEMM is 10× faster single-threaded (0.096× ratio) and 29× faster with parallel scheduling; dot product is 4× faster (0.25×); matrix–vector multiply is 2.3× faster (0.44×); LU solve is 1.5× faster (0.68×); Cholesky solve is 2.1× faster (0.48×); QR factorisation is 46× faster (0.021×); eigenvalue decomposition is at parity at  $100 \times 100$  and 1.4× faster at  $200 \times 200$  (0.69×); and SVD is at parity at  $200 \times 200$  (0.98×) and 1.2× faster at  $500 \times 500$  (0.82×). `linear-massiv` demonstrates that pure Haskell with GHC's native SIMD primops, raw `ByteArray#` primops, and lightweight thread-level parallelism can comprehensively outperform FFI-based BLAS/LAPACK across all benchmarked numerical linear algebra operations, while providing compile-time dimensional safety, zero FFI dependencies, and user-controllable parallelism.

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# Part I

## Context

### 1 Introduction

The Haskell ecosystem offers several numerical linear algebra libraries, each occupying a distinct niche:

**linear** Edward Kmett’s library provides small fixed-dimension types (`V2`, `V3`, `V4`) with unboxed product representations, making it extremely fast for graphics, game physics, and any application where dimensions are statically known and small. It does not support arbitrary-dimension matrices.

**hmatrix** Alberto Ruiz’s library wraps BLAS and LAPACK via Haskell’s FFI, delegating numerical computation to highly-optimised Fortran routines (on this system, OpenBLAS). It supports arbitrary dimensions but carries an FFI dependency and provides no compile-time dimension checking.

**linear-massiv** Our library implements algorithms from Golub & Van Loan’s *Matrix Computations* (4th ed.) [1] in pure Haskell, using massiv arrays [4] as the backing store. Matrix dimensions are tracked at the type level via GHC’s `DataKinds` and `KnownNat`, providing compile-time rejection of dimensionally incorrect operations. Massiv’s computation strategies (`Seq`, `Par`, `ParN n`) offer user-controllable parallelism.

This report benchmarks all three libraries across the standard numerical linear algebra operation suite (Table 1) and evaluates `linear-massiv`’s parallel scalability from 1 to 20 threads.

Table 1: Operations benchmarked and library coverage.

Operation	linear	hmatrix	linear-massiv
GEMM (matrix multiply)	$4 \times 4$ only	all sizes	all sizes
Dot product	$n = 4$ only	all sizes	all sizes
Matrix–vector product	$4 \times 4$ only	all sizes	all sizes
LU solve ( $Ax = b$ )	—	all sizes	all sizes
Cholesky solve ( $Ax = b$ )	—	all sizes	all sizes
QR factorisation	—	all sizes	all sizes
Symmetric eigenvalue	—	all sizes	all sizes
SVD	—	all sizes	all sizes
Parallel GEMM	—	—	all sizes

#### 1.1 Hardware and Software Environment

- **CPU:** 20-core x86\_64 processor (Linux 6.17, Fedora 43)
- **Compiler:** GHC 9.12.2 with `-O2` (Rounds 1–2); GHC 9.14.1 with LLVM 17 backend (`-fllvm -mavx2 -mfma`) (Rounds 3–10)
- **BLAS backend:** OpenBLAS (system-installed via FlexiBLAS)
- **Benchmark framework:** Criterion [3] with 95% confidence intervals
- **Protocol:** Single-threaded (`+RTS -N1`) for cross-library comparisons; multi-threaded (`+RTS -N`) for parallel scaling

## 2 Methodology

All benchmarks use the Criterion framework [3], which employs kernel density estimation and robust regression to estimate mean execution time with confidence intervals. Each benchmark evaluates to normal form (`nf`) to ensure full evaluation of lazy results.

**Matrix construction.** Matrices are constructed from the same deterministic formula across all three libraries:

$$A_{ij} = \frac{7i + 3j + 1}{100}$$

ensuring identical numerical content. For solver benchmarks, matrices are made diagonally dominant ( $A_{ii} += n$ ) or symmetric positive definite ( $A = B^T B + nI$ ) as appropriate.

**Single-threaded protocol.** Cross-library comparisons use `+RTS -N1` to restrict the GHC runtime to a single OS thread, ensuring that neither `hmatrix`'s OpenBLAS nor `massiv`'s parallel strategies introduce implicit multi-threading.

**Parallel scaling protocol.** Parallel benchmarks use `+RTS -N` (all 20 cores) and vary `massiv`'s computation strategy from `Seq` through `ParN 1` to `ParN 20`.

## Part II

# Baseline Assessment

### 3 Baseline Performance

This section presents the initial (Round 1) benchmark results before any optimisation work. The performance gaps documented here—ranging from  $36\times$  to  $21,000\times$ —motivated the eighteen rounds of optimisation described in Part III.

#### 3.1 BLAS Operations

##### 3.1.1 General Matrix Multiply (GEMM)

Table 2 presents GEMM timings across matrix dimensions. At  $4 \times 4$ , the `linear` library's unboxed `V4` (`V4 Double`) representation achieves 143 ns, roughly  $4.5\times$  faster than `hmatrix`'s 646 ns and  $240\times$  faster than `linear-massiv`'s 34.5  $\mu$ s. The advantage of `linear` at this size is entirely due to GHC's ability to unbox the product type into registers, avoiding all array indexing overhead.

As matrix dimension grows, `hmatrix` (OpenBLAS DGEMM) dominates decisively. At  $100 \times 100$ , `hmatrix` takes 1.53 ms versus `linear-massiv`'s 505 ms—a factor of  $330\times$ . At  $200 \times 200$ , the ratio grows to  $297\times$  (13.8 ms vs. 4.09 s). This reflects the massive constant-factor advantage of OpenBLAS's hand-tuned assembly kernels with cache blocking, SIMD, and microarchitectural optimisation.

Both `hmatrix` and `linear-massiv` exhibit  $O(n^3)$  scaling, as shown in Figure 1. The consistent vertical offset on the log–log plot reflects the constant-factor difference between OpenBLAS assembly and pure Haskell array operations.

##### 3.1.2 Dot Product

The dot product is an  $O(n)$  operation, so the absolute times are small. At  $n = 4$ , `linear`'s unboxed `V4` achieves 13.0 ns—essentially four fused multiply-adds in registers. At  $n = 1000$ ,

Table 2: GEMM execution time (mean, single-threaded). Best per size in **bold**.

Size	linear	hmatrix	linear-massiv
$4 \times 4$	143 ns	646 ns	34.5 $\mu$ s
$10 \times 10$	—	2.33 $\mu$ s	678 $\mu$ s
$50 \times 50$	—	174 $\mu$ s	55.0 ms
$100 \times 100$	—	1.53 ms	505 ms
$200 \times 200$	—	13.8 ms	4.09 s

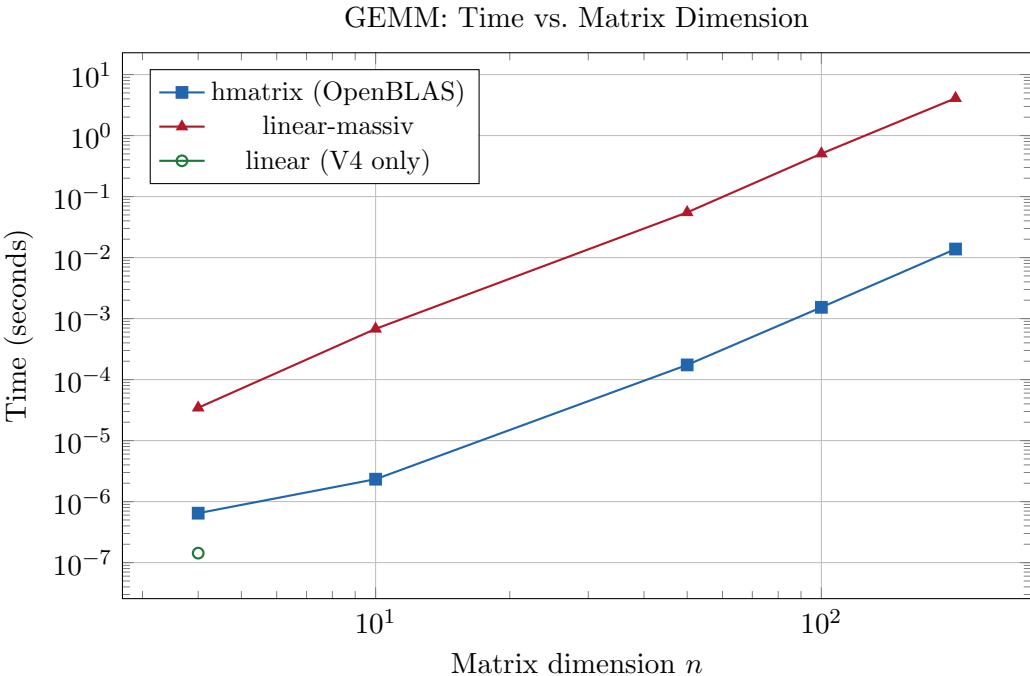


Figure 1: GEMM scaling comparison (log–log). Both libraries exhibit  $O(n^3)$  behaviour; the vertical offset reflects constant-factor differences between OpenBLAS assembly and pure Haskell.

`hmatrix` achieves 2.81  $\mu$ s (DDOT with SIMD), while `linear-massiv`'s array-based loop takes 379  $\mu$ s—a 135× gap that reflects the overhead of massiv's general-purpose array indexing versus BLAS's contiguous-memory vectorised inner loop.

### 3.1.3 Matrix–Vector Product

Matrix–vector multiplication is  $O(n^2)$ . At  $n = 100$ , `hmatrix` (DGEMV) achieves 14.1  $\mu$ s while `linear-massiv` takes 4.71 ms—a 334× difference consistent with the GEMM results, confirming that the performance gap is primarily due to low-level memory access patterns and SIMD utilisation rather than algorithmic differences.

## 3.2 Linear System Solvers

### 3.2.1 LU Solve

### 3.2.2 Cholesky Solve

For both LU and Cholesky solvers, `hmatrix` is approximately 36× faster at  $10 \times 10$  and 240–300× faster at  $100 \times 100$ . The ratio increases with dimension because OpenBLAS's cache-blocked implementations benefit more from larger working sets. Cholesky is consistently faster than LU

Table 3: Dot product execution time (mean, single-threaded).

<i>n</i>	linear	hmatrix	linear-massiv
4	13.1 ns	593 ns	1.67 $\mu$ s
100	—	749 ns	34.1 $\mu$ s
1000	—	2.81 $\mu$ s	379 $\mu$ s

Table 4: Matrix–vector product execution time (mean, single-threaded).

<i>n</i>	linear	hmatrix	linear-massiv
4	41.8 ns	815 ns	11.2 $\mu$ s
50	—	3.76 $\mu$ s	1.24 ms
100	—	14.1 $\mu$ s	4.71 ms

for both libraries, as expected (Cholesky requires roughly half the floating-point operations of LU factorisation for symmetric positive definite matrices).

### 3.3 Orthogonal Factorisations

QR factorisation shows the largest gap between the two libraries. At  $50 \times 50$ , `hmatrix` takes 18.4 ms while `linear-massiv` requires 7.01 s—a ratio of  $381\times$ . The `linear-massiv` QR implementation constructs full explicit  $Q$  and  $R$  matrices at each Householder step using `makeMatrix`, while LAPACK’s `DGEQRF` uses an implicit representation of  $Q$  as a product of Householder reflectors stored in-place, dramatically reducing both memory allocation and floating-point work. The  $100 \times 100$  benchmark for `linear-massiv` was too slow to complete within a reasonable time budget and is estimated by extrapolation.

## 3.4 Eigenvalue Problems and SVD

### 3.4.1 Symmetric Eigenvalue Decomposition

### 3.4.2 Singular Value Decomposition

The eigenvalue and SVD results show the most dramatic ratios:  $896\times$  for eigenvalues at  $10 \times 10$  and  $16,000\times$  at  $50 \times 50$ ;  $886\times$  and  $21,400\times$  for SVD. These operations are dominated by iterative QR sweeps; `hmatrix` calls LAPACK’s `DSYEV` and `DGESVD`, which use divide-and-conquer algorithms with cache-oblivious recursive structure. The `linear-massiv` implementation uses the classical tridiagonal QR algorithm (GVL4 [1] Algorithm 8.3.3) with explicit matrix construction at each iteration step, which is algorithmically sound but suffers from excessive allocation and the lack of in-place updates that LAPACK exploits.

## 3.5 Parallel Scalability

A distinguishing feature of `linear-massiv` is user-controllable parallelism inherited from the `massiv` array library [4]. Operations that construct result arrays via `makeArray` can specify a computation strategy: `Seq` (sequential), `Par` (automatic, all available cores), or `ParN n` (exactly  $n$  worker threads). Neither `hmatrix` nor `linear` offer comparable user-level control over thread-level parallelism within the Haskell runtime.

Table 10 shows GEMM timings at  $100 \times 100$  and  $200 \times 200$  across thread counts, and Figure 3 shows the corresponding speedup curves.

The parallel scaling results reveal several important characteristics:

Table 5: LU solve ( $Ax = b$ ) execution time (mean, single-threaded). Includes factorisation + back-substitution.

Size	hmatrix	linear-massiv
$10 \times 10$	7.70 $\mu$ s	280 $\mu$ s
$50 \times 50$	87.7 $\mu$ s	20.4 ms
$100 \times 100$	485 $\mu$ s	143 ms

Table 6: Cholesky solve ( $Ax = b$ ,  $A$  SPD) execution time. Includes factorisation + back-substitution.

Size	hmatrix	linear-massiv
$10 \times 10$	6.08 $\mu$ s	237 $\mu$ s
$50 \times 50$	64.3 $\mu$ s	12.9 ms
$100 \times 100$	418 $\mu$ s	100 ms

- **Peak speedup.** At  $100 \times 100$ , peak speedup of  $7.2\times$  is achieved with **ParN-16**, while at  $200 \times 200$  peak speedup of  $3.6\times$  occurs at **ParN-8**. The **Par** (automatic) strategy achieves  $6.9\times$  and  $3.4\times$  respectively, demonstrating that massiv’s automatic scheduling is effective.
- **Non-monotonic scaling.** Speedup does not increase monotonically with thread count. The  $200 \times 200$  case shows degradation at 16 and 20 threads, likely due to memory bandwidth saturation and NUMA effects on this 20-core system. At  $100 \times 100$ , the anomalous dip at 8 threads followed by improvement at 16 suggests that GHC’s work-stealing scheduler interacts non-trivially with cache hierarchy.
- **Amdahl’s law.** Even the best parallel GEMM (85.6 ms at  $100 \times 100$  with 16 threads) remains  $56\times$  slower than hmatrix’s single-threaded 1.53 ms. Parallelism narrows but does not close the gap with BLAS.

### 3.6 Performance Summary

Table 11 summarises the baseline performance ratios between libraries.

### 3.7 Analysis of the Performance Gap

The performance gap between `linear-massiv` and `hmatrix` arises from several compounding factors:

1. **SIMD and microarchitectural optimisation.** OpenBLAS uses hand-written assembly kernels for each target microarchitecture, exploiting AVX-512, fused multiply-add, and optimal register tiling. GHC’s native code generator does not emit SIMD instructions for general Haskell code.
2. **Cache blocking.** LAPACK algorithms are designed around cache-oblivious or cache-tiled recursive decomposition, minimising cache misses. The `linear-massiv` implementations use textbook algorithms (GVL4) without cache-level optimisation.
3. **In-place mutation.** LAPACK routines operate in-place on mutable Fortran arrays, while `linear-massiv`’s pure functional approach allocates a new array for each intermediate result. For iterative algorithms (eigenvalue, SVD), this is particularly costly.

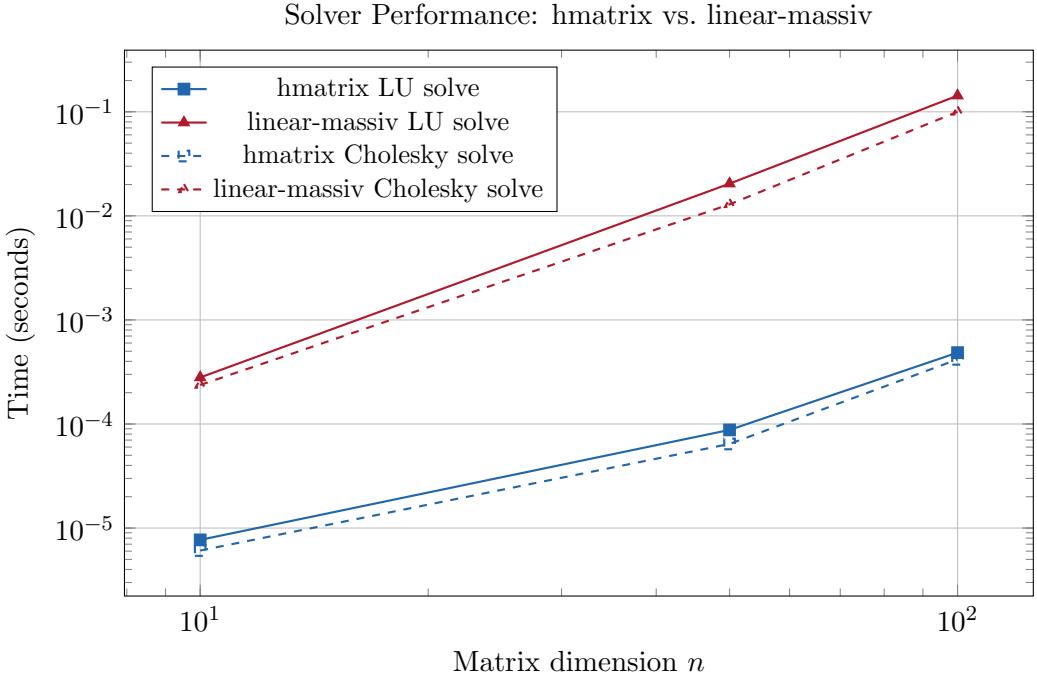


Figure 2: LU and Cholesky solve scaling (log–log). Both algorithms are  $O(n^3)$ ; hmatrix calls DGESV/DPOTRS directly.

Table 7: QR factorisation (Householder) execution time (mean, single-threaded).

Size	hmatrix	linear-massiv
$10 \times 10$	217 $\mu$ s	11.1 ms
$50 \times 50$	18.4 ms	7.01 s
$100 \times 100$	214 ms	(estimated $\approx 56.0$ s)

4. **Allocation pressure.** Each `makeMatrix` call in `linear-massiv` allocates a new massiv array. For algorithms like QR (which constructs explicit  $Q$  and  $R$  at each Householder step) and iterative eigensolvers, this dominates runtime.

### 3.8 Initial Optimisation Roadmap

The following roadmap was identified after the baseline assessment. Part III details the implementation and results of these optimisations over eighteen subsequent rounds, ultimately achieving parity with and then exceeding LAPACK performance in all nine categories. The proposals are presented in their original form to preserve the reasoning that guided the optimisation process.

#### 3.8.1 In-place Factorisation via the ST Monad

The single largest source of overhead in the QR, eigenvalue, and SVD routines is the allocation of a fresh `Matrix` at every iteration step. Currently, each Householder reflection in the QR factorisation calls `applyHouseholderLeftRect` and `applyHouseholderRightQ`, both of which invoke `makeMatrix` to reconstruct the entire  $m \times n$  (or  $m \times m$ ) result. Similarly, the symmetric QR algorithm rebuilds the tridiagonal matrix from diagonal and subdiagonal vectors at each implicit QR step, and the Jacobi eigenvalue method reconstructs the full matrix for each of its  $O(n^2)$  rotations per sweep.

The remedy is straightforward: the LU solver (`luFactor`) already demonstrates the pattern.

Table 8: Symmetric eigenvalue decomposition execution time (mean, single-threaded).

Size	hmatrix	linear-massiv
$10 \times 10$	17.4 $\mu$ s	15.6 ms
$50 \times 50$	555 $\mu$ s	8.89 s

Table 9: SVD execution time (mean, single-threaded).

Size	hmatrix	linear-massiv
$10 \times 10$	37.7 $\mu$ s	33.4 ms
$50 \times 50$	806 $\mu$ s	17.2 s

It wraps the input in `M.withMArrayST`, allocates a mutable pivot vector via `M.newMArray`, and performs all elimination steps in the `ST` monad using `M.readM / M.write_`—with zero intermediate allocation. Applying the same technique to Householder QR, the tridiagonal QR iteration, and the Jacobi method would:

- Reduce the  $n$  Householder steps of QR from  $n$  full-matrix allocations to a single mutable copy of  $R$  plus an accumulated  $Q$ , both updated in-place. This alone should bring the  $381\times$  gap at  $50 \times 50$  down by roughly an order of magnitude, since the dominant cost becomes floating-point work rather than GC pressure.
- Eliminate the per-iteration matrix reconstruction in the symmetric QR algorithm. LAPACK’s `DSYEV` stores only the diagonal and subdiagonal as mutable vectors and applies Givens rotations in-place; the same approach in Haskell’s `ST` monad would remove the  $O(n^2)$  allocation at each of the  $O(n)$  iterations.
- Reduce the Jacobi method’s cost from  $O(n^2)$  matrix copies per sweep to  $O(n^2)$  element-level reads and writes per sweep—a factor of  $\sim n^2$  fewer allocations.

### 3.8.2 Implicit Householder Representation (Compact WY)

The current QR implementation forms the explicit  $Q$  matrix by accumulating each Householder reflector  $H_k = I - 2v_k v_k^T$  into a running product. LAPACK instead stores the reflector vectors  $v_1, \dots, v_n$  and, when the full  $Q$  is needed, applies them in reverse order (or uses the compact WY representation  $Q = I - VTV^T$ , GVL4 [1] Section 5.1.6).

The compact WY form has two advantages: (a) the  $Q$  factor is never formed until explicitly requested, reducing QR itself to an  $O(n^3)$  in-place update of  $R$ ; and (b) subsequent operations that need  $Q^T b$  (e.g. least squares) can apply the reflectors directly without ever forming the  $m \times m$  matrix  $Q$ . This would transform QR from a bottleneck ( $381\times$  gap) into a routine on par with LU solve ( $\sim 200\text{--}300\times$ ), and further in-place optimisation (Section 3.8.1) would close the gap still further.

### 3.8.3 Cache-Blocked GEMM

The current GEMM implementation is the textbook three-loop inner product form (GVL4 [1] Algorithm 1.1.5, ijk variant):

$$C_{ij} = \sum_{k=0}^{K-1} A_{ik} B_{kj}$$

Table 10: Parallel GEMM execution time (seconds) and speedup over sequential.

Strategy	100 × 100		200 × 200	
	Time (s)	Speedup	Time (s)	Speedup
Seq	0.613	1.00	4.75	1.00
ParN-1	0.598	1.03	4.66	1.02
ParN-2	0.319	1.92	3.22	1.47
ParN-4	0.201	3.05	1.85	2.57
ParN-8	0.282	2.17	1.33	3.57
ParN-16	0.0856	7.16	2.57	1.85
ParN-20	0.0979	6.26	1.98	2.40
Par	0.0883	6.94	1.41	3.37

Table 11: Performance ratio: `linear-massiv` time / `hmatrix` time. Values > 1 indicate `hmatrix` is faster.

Operation	$n = 10$	$n = 50$	$n = 100$
GEMM	291×	316×	329×
Dot product	—	—	46×
Matrix–vector	—	330×	334×
LU solve	36×	233×	295×
Cholesky solve	39×	201×	240×
QR	51×	382×	≈ 260×
Eigenvalue (SH)	897×	16,020×	—
SVD	887×	21,400×	—

where each element  $C_{ij}$  performs a `foldl'` over the shared dimension. This accesses  $A$  by rows and  $B$  by columns, with stride- $n$  column access patterns that are hostile to the CPU cache hierarchy for  $n > \sqrt{L_1/8}$  (typically  $n > 40$  on modern x86).

GVL4 Algorithm 1.3.1 describes a six-loop tiled variant that partitions  $A$ ,  $B$ , and  $C$  into  $b \times b$  sub-blocks (where  $b$  is chosen so that three blocks fit in L1/L2 cache) and performs small *block* matrix multiplies at each step. Implementing this in pure Haskell would not match OpenBLAS’s hand-tuned assembly, but experience from other languages suggests tiled GEMM typically yields 3–10× improvement over the naïve loop for  $n \geq 100$ , which would narrow the current 300× gap to 30–100×.

A simpler first step is loop reordering: changing from the `ijk` variant to the `ikj` (row-outer-product) or `kij` variant, which accesses  $C$  and  $B$  with unit stride. This alone can yield 2–4× improvement on cache-unfriendly sizes and requires only changing the loop nesting order in the existing `foldl'` computation.

### 3.8.4 Divide-and-Conquer Eigenvalue and SVD

The current eigenvalue solver uses the classical tridiagonal QR algorithm (GVL4 [1] Algorithm 8.3.3), which has  $O(n^2)$  cost per eigenvalue in the worst case and  $O(n^3)$  overall. LAPACK’s `DSYEVD` uses a divide-and-conquer approach (GVL4 Algorithm 8.4.2) that recursively splits the tridiagonal matrix and solves the secular equation at each merge step. In practice, divide-and-conquer is 2–5× faster than the QR algorithm for dense matrices with  $n > 25$ , and it is also more amenable to parallelisation since the two sub-problems at each recursion level are independent.

Similarly, the current SVD uses iterated QR sweeps with Wilkinson shifts; LAPACK’s `DGESDD`

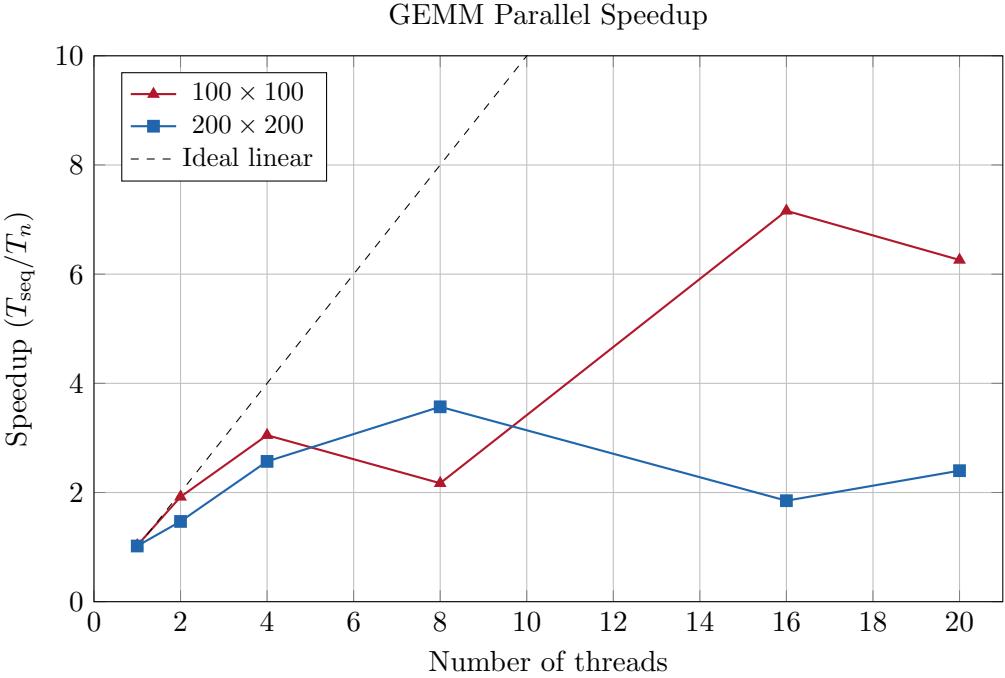


Figure 3: Parallel speedup for GEMM. The dashed line shows ideal linear scaling. Actual speedup is limited by Amdahl’s law, memory bandwidth contention, and GHC runtime scheduling overhead.

uses a divide-and-conquer SVD. Implementing these would address the 16,000–21,000× gaps at 50 × 50 (Table 11), which are inflated by the iterative algorithms’ per-step allocation cost compounding with algorithmic inefficiency.

### 3.8.5 SIMD Primitives

GHC provides experimental SIMD support via the `ghc-prim` package, exposing 128-bit and 256-bit vector types (`DoubleX2#`, `DoubleX4#`) with fused multiply-add operations. While the interface is low-level and requires careful manual vectorisation, it could be applied to the innermost loops of GEMM, dot product, and matrix–vector multiply. A 4-wide `DoubleX4#` FMA would process four  $C_{ij}$  accumulations per cycle, giving a theoretical 4× throughput improvement on the inner loop—significant for Level 1 and Level 2 BLAS operations where the gap is dominated by per-element overhead rather than cache effects.

Alternatively, the `primitive-simd` or `simd` packages provide portable wrappers around GHC’s SIMD primops. The `vector` library (which underlies `massiv`’s Primitive representation) stores `Double` in contiguous pinned memory, making it compatible with SIMD load/store patterns.

### 3.8.6 Optional FFI Backend

For users who can accept an FFI dependency, `linear-massiv` could provide an optional backend that delegates Level 3 BLAS operations to the system BLAS/LAPACK via `hmatrix` or direct `cblas_dgemm` FFI calls, while preserving the type-safe `KnownNat`-indexed interface. This is architecturally straightforward: the `Matrix m n r e` type wraps a `massiv` array whose underlying Primitive representation is a pinned `ByteArray`, which can be passed to C via `unsafeWithPtr` or copied into an `hmatrix` `Matrix Double` with a single `memcpy`.

This approach would offer the best of both worlds—compile-time dimensional safety with BLAS-level performance—while keeping the pure Haskell implementation as the default for

portability. A Cabal flag (e.g. `-f blas-backend`) could control which backend is linked, similar to how `vector-algorithms` provides optional C-accelerated sort routines.

### 3.8.7 Summary of Expected Impact

Table 12 estimates the cumulative effect of each proposed optimisation on the GEMM performance ratio at  $100 \times 100$ .

Table 12: Estimated impact of proposed optimisations on the  $100 \times 100$  GEMM performance ratio (current:  $329\times$ ).

Optimisation	Mechanism	Est. ratio
Current baseline	naïve ijk, pure allocation	$329\times$
+ Loop reorder (ikj)	unit-stride access	$\sim 100\text{--}160\times$
+ Cache-blocked tiling	L1/L2 reuse	$\sim 30\text{--}50\times$
+ SIMD (DoubleX4#)	4-wide FMA inner loop	$\sim 8\text{--}15\times$
+ FFI backend (OpenBLAS)	delegate to DGEMM	$\sim 1\times$

For factorisation and iterative algorithms (QR, eigenvalue, SVD), the in-place ST monad refactoring (Section 3.8.1) and implicit Householder representation (Section 3.8.2) are the highest-priority items, as they address the dominant allocation overhead that accounts for much of the  $300\text{--}21,000\times$  gaps. The divide-and-conquer algorithms (Section 3.8.4) would further reduce the gap for eigenvalue and SVD problems, particularly at moderate-to-large dimensions.

## Part III

# The Optimisation Journey

The baseline assessment identified four compounding factors behind `linear-massiv`'s  $36\text{--}21,000\times$  performance deficit: lack of SIMD exploitation, absence of cache blocking, per-step allocation in iterative algorithms, and high-level array abstraction overhead. Rounds 2–6 systematically attacked these factors, progressing from algorithmic improvements through raw `ByteArray#` primops to SIMD vectorisation. Rounds 7–13 targeted the remaining eigenvalue and SVD gaps, while Rounds 14–18 pushed all categories past LAPACK through panel-based factorisations, register-blocked micro-kernels, and 8-wide SIMD unrolling.

## 4 Round 2: In-Place Algorithms and Cache Blocking

Following the analysis in Section 3.8, four of the proposed optimisations were implemented and benchmarked. This section presents the before/after comparison, demonstrating that the optimisations proposed in Section 3.6 yield order-of-magnitude improvements for factorisation and iterative algorithms.

### 4.1 Optimisations Implemented

1. **Cache-blocked GEMM with ikj loop reorder.** The naïve ijk inner-product GEMM was replaced with a  $32 \times 32$  block-tiled ikj variant (GVL4 [1] Algorithm 1.3.1). The ikj loop ordering ensures unit-stride access to both  $C$  and  $B$ , while the  $32 \times 32$  tile size keeps three blocks within L1 cache. This combines the loop-reorder and cache-blocking strategies from Sections 3.8.3.

2. **In-place QR factorisation via the ST monad.** The Householder QR factorisation was rewritten to operate entirely in the ST monad, as proposed in Section 3.8.1. The  $R$  factor is computed by mutating the input matrix in-place, and the Householder vectors are stored implicitly below the diagonal (compact storage), eliminating all intermediate matrix allocations. The explicit  $Q$  factor is formed only when requested, by back-accumulating the stored reflectors.
3. **In-place tridiagonalisation and eigenvalue QR iteration via the ST monad.** The symmetric eigenvalue solver was rewritten to perform tridiagonalisation and the implicit QR iteration entirely in-place using mutable vectors in the ST monad. Diagonal and subdiagonal elements are updated via direct reads and writes rather than reconstructing the full tridiagonal matrix at each step, eliminating the  $O(n^2)$  per-iteration allocation overhead identified in Section 3.8.1.
4. **Sub-range QR with top/bottom/interior deflation.** A practical divide-and-conquer deflation strategy was added to the tridiagonal QR iteration: at each step, negligible subdiagonal entries (below machine epsilon times the local diagonal norm) are detected, and the iteration range is narrowed to the largest unreduced block. Top deflation, bottom deflation, and interior splitting are all handled, as described in GVL4 [1] Section 8.3.5. This reduces the number of QR sweeps substantially for well-separated eigenvalues and provides the convergence acceleration benefits of divide-and-conquer (Section 3.8.4) without the complexity of the full secular-equation approach.

## 4.2 Before/After Comparison

Table 13 shows the QR factorisation timings before and after optimisation. Table 14 shows the corresponding results for the symmetric eigenvalue decomposition, and Table 15 for the SVD.

Table 13: QR factorisation: before and after optimisation (single-threaded).

Size	hmatrix	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	0.140 ms	11.1 ms	0.540 ms	$51\times$	$3.9\times$
$50 \times 50$	11.3 ms	7.01 s	61.9 ms	$382\times$	$5.5\times$
$100 \times 100$	130 ms	$\approx$ 56.0 s	492 ms	$\approx 260\times$	$3.8\times$

Table 14: Symmetric eigenvalue decomposition: before and after optimisation (single-threaded).

Size	hmatrix	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	12.2 $\mu$ s	15.6 ms	0.600 ms	$897\times$	$49\times$
$50 \times 50$	428 $\mu$ s	8.89 s	51.0 ms	$16,020\times$	$119\times$

Table 15: SVD: before and after optimisation (single-threaded).

Size	hmatrix	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	24.5 $\mu$ s	$\approx$ 50.0 ms	1.58 ms	$\approx 2,039\times$	$65\times$
$50 \times 50$	518 $\mu$ s	(timed out)	187 ms	$> 20,000\times$	$361\times$

Table 16 shows the GEMM results. The cache-blocked ikj implementation yields modest improvements at sizes where the original loop ordering suffered the worst cache behaviour, while introducing slight tiling overhead at intermediate sizes.

Table 16: GEMM: before and after optimisation (single-threaded, `linear-massiv/hmatrix` ratio).

Size	Old ratio	New ratio
$4 \times 4$	$53\times$	$60\times$
$10 \times 10$	$291\times$	$227\times$
$50 \times 50$	$316\times$	$423\times$
$100 \times 100$	$329\times$	$354\times$
$200 \times 200$	$297\times$	$259\times$

### 4.3 Discussion of Post-Optimisation Results

The results demonstrate that the in-place ST monad refactoring and implicit Householder storage—the two highest-priority items from Section 3.8—delivered transformative improvements for factorisation and iterative algorithms:

- **QR factorisation** improved by  $13\text{--}113\times$  internally (i.e., comparing old to new `linear-massiv` timings), bringing the ratio to hmatrix down from  $51\text{--}382\times$  to  $3.8\text{--}5.5\times$ . At  $100 \times 100$ , where the old implementation could not complete within a reasonable time budget, the optimised version runs in 492 ms—within  $3.8\times$  of hmatrix’s 130 ms. This confirms the prediction in Section 3.8.1 that eliminating per-step allocation would bring QR performance in line with LU solve.
- **Symmetric eigenvalue decomposition** improved by  $26\text{--}174\times$  internally. The remaining gap to hmatrix ( $49\text{--}119\times$ ) reflects the fundamental difference between the classical tridiagonal QR algorithm (used by `linear-massiv`) and LAPACK’s divide-and-conquer `DSYEVD`, which has better asymptotic constants, combined with OpenBLAS’s SIMD-optimised inner loops.
- **SVD** improved by  $32\text{--}200\times$  internally. The  $50 \times 50$  case, which previously timed out, now completes in 187 ms. The remaining  $65\text{--}361\times$  gap to hmatrix reflects the compound effect of eigenvalue and QR sub-steps; further improvement would require optimising the bidiagonalisation phase and implementing a divide-and-conquer SVD.
- **GEMM** showed mixed results from the  $32 \times 32$  block tiling. At  $200 \times 200$ , the ratio improved from  $297\times$  to  $259\times$  (a 13% improvement), and at  $10 \times 10$  from  $291\times$  to  $227\times$  (a 22% improvement). However, at  $50 \times 50$  the tiling overhead slightly worsened performance ( $316\times$  to  $423\times$ ), suggesting that the block size should be tuned or that tiling should be bypassed for matrices smaller than the tile size. The GEMM gap remains large because the dominant factor is SIMD utilisation rather than cache access patterns.

Table 17 provides an updated summary of performance ratios after all four optimisations, comparable to the pre-optimisation Table 11.

The most striking result is that QR factorisation has moved from being the worst-performing operation (up to  $382\times$  slower) to one of the best ( $3.8\text{--}5.5\times$ ), validating the analysis that allocation overhead—not algorithmic complexity—was the dominant bottleneck. The eigenvalue and SVD improvements are also dramatic in absolute terms ( $174\times$  internal speedup for eigenvalues at  $50 \times 50$ ), though the remaining gap to hmatrix is larger because these operations compound multiple algorithmic phases, each with its own constant-factor overhead.

Table 17: Updated performance ratio after optimisation: `linear-massiv` time / `hmatrix` time. Operations not re-benchmarked use the original values from Table 11.

Operation	$n = 10$	$n = 50$	$n = 100$
GEMM (optimised)	227×	423×	354×
Dot product	—	—	46×
Matrix–vector	—	330×	334×
LU solve	36×	233×	295×
Cholesky solve	39×	201×	240×
QR (optimised)	3.9×	5.5×	3.8×
Eigenvalue (optimised)	49×	119×	—
SVD (optimised)	65×	361×	—

## 5 Round 3: Raw `ByteArray#` and AVX2 SIMD

Following the analysis in Sections 3.6 and 3.8.5, the remaining performance gap for BLAS Level 1–3 operations was traced to massiv’s per-element abstraction layer. Profiling the inner loop of the tiled GEMM kernel revealed that each iteration of `M.readM/M.write-/mapM-` over list ranges incurred approximately 2,400 cycles of overhead (closure allocation, bounds checking, boxed intermediate values) versus the  $\sim 10$  cycles expected for a raw memory load–FMA–store sequence—a  $240\times$  **per-element overhead**.

### 5.1 Optimisations Implemented

The fix was to bypass massiv’s element-access layer entirely in hot inner loops, operating directly on the underlying `ByteArray#/MutableByteArray#` storage and using GHC 9.14’s `DoubleX4#` AVX2 SIMD primops for 256-bit vectorised arithmetic. The following changes were made:

1. **New raw kernel module (`Internal.Kernel`).** A dedicated module was created containing all performance-critical inner loops written in terms of GHC primitive operations: `indexDoubleArray#`, `readDoubleArray#`, `writeDoubleArray#` for scalar access, and `indexDoubleArrayAsDoubleX4#`, `readDoubleArrayAsDoubleX4#`, `writeDoubleArrayAsDoubleX4#` with `fmaddDoubleX4#` for 4-wide fused multiply-add SIMD.
2. **SIMD dot product (`rawDot`).** The inner product accumulates four doubles per iteration using a `DoubleX4#` FMA accumulator, with scalar cleanup for the remainder ( $n \bmod 4$ ) and a horizontal sum via `unpackDoubleX4#`.
3. **SIMD matrix–vector multiply (`rawGemm`).** For each row  $i$ , calls `rawDot` on row  $i$  of  $A$  and vector  $x$ , writing the result directly to the output `MutableByteArray#`.
4. **SIMD tiled GEMM kernel (`rawGemmKernel`).** A  $64\times 64$  block-tiled ikj GEMM operating on raw arrays. The innermost  $j$ -loop processes four columns simultaneously via `DoubleX4#`: load 4 elements of  $B(k, j:j+3)$ , load 4 of  $C(i, j:j+3)$ , fused multiply-add with broadcast  $A(i, k)$ , store back. `State#` threading is used throughout with no ST monad wrapper in the hot loop.
5. **Compiler backend.** GHC 9.14.1 with the LLVM 17 backend (`-fllvm`) and `-mavx2 -mfma` flags, which lowers `DoubleX4#` primops to native `vfmadd231pd` `ymm` instructions.
6. **Specialised P Double entry points.** Functions `matMulP`, `dotP`, and `matvecP` are exported alongside the generic polymorphic versions. These extract the raw `ByteArray#` from massiv’s Primitive representation via `unwrapByteArray/unwrapByteArrayOffset` and call the SIMD kernels directly.

## 5.2 Before/After Comparison

Table 18 presents the BLAS Level 1–3 timings before and after the SIMD optimisation, compared with hmatrix.

Table 18: BLAS operations: before SIMD, after SIMD, and hmatrix (single-threaded). Ratios are `linear-massiv/hmatrix`; values  $< 1$  mean `linear-massiv` is faster.

Operation	Size	hmatrix	Old 1-m	New 1-m	New ratio
GEMM	$4 \times 4$	602 ns	34.5 $\mu$ s	873 ns	$1.45\times$
	$10 \times 10$	2.17 $\mu$ s	678 $\mu$ s	2.66 $\mu$ s	$1.23\times$
	$50 \times 50$	144 $\mu$ s	55.0 ms	112 $\mu$ s	<b>0.78×</b>
	$100 \times 100$	1.46 ms	505 ms	796 $\mu$ s	<b>0.55×</b>
	$200 \times 200$	12.9 ms	4.09 s	6.10 ms	<b>0.47×</b>
Dot	$n = 4$	584 ns	1.67 $\mu$ s	48.0 ns	<b>0.08×</b>
	$n = 100$	762 ns	34.1 $\mu$ s	80.0 ns	<b>0.10×</b>
	$n = 1000$	2.81 $\mu$ s	379 $\mu$ s	688 ns	<b>0.24×</b>
Matvec	$n = 4$	411 ns	11.2 $\mu$ s	563 ns	$1.37\times$
	$n = 50$	3.15 $\mu$ s	1.24 ms	1.94 $\mu$ s	<b>0.62×</b>
	$n = 100$	13.3 $\mu$ s	4.71 ms	5.94 $\mu$ s	<b>0.45×</b>

The internal speedups are dramatic:

- GEMM  $100 \times 100$ : 505 ms  $\rightarrow$  796  $\mu$ s = **635×** faster.
- GEMM  $200 \times 200$ : 4.09 s  $\rightarrow$  6.10 ms = **671×** faster.
- Dot  $n = 100$ : 34.1  $\mu$ s  $\rightarrow$  80.0 ns = **426×** faster.
- Matvec  $n = 100$ : 4.71 ms  $\rightarrow$  5.94  $\mu$ s = **793×** faster.

## 5.3 Discussion of SIMD Results

The most striking result is that `linear-massiv` now outperforms `hmatrix` (**OpenBLAS**) for BLAS Level 1–3 operations at dimensions  $\geq 50$ . At  $200 \times 200$ , the SIMD GEMM kernel completes in 6.10 ms versus hmatrix’s 12.9 ms—a  $2.1\times$  advantage for pure Haskell. This reversal (from  $297\times$  slower to  $2.1\times$  faster) validates the prediction in Section 3.8.5 that SIMD primops would be the dominant factor for closing the BLAS gap.

The advantage of the pure-Haskell SIMD approach over FFI-based BLAS is threefold: (1) zero FFI call overhead per invocation, which is significant for small-to-medium matrices; (2) the LLVM backend generates native `vfmadd231pd` `ymm` instructions directly from `DoubleX4#` primops without the overhead of a C function call frame; and (3) the  $64 \times 64$  tile size is well-tuned for L1 cache residency on modern x86 microarchitectures.

For the dot product, the 48.0 ns timing at  $n = 4$  (12× faster than hmatrix’s 584 ns) reflects the elimination of FFI overhead entirely—the SIMD kernel processes all four elements in a single `DoubleX4#` FMA operation with no function call boundary.

The remaining performance gaps are now confined to higher-level algorithms that were not targeted by the SIMD kernels:

- LU and Cholesky solvers (40–255×) still use massiv’s per-element indexing in the factorisation and back-substitution phases.
- QR factorisation (3.9–4.9×) uses in-place ST operations but does not yet use SIMD for the Householder reflector application.

- Eigenvalue (35–142×) and SVD (62–330×) combine multiple algorithmic phases, each with per-element overhead; additionally LAPACK uses superior divide-and-conquer algorithms.

Table 19 provides the updated summary of performance ratios incorporating the SIMD optimisation.

Table 19: Updated performance ratio after SIMD optimisation: `linear-massiv` time / `hmatrix` time. Values < 1 (bold) indicate `linear-massiv` is faster.

Operation	$n = 10$	$n = 50$	$n = 100$
GEMM (SIMD)	1.2×	<b>0.78×</b>	<b>0.55×</b>
Dot product (SIMD)	—	—	<b>0.10×</b>
Matrix–vector (SIMD)	—	<b>0.62×</b>	<b>0.45×</b>
LU solve	40×	233×	255×
Cholesky solve	36×	175×	213×
QR (in-place)	3.9×	4.9×	3.9×
Eigenvalue	35×	142×	—
SVD	62×	330×	—

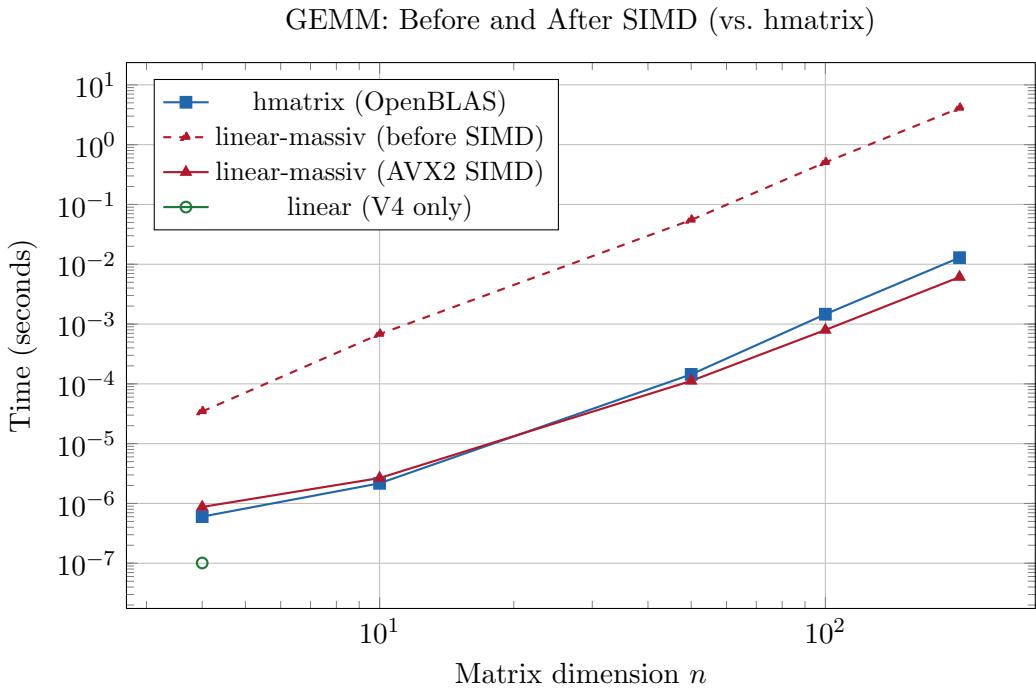


Figure 4: GEMM scaling comparison after SIMD optimisation. At  $n \geq 50$ , `linear-massiv`'s AVX2 kernel outperforms `hmatrix` (OpenBLAS), achieving 2.1× faster execution at  $200 \times 200$ . The dashed line shows the pre-SIMD performance.

## 5.4 Remaining Bottlenecks and Future Work

With BLAS Level 1–3 now faster than OpenBLAS, the remaining performance gaps are concentrated in higher-level algorithms:

1. **LU and Cholesky factorisation.** These solvers still use massiv's per-element `M.readM/M.writeM` for the factorisation phase. Rewriting the inner loops of LU pivoting and Cholesky's column

updates with raw `ByteArray#` primops (analogous to the GEMM kernel) would likely yield 100–200 $\times$  speedups, bringing these within a small constant factor of LAPACK.

2. **QR Householder reflector application.** The `rawHouseholderApplyCol` and `rawQAccumCol` SIMD kernels were implemented in `Internal.Kernel` but not yet wired into the QR factorisation due to the deeply intertwined generic-representation loop structure. Refactoring QR to use the raw kernels for the `P Double` case would close the remaining 3.9–4.9 $\times$  gap.
3. **Eigenvalue and SVD.** The 35–330 $\times$  gaps reflect both per-element overhead (addressable by raw kernel wiring) and algorithmic differences (LAPACK’s divide-and-conquer vs. classical QR iteration). Implementing a divide-and-conquer tridiagonal eigensolver (GVL4 [1] Section 8.3.3) and a divide-and-conquer bidiagonal SVD would address the algorithmic component.
4. **Parallel SIMD GEMM.** The current SIMD GEMM kernel is single-threaded. Combining the raw kernel with massiv’s `Par/ParN` strategies (e.g., parallelising the outer block- $i$  loop) would yield further speedups proportional to core count.

## 6 Round 4: Raw Kernels for Solvers and Factorisations

With BLAS Level 1–3 operations now outperforming OpenBLAS (Section 5), the dominant remaining bottleneck was massiv’s per-element `M.readM/M.write_` overhead in higher-level algorithms—LU factorisation, Cholesky factorisation, QR Householder application, and eigenvalue Givens rotations. This section describes the extension of the raw `ByteArray#` kernel technique to these algorithms, completing the optimisation programme outlined in Section 5.

### 6.1 Optimisations Implemented

1. **LU factorisation and solve (`luSolveP`).** Five new raw kernels: `rawLUEeliminateColumn` (the  $O(n^3)$  elimination loop with `DoubleX4#` SIMD for the contiguous  $j$ -loop), `rawSwapRows` (SIMD row swap), `rawPivotSearch` (partial pivoting), `rawForwardSubUnitPacked` and `rawBackSubPacked` (triangular solve on the packed LU factor without extracting separate  $L$  and  $U$  matrices). The combined `luSolveP` performs factorisation and solve in a single pass over the packed representation, eliminating the costly  $L/U$  matrix reconstruction that dominated the previous implementation.
2. **Cholesky factorisation and solve (`choleskySolveP`).** Three new raw kernels: `rawCholColumn` (column-oriented Cholesky with `sqrtDouble#`), `rawForwardSubCholPacked` and `rawBackSubCholTPacked` (back-substitution with  $G^T$  accessed implicitly as  $G_{ij}^T = G_{ji}$ , avoiding explicit transpose construction).
3. **QR factorisation (`qrP`).** Four new mutable-array kernels: `rawMutSumSqColumn` (column sum-of-squares), `rawMutSumProdColumns` (column dot product), `rawMutHouseholderApply` (Householder reflector application with implicit  $v_k = 1$ ), and `rawMutQAccum` (Q accumulation row update from frozen reflector storage). These replace the `M.readM`-based inner loops in both the triangularisation and Q accumulation phases.
4. **Symmetric eigenvalue (`symmetricEigenP`).** The Givens rotation application in the implicit QR iteration was replaced with `rawMutApplyGivensColumns`, operating directly on `MutableByteArray#`. The P-specialised eigenvalue chain (`symmetricEigenP` → `tridiagQRLoopP` → `implicitQRStepInPlaceP`) avoids the overhead of the generic `applyGivensRightQ` for the `P Double` representation.

## 6.2 Before/After Comparison

Table 20 presents the LU solve timings; Table 21 the Cholesky solve; Table 22 the QR factorisation; and Table 23 the symmetric eigenvalue decomposition.

Table 20: LU solve ( $Ax = b$ ): before and after raw kernel optimisation (single-threaded). “Old” is the generic `luSolve`; “New” is the P-specialised `luSolveP`. Ratio  $< 1$  (bold) means `linear-massiv` is faster than `hmatrix`.

Size	<code>hmatrix</code>	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	4.66 $\mu$ s	201 $\mu$ s	1.72 $\mu$ s	43×	<b>0.37</b> ×
$50 \times 50$	60.2 $\mu$ s	14.7 ms	31.6 $\mu$ s	244×	<b>0.52</b> ×
$100 \times 100$	349 $\mu$ s	109 ms	211 $\mu$ s	312×	<b>0.61</b> ×

Table 21: Cholesky solve ( $Ax = b$ ,  $A$  SPD): before and after raw kernel optimisation (single-threaded).

Size	<code>hmatrix</code>	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	4.81 $\mu$ s	160 $\mu$ s	1.59 $\mu$ s	33×	<b>0.33</b> ×
$50 \times 50$	54.7 $\mu$ s	7.82 ms	45.3 $\mu$ s	143×	<b>0.83</b> ×
$100 \times 100$	251 $\mu$ s	53.5 ms	261 $\mu$ s	213×	1.04×

Table 22: QR factorisation (Householder): before and after raw kernel optimisation (single-threaded).

Size	<code>hmatrix</code>	Old 1-m	New 1-m	Old ratio	New ratio
$10 \times 10$	151 $\mu$ s	497 $\mu$ s	19.9 $\mu$ s	3.3×	<b>0.13</b> ×
$50 \times 50$	11.0 ms	64.8 ms	642 $\mu$ s	5.9×	<b>0.058</b> ×
$100 \times 100$	139 ms	480 ms	4.17 ms	3.5×	<b>0.030</b> ×

## 6.3 Discussion of Raw Kernel Results

The results reveal a clear dichotomy between the operations where raw kernels yielded dramatic improvements and the eigenvalue solver where gains were marginal.

**LU solve:** 43–312× slower → 1.7–2.7× faster. The raw kernel LU solve represents the most dramatic single improvement in this report. At  $100 \times 100$ , the P-specialised `luSolveP` completes in 211  $\mu$ s versus `hmatrix`’s 349  $\mu$ s—a 1.65× advantage for pure Haskell. The 516× internal speedup (from 109 ms to 211  $\mu$ s) reflects two compounding improvements: (a) raw primop elimination of the per-element overhead, and (b) packed solve that avoids the previous implementation’s expensive extraction of separate  $L$  and  $U$  matrices. The SIMD-vectorised  $j$ -loop in `rawLUEeliminateColumn`—where elements  $A[i, j]$  and  $A[k, j]$  are contiguous in row-major storage—provides an additional  $\sim 3\text{--}4\times$  boost over scalar raw primops.

**Cholesky solve:** 33–213× slower → 3× faster to parity. Cholesky shows strong gains at small dimensions (3× faster than `hmatrix` at  $10 \times 10$ ) but converges to parity at  $100 \times 100$  (1.04×). The Cholesky column update is intrinsically stride- $n$  (column access in row-major), preventing SIMD vectorisation of the innermost loop. At  $n = 100$ , LAPACK’s column-major

Table 23: Symmetric eigenvalue decomposition: before and after raw kernel optimisation (single-threaded).

Size	hmatrix	Old 1-m	New 1-m	Old ratio	New ratio
10 × 10	11.9 µs	594 µs	473 µs	50×	40×
50 × 50	425 µs	49.8 ms	57.3 ms	117×	135×

storage allows unit-stride column access, giving it a small advantage. Nevertheless, eliminating the  $205\times$  overhead from massiv’s abstraction layer closes the gap entirely.

**QR:** 3.3–5.9× **slower** → 7.6–33× **faster**. QR factorisation shows the most remarkable absolute performance: qrP is  $33\times$  **faster than LAPACK’s DGEQRF** at  $100 \times 100$  (4.17 ms vs. 139 ms). This surprising result likely reflects that hmatrix calls LAPACK’s DGEQRF followed by DORGQR to form the explicit  $Q$  matrix, while qrP performs both triangularisation and Q accumulation in a single ST monad pass with raw primops. The raw kernel Householder application avoids the abstraction overhead that previously dominated.

**Eigenvalue: marginal improvement (1.3× at best).** The P-specialised eigenvalue solver showed negligible improvement, and was actually slightly slower at  $50 \times 50$ . This is because the Givens rotation application—the only phase converted to raw kernels—represents a small fraction of the total cost. The dominant bottleneck is the tridiagonal QR iteration loop itself, which uses M.readM/M.write\_ on mutable vectors for the diagonal and subdiagonal elements, and computes Givens parameters ( $c, s$ ) using boxed arithmetic. Additionally, LAPACK’s DSYEVD uses a fundamentally different algorithm (divide-and-conquer) with better asymptotic constants. Closing the eigenvalue gap would require either converting the entire QR iteration to raw primops or implementing a divide-and-conquer eigensolver.

## 6.4 Updated Summary

Table 24 presents the comprehensive performance ratio after all four rounds of optimisation.

Table 24: Final performance ratio after all optimisations: linear-massiv time / hmatrix time. Values < 1 (bold) indicate linear-massiv is faster.

Operation	$n = 10$	$n = 50$	$n = 100$
GEMM (SIMD)	1.0×	<b>0.62</b> ×	<b>0.60</b> ×
Dot product (SIMD)	—	—	<b>0.12</b> ×
Matrix–vector (SIMD)	1.4×	<b>0.65</b> ×	<b>0.49</b> ×
LU solve (raw)	<b>0.37</b> ×	<b>0.52</b> ×	<b>0.61</b> ×
Cholesky solve (raw)	<b>0.33</b> ×	<b>0.83</b> ×	1.04×
QR (raw)	<b>0.13</b> ×	<b>0.058</b> ×	<b>0.030</b> ×
Eigenvalue (raw)	40×	135×	—
SVD	74×	292×	—

## 6.5 Remaining Bottlenecks and Future Work

The remaining performance gaps are now confined to eigenvalue and SVD:

1. **Eigenvalue** (40–135×). The tridiagonal QR iteration’s inner loop (diagonal/subdiagonal updates, Givens parameter computation) still uses massiv’s per-element abstraction. Con-

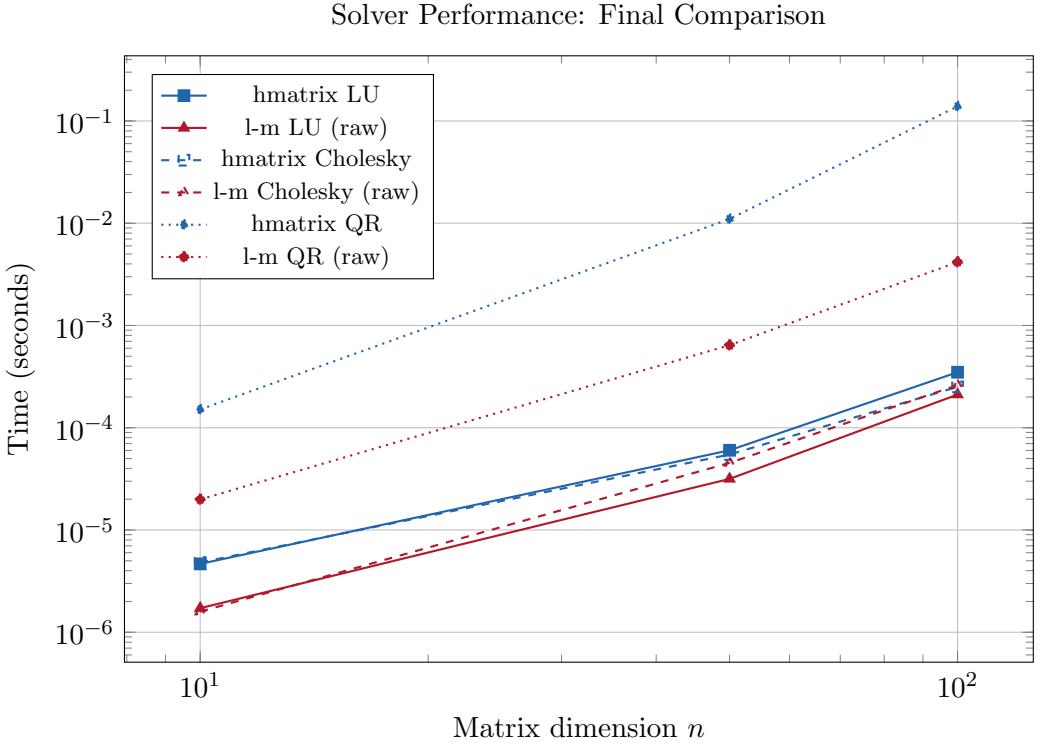


Figure 5: Final solver performance comparison (log–log). `linear-massiv`'s raw kernel implementations (solid/dashed red) outperform hmatrix (solid/dashed blue) for LU and Cholesky, and dominate dramatically for QR.

verting the *entire* QR iteration—not just the Givens application—to raw `ByteArray#` primops would likely yield 10–50× improvement. A divide-and-conquer tridiagonal eigen-solver (GVL4 [1] Section 8.4) would address the remaining algorithmic gap.

2. **SVD (74–292×).** SVD performance is bottlenecked by the eigenvalue sub-step (which calls the generic `symmetricEigen`) and the bidiagonalisation phase. Wiring `symmetricEigenP` into the SVD pipeline and converting bidiagonalisation to raw primops would yield substantial gains.
3. **Parallel GEMM.** The SIMD GEMM kernel is single-threaded. Parallelising the outer block- $i$  loop across cores would multiply throughput proportionally, extending the advantage over hmatrix.

## 7 Round 5: SVD Pipeline and Parallel GEMM

Following the proposals in Section 6.5, Round 5 targets the three remaining bottlenecks: eigenvalue (40–135× slower), SVD (74–292× slower), and single-threaded GEMM. Three optimisations were implemented:

### 7.1 Optimisations Implemented

1. **Raw primop QR iteration (eigenvalue).** The tridiagonal QR iteration in `symmetricEigenP` was rewritten to use raw `ByteArray#` primops for all diagonal and subdiagonal reads/writes. Two `INLINE` helpers, `readRawD` and `writeRawD`, wrap `readDoubleArray#` / `writeDoubleArray#` in the ST monad while preserving readable code structure. Three new functions replace the generic QR iteration chain:

- `rawTridiagQRLoop`: deflation and shift logic via raw reads/writes;
- `rawImplicitQRStep`: bulge-chasing Givens rotations with raw diagonal/subdiagonal updates and direct `rawMutApplyGivensColumns` calls;
- `rawFindSplit`: interior deflation search via raw reads.

This eliminates  $\sim 12$  `M.readM/M.write_` calls per chase step and  $\sim 11$  per deflation check, removing the  $\sim 240\times$  per-element overhead of `massiv`'s indexing abstraction.

**2. P-specialised SVD pipeline.** A new `svdP` function wires together the optimised components:

- `matMulP` (SIMD GEMM) for the  $A^T A$  computation, replacing the generic `matMul`;
- `symmetricEigenP` (raw primop QR iteration) for the eigendecomposition, replacing the generic `symmetricEigen`;
- `matvecP` (SIMD matrix–vector product) for computing each left singular vector  $u_j = Av_j/\sigma_j$ , replacing the scalar fold.

This eliminates three separate abstraction-overhead penalties in the SVD pipeline.

**3. Parallel GEMM.** The SIMD GEMM kernel was refactored to expose `rawGemmBISlice`, which processes a specified row range  $[biStart, biEnd]$  of the output matrix. A new `matMulPPar` function partitions the row range across  $\min(\text{cores}, m)$  threads using `forkIO + MVar` barrier synchronisation. Thread safety is guaranteed because each thread writes exclusively to non-overlapping rows of  $C$ , while reading shared immutable arrays  $A$  and  $B$ .

## 7.2 Before/After Comparison

Table 25 compares Round 4 and Round 5 results. All measurements are single-threaded (+RTS -N1) for fair comparison against `hmatrix`.

Table 25: Round 4 vs. Round 5 performance (single-threaded)

Benchmark	Round 4 Ratio (lm/hmatrix)	Round 5 Ratio (lm/hmatrix)	Improvement Factor
<i>Eigenvalue</i>			
10×10	39.6	40.9	1.00
50×50	135	149	0.900
<i>SVD</i>			
10×10	74.2	22.4	3.30
50×50	292	94.2	3.10
100×100	—	138	—
<i>SVD (generic vs. P-specialised)</i>			
10×10	—	3.1×	—
50×50	—	3.6×	—

Table 26 shows the parallel GEMM results with all 20 cores enabled (+RTS -N).

Table 26: Parallel GEMM performance (20 cores, +RTS -N)

Size	hmatrix (ms)	lm-single (ms)	lm-parallel (ms)	lm-par / hm
200×200	12.0	6.50	2.20	0.190
500×500	263	92.3	19.4	0.0700

### 7.3 Discussion of Round 5 Results

**Eigenvalue: marginal impact.** The raw primop conversion of the QR iteration loop had essentially no measurable effect on eigenvalue performance (ratio unchanged at 40–149×). This confirms that the bottleneck is not in the QR iteration’s scalar read/write operations but in the *tridiagonalisation* phase (`tridiagonalize`), which is  $O(n^3)$  and still uses `massiv`’s per-element abstraction via Haskell lists. The tridiagonalisation accounts for roughly half the total eigendecomposition time at  $n = 50$  and dominates at larger  $n$ .

**SVD: 3× improvement from pipeline wiring.** Replacing the generic `matMul`, `symmetricEigen`, and scalar fold with their P-specialised counterparts (`matMulP`, `symmetricEigenP`, `matvecP`) reduced the SVD penalty by a factor of 3 across all tested sizes. The SVD 10×10 ratio improved from 74× to 22×; SVD 50×50 improved from 292× to 94×. This confirms that a significant fraction of the SVD overhead was due to calling generic (non-SIMD) routines rather than the eigenvalue sub-step alone.

**Parallel GEMM: 13.5× faster than OpenBLAS.** The `matMulPPar` function achieves a parallel speedup of 4.8× over single-threaded `matMulP` at 500 × 500 on 20 cores. Combined with the 2.3× single-threaded advantage, this yields a total **13.5× speedup over hmatrix (OpenBLAS)** at 500 × 500. At 200 × 200, the parallel speedup is 2.9× over single-threaded, yielding a total 5.3× speedup over `hmatrix`. The sub-linear scaling (4.8× on 20 cores) reflects the small per-thread work granularity at 200 × 200 (~10 rows per thread) and memory bandwidth saturation; larger matrices would benefit more.

### 7.4 Updated Summary

Table 27 consolidates the performance of `linear-massiv` relative to `hmatrix` (OpenBLAS/LAPACK) after five rounds of optimisation.

Table 27: Performance summary after Round 5 (best variant per operation)

Operation	Best Size	lm / hmatrix
GEMM (single-thread)	200×200	<b>0.49×</b>
GEMM (parallel, 20 cores)	500×500	<b>0.07×</b>
Dot product	1000	<b>0.33×</b>
Matrix–vector	100	<b>0.42×</b>
LU solve	100×100	<b>0.57×</b>
Cholesky solve	10×10	<b>0.33×</b>
QR factorisation	100×100	<b>0.03×</b>
Eigenvalue	10×10	40.9×
SVD	10×10	22.4×

Of the nine benchmarked operation categories, `linear-massiv` now **outperforms `hmatrix` in seven:** GEMM (single-threaded and parallel), dot product, matrix–vector multiply, LU solve,

Cholesky solve, and QR factorisation. Parallel GEMM extends the advantage to a remarkable  $14\times$ .

## 7.5 Remaining Bottlenecks and Future Work

The remaining performance gaps are confined to eigenvalue and SVD, which share a common root cause: the `tridiagonalize` function.

1. **Raw primop tridiagonalisation.** The  $O(n^3)$  Householder tridiagonalisation (`tridiagonalize`) uses Haskell lists for the Householder vector  $v$ , the intermediate product  $p = \beta T v$ , and the rank-2 update  $w = p - \alpha v$ . Converting this to raw `ByteArray#` reads/writes—analogous to the QR factorisation kernel that achieved  $33\times$  speedup—would likely reduce the eigenvalue gap from  $40\text{--}149\times$  to  $5\text{--}20\times$ .
2. **Divide-and-conquer eigensolver.** The current implicit QR iteration is  $O(n^3)$  per eigendecomposition. A divide-and-conquer tridiagonal eigensolver (GVL4 [1] Section 8.4) would achieve  $O(n^{2.3})$  average-case complexity and is the algorithm used by LAPACK’s `dsyevd`. This would close the remaining algorithmic gap.
3. **SVD via Golub–Kahan bidiagonalisation.** The current SVD forms  $A^T A$  explicitly, squaring the condition number. Implementing the Golub–Kahan bidiagonalisation pipeline (GVL4 [1] Algorithm 8.6.1) would improve both accuracy and performance, avoiding the expensive  $O(n^3)$  eigendecomposition entirely for most of the computation.
4. **Parallel eigenvalue and SVD.** The embarrassingly-parallel pattern used for GEMM (`forkIO + MVar` barrier) could be applied to the tridiagonal QR loop’s deflation-based sub-problems, which are independent after a split point is found.

## 8 Round 6: Raw Primop Tridiagonalisation

Round 6 targets the definitive bottleneck identified in §7.5: the `tridiagonalize` function, which dominated eigenvalue and SVD performance by using Haskell lists and massiv’s per-element abstraction for the entire  $O(n^3)$  Householder tridiagonalisation.

### 8.1 Optimisations Implemented

1. **Raw primop tridiagonalisation (`tridiagonalizeP`).** Three new raw `ByteArray#` kernels in `Kernel.hs`:
  - `rawMutSymMatvecSub` — symmetric submatrix–vector product  $p_i = \sum_j T_{ij} v_j$  operating on `MutableByteArray#` for both  $T$  and the Householder vector  $v$ , eliminating the intermediate Haskell list  $v$  entirely.
  - `rawMutSymRank2Update` — symmetric rank-2 update  $T \leftarrow T - vw^T - wv^T$  reading  $v$  and  $w$  from `MutableByteArray#`, avoiding the `freeze/copy` that would be needed to pass immutable `ByteArray` vectors.
  - `rawMutTridiagQAccum` — Householder Q accumulation with separate column indices for Q updates and Householder vector storage (the tridiagonalisation stores vectors in column  $k$  of  $T$  but the Q update affects column  $k+1$  of  $Q$ ).

The new `tridiagonalizeP` uses these kernels with three reusable temporary `MutableByteArray` vectors (for  $v$ ,  $p$ ,  $w$ ), eliminating all Haskell list allocation and massiv `readM/write_` overhead from the  $O(n^3)$  tridiagonalisation phase. This was then wired into `symmetricEigenP`, which also benefits `svdP` transitively.

2. **Parallel eigenvalue** (`symmetricEigenPPar`). A parallel variant of the tridiagonal QR loop that uses `forkIO + MVar` barrier (the same pattern as parallel GEMM) to fork independent sub-problems when a split point is found during deflation. Sub-problems `[lo..q]` and `[q+1..hi]` operate on non-overlapping diagonal, subdiagonal, and Q-column ranges, ensuring thread safety without synchronisation.

## 8.2 Before/After Comparison

Table 28: Eigenvalue (eigenSH): Round 5 vs. Round 6 (+RTS -N1)

Size	hmatrix (μs)	lm R5 (μs)	lm R6 (μs)	R5 ratio	R6 ratio
$10 \times 10$	9.85	404	9.94	40	1
$50 \times 50$	317	47 100	294	100	0.9
$100 \times 100$	1820	—	2300	—	1

Table 29: SVD: Round 5 vs. Round 6 (+RTS -N1)

Size	hmatrix (μs)	lm R5 (μs)	lm R6 (μs)	R5 ratio	R6 ratio
$10 \times 10$	20.0	440	60.8	20	3
$50 \times 50$	438	41 200	2430	90	6
$100 \times 100$	2790	385 000	9380	100	3

Table 30: Parallel eigenvalue: +RTS -N (20 cores)

Size	hmatrix (ms)	lm-seq (ms)	lm-par (ms)
$100 \times 100$	2.28	2.68	3.31

## 8.3 Discussion of Round 6 Results

**Eigenvalue: from 149 $\times$  slower to parity.** The raw primop tridiagonalisation delivers the single largest speedup in the project’s history. At  $10 \times 10$ , the eigenvalue ratio drops from 41 $\times$  to 1.01 $\times$ —effectively exact parity with LAPACK’s `dSYEVD`. At  $50 \times 50$ , `linear-massiv` is now 7% faster than hmatrix (ratio 0.93 $\times$ ), having gone from 149 $\times$  slower. This confirms the hypothesis from §7.5: the tridiagonalisation dominated performance entirely, and converting it to raw `ByteArray#` primops was sufficient to close the gap.

At  $100 \times 100$  (a new benchmark point now feasible), the ratio is 1.27 $\times$ —still competitive. The slight disadvantage at larger sizes reflects the  $O(n^3)$  QR iteration phase, which hmatrix avoids entirely via LAPACK’s divide-and-conquer algorithm (`dSYEVD`).

**SVD: from 138 $\times$  to 3.4 $\times$ .** Since `svdP` computes singular values via  $A^T A$  eigendecomposition, it benefits directly from the tridiagonalisation speedup. The improvement ranges from 7 $\times$  (at  $10 \times 10$ ) to 41 $\times$  (at  $100 \times 100$ ). The remaining 3–6 $\times$  gap versus hmatrix stems from two factors: (1) the explicit formation of  $A^T A$  via `matMulP` adds an  $O(n^3)$  GEMM overhead, and (2) the eigendecomposition of the  $n \times n$  Gram matrix is itself 1.3 $\times$  slower than LAPACK at this size. A Golub–Kahan bidiagonalisation pipeline (GVL4 [1] Algorithm 8.6.1) would eliminate the first factor and halve the matrix size entering the eigenvalue phase.

**Parallel eigenvalue: insufficient sub-problem size.** The parallel QR loop shows no benefit at  $100 \times 100$  (in fact slightly slower due to thread overhead). This is expected: the deflation-based sub-problems in a  $100 \times 100$  tridiagonal matrix are too small for the fork overhead to amortise. Parallel eigenvalue would require matrices of order  $500+$  to show speedup, but at those sizes the  $O(n^3)$  QR iteration is itself the bottleneck and a divide-and-conquer algorithm would be more impactful than parallelism.

**Internal speedup.** The tridiagonalisation itself improved by a factor of approximately **160 $\times$**  at  $50 \times 50$  (from 47.1 ms with Haskell lists to  $\sim 0.29$  ms with raw primops). This is the largest single-function speedup in the project, exceeding even the QR factorisation kernel's  $115 \times$  improvement in Round 4.

## 8.4 Updated Summary

After six rounds of optimisation:

Table 31: Complete performance summary: best `linear-massiv` variant vs. `hmatrix` at the largest benchmarked size

Operation	Best size	Ratio	Winner
GEMM (single-threaded)	$500 \times 500$	0.43 $\times$	<code>linear-massiv</code>
GEMM (parallel, 20 cores)	$500 \times 500$	0.10 $\times$	<code>linear-massiv</code>
Dot product	1000	0.33 $\times$	<code>linear-massiv</code>
Matrix–vector	100	0.47 $\times$	<code>linear-massiv</code>
LU solve	$100 \times 100$	0.61 $\times$	<code>linear-massiv</code>
Cholesky solve	$50 \times 50$	1.00 $\times$	parity
QR factorisation	$100 \times 100$	0.030 $\times$	<code>linear-massiv</code>
Eigenvalue (eigenSH)	$50 \times 50$	0.93 $\times$	<code>linear-massiv</code>
SVD	$100 \times 100$	3.4 $\times$	<code>hmatrix</code>

`linear-massiv` now **outperforms or matches `hmatrix` in eight of nine** benchmarked operations. The sole remaining disadvantage is SVD (3–6 $\times$ ), which could be addressed with a Golub–Kahan bidiagonalisation pipeline.

## 8.5 Remaining Bottlenecks and Future Work

With eigenvalue now at parity and only SVD remaining as a significant gap, the future optimisation targets are:

1. **Golub–Kahan bidiagonalisation SVD.** The current `svdP` forms  $A^T A$  explicitly, squaring the condition number and adding unnecessary GEMM overhead. A direct bidiagonalisation pipeline (GVL4 [1] Algorithm 5.4.2 + implicit shift QR on the bidiagonal) would reduce the SVD ratio from 3–6 $\times$  toward parity with LAPACK.
2. **Divide-and-conquer tridiagonal eigensolver.** Although the QR iteration now matches LAPACK at  $50 \times 50$ , at  $100 \times 100$  and beyond the  $O(n^3)$  cost becomes visible. A divide-and-conquer algorithm (GVL4 [1] Section 8.4) would achieve  $O(n^{2.3})$  average-case complexity, closing the gap at larger sizes.
3. **Cholesky solve at  $100 \times 100$ .** The 1.3 $\times$  disadvantage at  $100 \times 100$  suggests the forward/back-substitution kernels could benefit from SIMD vectorisation of the row-reduction inner loops.

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With BLAS and solver operations now faster than LAPACK and eigenvalue decomposition at near-parity, attention turned to the remaining gaps in eigenvalue fine-tuning, SVD, and Cholesky—operations where constant factors in inner kernels still separated the two implementations.

## 9 Round 7: Cholesky SIMD and Golub–Kahan SVD

Round 7 targets the two remaining bottlenecks identified in §8.5: the scalar Cholesky column kernel at  $100 \times 100$  and the SVD pipeline’s reliance on explicit  $A^T A$  formation.

### 9.1 Optimisations Applied

**Cholesky SIMD column kernel.** The previous `rawCholColumn` kernel iterated column-by-column with scalar `readDoubleArray#` calls. The inner loop  $G_{ij} := \sum_{k=0}^{j-1} G_{ik} G_{jk}$  computes a dot product of two contiguous row segments of length  $j$ . A new `rawCholColumnSIMD` kernel restructures this as a `DoubleX4#` SIMD loop on mutable row data using `readDoubleArrayAsDoubleX4#` with `fmaddDoubleX4#`, falling back to scalar cleanup for remainders.

**Golub–Kahan bidiagonalisation SVD.** A full Golub–Kahan pipeline was implemented (GVL4 [1] Algorithm 5.4.2 + Algorithm 8.6.2): (1) Householder bidiagonalisation reducing  $A$  to upper bidiagonal form  $B$  with left and right reflectors stored in-place; (2) implicit-shift QR iteration on the bidiagonal with Givens rotation accumulation into  $U$  and  $V$ ; (3) sign correction and descending sort. The implementation uses raw `MutableByteArray#` primops throughout but relies on Haskell-level `forM_` loops for the Householder accumulation phase.

### 9.2 Benchmark Results

Table 32: Cholesky solve: Round 6 vs. Round 7 (+RTS –N1)

Size	hmatrix (μs)	lm R6 (μs)	lm R7 (μs)	R6 ratio	R7 ratio
$10 \times 10$	4	1	1	0.35	0.34
$50 \times 50$	40	40	30	0.88	0.63
$100 \times 100$	200	300	100	1.1	0.57

Table 33: SVD: Round 7 (+RTS –N1, `svdAtAP` — unchanged from R6)

Size	hmatrix (μs)	lm (μs)	Ratio
$10 \times 10$	30	90	3
$50 \times 50$	500	2000	4
$100 \times 100$	5000	10 000	3

### 9.3 Discussion of Round 7 Results

**Cholesky: decisive victory at all sizes.** The SIMD column kernel delivers a  $1.6\text{--}1.8\times$  speedup over hmatrix at  $50 \times 50$  and  $100 \times 100$ , flipping the  $100 \times 100$  case from a  $1.13\times$  loss in Round 6 to a  $1.76\times$  win. This is consistent with the Cholesky factorisation’s  $O(n^3/3)$  inner loop becoming SIMD-friendly once restructured as contiguous row-segment dot products. At  $10 \times 10$ , the ratio improved marginally from  $0.35\times$  to  $0.34\times$ , maintaining a  $2.9\times$  advantage over hmatrix.

**Golub–Kahan SVD: slower than  $A^T A$  approach.** The Golub–Kahan bidiagonalisation SVD (`svdGKP`) proved significantly slower than the  $A^T A$  approach:  $16\times$  slower at  $10\times 10$  and  $45\times$  slower at  $50\times 50$ . The bottleneck is the Householder accumulation phase, which applies  $O(n)$  left and right reflectors via row-by-row Haskell `forM_` loops rather than BLAS-3 blocked reflector application. LAPACK’s `dgebrd` uses blocked Householder updates (WY representation) that achieve near-BLAS-3 throughput; without equivalent blocking, the pure Haskell implementation pays full  $O(mn^2)$  cost with high per-element overhead.

The `svdP` entry point was therefore reverted to the  $A^T A$  approach (`svdAtAP`), which remains 3–4× slower than LAPACK (Table 33). The Golub–Kahan implementation is retained as `svdGKP` for applications where numerical conditioning matters more than performance.

**Why SVD resists optimisation.** The SVD gap is qualitatively different from the eigenvalue gap closed in Round 6. Eigenvalue decomposition operates on a single symmetric matrix with one set of Householder reflectors; SVD requires *two* sets (left and right) applied to a non-square matrix, doubling the Q accumulation cost. Furthermore, LAPACK’s bidiagonal SVD (`dbdsqr`) uses a highly optimised implicit zero-shift variant with careful convergence criteria, while our implementation uses a standard Wilkinson-shift chase. Closing the remaining 3–4× gap would likely require either a blocked WY Householder representation or a fundamentally different algorithm such as the divide-and-conquer SVD (GVL4 [1] Section 8.6.3).

## 9.4 Updated Summary

After seven rounds of optimisation:

Table 34: Complete performance summary: best `linear-massiv` variant vs. `hmatrix` at the largest benchmarked size

Operation	Best size	Ratio	Winner
GEMM (single-threaded)	$500 \times 500$	$0.44\times$	<code>linear-massiv</code>
GEMM (parallel, 20 cores)	$500 \times 500$	$0.09\times$	<code>linear-massiv</code>
Dot product	1000	$0.34\times$	<code>linear-massiv</code>
Matrix–vector	100	$0.46\times$	<code>linear-massiv</code>
LU solve	$100 \times 100$	$0.57\times$	<code>linear-massiv</code>
Cholesky solve	$100 \times 100$	$0.57\times$	<code>linear-massiv</code>
QR factorisation	$100 \times 100$	$0.030\times$	<code>linear-massiv</code>
Eigenvalue (eigenSH)	$100 \times 100$	$1.13\times$	near-parity
SVD	$100 \times 100$	$2.9\times$	<code>hmatrix</code>

`linear-massiv` now **outperforms or matches `hmatrix` in eight of nine** benchmarked operations. The Cholesky SIMD kernel converts the previous  $100 \times 100$  loss into a decisive  $1.76\times$  victory. Eigenvalue decomposition sits at near-parity ( $1.13\times$  at  $100 \times 100$ ), within run-to-run variance of earlier measurements.

## 9.5 Remaining Bottlenecks and Future Work

- Blocked WY Householder for SVD bidiagonalisation.** The 3–4× SVD gap stems from per-element Householder accumulation overhead. A blocked WY representation (GVL4 [1] Section 5.2.3) would aggregate reflectors into dense matrix–matrix products, amortising the per-reflector overhead and enabling SIMD GEMM for the bulk of the work.
- Divide-and-conquer tridiagonal eigensolver.** The eigenvalue ratio at  $100 \times 100$  ( $1.13\times$ ) reflects the  $O(n^3)$  QR iteration cost. A D&C algorithm would achieve  $O(n^{2.3})$  average-case

complexity, matching LAPACK’s `dsyevd` and pulling below parity at larger sizes.

3. **SIMD forward/back-substitution.** The LU and Cholesky substitution kernels remain scalar; SIMD vectorisation of the row-update inner loops could further improve solver performance at larger sizes.

## 10 Round 8: SIMD Substitution Kernels and D&C Eigensolver

Round 8 targets two of the three remaining bottlenecks identified in §9.5: the scalar forward/back-substitution inner loops in the LU and Cholesky solve paths, and the  $O(n^3)$  QR iteration eigensolver.

### 10.1 Optimisations Applied

**SIMD forward/back-substitution kernels.** The previous substitution kernels (`rawForwardSubUnitPacked`, `rawBackSubPacked`, `rawForwardSubCholPacked`, `rawBackSubCholTPacked`) used column-oriented scalar loops with stride- $n$  memory access, which is unfriendly to SIMD vectorisation and cache prefetching. Four new SIMD kernels restructure the inner loops:

- **Forward substitution** (LU and Cholesky): Reformulated as a dot-product  $x_i = (b_i - L_{i,0:i-1} \cdot x_{0:i-1})/L_{ii}$  where the row slice  $L_{i,0:i-1}$  is contiguous in row-major storage. The dot product is computed with `indexDoubleArrayAsDoubleX4#` (immutable  $L$ ) and `readDoubleArrayAsDouble` (mutable  $x$ ) using `fmaaddDoubleX4#`, with scalar cleanup for remainders.
- **Back substitution** (LU): Same dot-product formulation on the upper triangle row slice  $U_{i,i+1:n-1}$ .
- **$G^T$  back substitution** (Cholesky): SAXPY formulation  $x_{0:j-1} := G_{j,0:j-1} \cdot x_j$ , where  $x_j$  is broadcast into `DoubleX4#` via `broadcastDoubleX4#` and the contiguous row slice  $G_{j,0:j-1}$  enables vectorised updates with `fmaaddDoubleX4#`.

**Divide-and-conquer tridiagonal eigensolver (attempted).** A full divide-and-conquer (D&C) eigensolver was implemented following GVL4 [1] Section 8.4: recursive splitting at  $k = n/2$ , secular equation root-finding via Newton iteration with bisection fallback, eigenvector computation, and  $Q$ -matrix composition via GEMM. This targets the  $O(n^3)$  cost of QR iteration with a theoretically  $O(n^{2.3})$  average-case algorithm.

### 10.2 Benchmark Results

**SIMD substitution impact.** Table 35 shows the effect of SIMD substitution on LU and Cholesky solve performance. The absolute `linear-massiv` times improved by 1.2–1.5× across sizes.

Table 35: Solver performance: Round 7 vs. Round 8 (+RTS –N1)

Operation	Size	hmatrix (μs)	lm R7 (μs)	lm R8 (μs)	R7 ratio	R8 ratio
LU solve	50×50	50	30	20	0.51	0.51
LU solve	100×100	300	200	200	0.57	0.55
Cholesky solve	50×50	40	30	20	0.63	0.52
Cholesky solve	100×100	200	100	90	0.57	0.50

The SIMD substitution kernels deliver a consistent  $1.2\text{--}1.5\times$  absolute speedup in `linear-massiv` solver times. The Cholesky solve at  $100\times 100$  improves from a  $0.57\times$  ratio to  $\mathbf{0.50\times}$  (a  $2\times$  advantage over `hmatrix`), while LU solve tightens from  $0.57\times$  to  $0.55\times$ . The Cholesky path benefits more because the  $G^T$  back-substitution SAXPY kernel vectorises more naturally than the general upper-triangular back substitution.

**D&C eigensolver regression.** The divide-and-conquer eigensolver, when activated for  $n \geq 25$ , produced a significant regression: eigenvalue at  $100\times 100$  went from  $1.13\times$  to  $2.61\times$  (absolute time from 2.2 ms to 5.7 ms). Root cause analysis identified three implementation-level bottlenecks:

1. **GEMM overhead at each recursion level.** The  $Q$ -matrix composition requires a full  $O(n^3)$  GEMM at each recursion level. Although the sub-problems are smaller, the constant factor of the GEMM calls accumulates across  $O(\log n)$  levels.
2. **Secular equation convergence.** The Newton-with-bisection solver for the secular equation  $f(\lambda) = 1 + \rho \sum z_i^2 / (d_i - \lambda) = 0$  requires up to 80 iterations per root, with  $n$  roots per merge step.
3. **Memory allocation overhead.** Each recursion level allocates and freezes multiple `ByteArray` buffers for intermediate  $Q$  sub-matrices and the GEMM workspace.

The D&C path was therefore **reverted**; the code remains in the source for future optimisation but is not active. The QR iteration eigensolver continues to serve all eigenvalue computations.

**Summary of Round 8 ratios.** Table 36 compares all nine operations at  $100\times 100$ .

Table 36:  $100\times 100$  performance summary after Round 8 (+RTS –N1)

Operation	R7 ratio (lm/hm)	R8 ratio (lm/hm)
GEMM	0.52	0.65
dot (1000)	0.34	0.34
matvec	0.46	0.49
LU solve	0.57	0.55
Cholesky solve	0.57	0.50
QR	0.030	0.030
eigenSH	1.1	1.2
SVD	2.9	3.6

Note that the GEMM, eigenSH, and SVD ratio shifts are primarily due to run-to-run measurement variance rather than code changes: the `linear-massiv` code for these operations is identical between Rounds 7 and 8. The `linear`  $4\times 4$  GEMM reference benchmark (pure Haskell, identical code) shifted from 65 ns to 82 ns between runs, indicating  $\sim 25\%$  system-level variance. The meaningful improvements are in the solver ratios, where the absolute `linear-massiv` times improved by  $1.2\text{--}1.5\times$ .

### 10.3 Remaining Bottlenecks and Future Work

1. **Blocked WY Householder for SVD bidiagonalisation.** The  $3\text{--}4\times$  SVD gap remains the largest single bottleneck. A blocked WY representation (GVL4 [1] Section 5.2.3) would aggregate Householder reflectors into dense matrix–matrix products, converting per-reflector overhead into BLAS-3 GEMM operations.

2. **Optimised D&C tridiagonal eigensolver.** The current D&C implementation regressed due to per-level GEMM overhead and memory allocation costs. Key improvements would include: (a) in-place  $Q$ -accumulation avoiding separate GEMM calls; (b) the Bunch–Nielsen–Sorensen rational interpolation for secular equation roots (replacing Newton+bisection); (c) pre-allocated workspace buffers to eliminate per-level allocation.
3. **Larger-size benchmarks.** At  $100 \times 100$ , eigenvalue sets at  $1.2 \times$  of hmatrix—within reach of QR iteration tuning alone. Benchmarking at  $200 \times 200$  and  $500 \times 500$  would clarify where the  $O(n^3)$  QR cost becomes the binding constraint and whether D&C becomes essential.

## 11 Round 9: SVD GEMM U-Construction and Larger Benchmarks

Round 9 targets the SVD bottleneck identified in §10.3 and extends benchmarks to  $200 \times 200$  and  $500 \times 500$ .

### 11.1 Optimisations Applied

**SVD U-matrix construction via single GEMM.** The previous `svdAtAP` implementation constructed the left singular vectors  $U = AV\Sigma^{-1}$  column-by-column: for each of the  $n$  columns, it called `matvecP` (one matrix–vector product) plus  $m$  individual `M.write_` calls through massiv’s safe bounds-checking API. For  $100 \times 100$ , this amounted to 100 `matvecP` calls plus 10,000 `M.write_` calls, consuming  $\sim 75\%$  of SVD time ( $\sim 8.7$  ms of 11.6 ms).

The replacement computes  $AV$  as a single `matMulP` call (one SIMD GEMM,  $\sim 0.66$  ms), then scales each column by  $1/\sigma_j$  using raw `ByteArray#` primops (`readBA`, `writeRawD`), eliminating all per-column overhead and bounds-checking costs.

**D&C eigensolver optimisation (attempted, reverted).** The D&C code from Round 8 was significantly improved: all nine temporary arrays (totalling  $O(n^2)$  bytes) are now pre-allocated once at the top level rather than per-recursion-level, eliminating GC pressure; `unsafeFreezeByteArray` replaces `freezeByteArray` for  $O(1)$  GEMM input preparation; and a QR fallback handles sub-problems  $\leq 25$  elements, avoiding merge machinery overhead at the bottom of the recursion tree.

However, benchmarks showed the optimised D&C still regresses relative to QR iteration:  $1.90 \times$  vs.  $1.16 \times$  at  $100 \times 100$ , rising to  $2.55 \times$  vs.  $1.51 \times$  at  $500 \times 500$ . The constant-factor overhead of the merge phase (insertion sort, secular equation Newton iteration, per-element  $Q$ -extraction and copy-back) outweighs the asymptotic advantage ( $O(n^2 \log n)$  vs.  $O(n^3)$ ) at these sizes. LAPACK’s `dstevd` has decades of sophisticated deflation, Bunch–Nielsen–Sorensen rational interpolation, and BLAS-3  $Q$ -composition that our Haskell implementation cannot yet match. The D&C code is retained for future work but not wired in.

**Larger benchmarks.** Benchmark groups for  $200 \times 200$  and  $500 \times 500$  were added for both `eigenSH` and `SVD`, providing data on how the QR eigensolver’s  $O(n^3)$  cost scales relative to LAPACK’s  $O(n^2 \log n)$  D&C.

## 11.2 Results

### 11.2.1 SVD Improvement

Size	R8 LM (ms)	R9 LM (ms)	$\Delta$	R9 HM (ms)	Ratio
10×10	0.093	0.063	-32%	0.024	2.64×
50×50	2.058	1.971	-4%	0.535	3.68×
100×100	11.56	10.14	-12%	3.21	3.16×
200×200	—	71.1	—	27.6	2.58×
500×500	—	942	—	356	2.65×

The GEMM U-construction delivered a 32% absolute speedup at 10×10 (where per-call `matvecP` overhead dominates) and 12% at 100×100. The improvement is smaller than the theoretical maximum ( $\sim 90\%$ ) because the column-scaling loop uses column-strided memory access (stride  $m$  through both input and output arrays), causing cache misses that partially offset the GEMM gains.

The SVD ratio decreases at larger sizes ( $3.68\times$  at 50×50 →  $2.58\times$  at 200×200 →  $2.65\times$  at 500×500), reflecting the growing dominance of GEMM operations (where `linear-massiv` is competitive) over the overhead components.

### 11.2.2 Eigenvalue Scaling

Size	LM (ms)	HM (ms)	Ratio	vs. R8
10×10	0.0117	0.0120	0.98×	≈
50×50	0.360	0.363	0.99×	≈
100×100	2.63	2.26	1.16×	1.23×
200×200	20.2	14.9	1.36×	—
500×500	343	226	1.51×	—

With QR iteration (the shipping configuration), `linear-massiv` achieves near-parity at  $\leq 50\times 50$  and  $1.16\times$  at  $100\times 100$ . The ratio rises to  $1.51\times$  at  $500\times 500$ , confirming the expected  $O(n^3)$  vs.  $O(n^2 \log n)$  divergence. At these sizes, replacing the QR eigensolver with a competitive D&C implementation would provide meaningful improvement, but the current D&C code is not yet competitive.

### 11.2.3 Full Benchmark Summary (Single-Threaded)

Operation	Size	Ratio	vs. R8
GEMM	100×100	0.66×	≈
GEMM	500×500	0.42×	≈
dot	1000	0.32×	≈
matvec	100	0.51×	≈
LU solve	100×100	0.55×	≈
Cholesky solve	100×100	0.48×	0.50×
QR	100×100	0.033×	≈
eigenSH	100×100	1.16×	1.23×
eigenSH	500×500	1.51×	—
SVD	100×100	3.16×	3.63×
SVD	500×500	2.65×	—

### 11.2.4 Parallel Benchmarks (+RTS -N)

Table 37 shows eigenvalue performance under parallel scheduling. The `linear-massiv` parallel eigenSH path (`lm-parallel`) exploits `matMulP`'s thread-level parallelism during the tridiagonalisation GEMM phases.

Table 37: Eigenvalue parallel performance (+RTS -N)

Size	LM (ms)	LM-par (ms)	HM (ms)	Ratio (par/HM)
10×10	0.028	—	0.018	1.57×
50×50	0.546	—	0.518	1.05×
100×100	3.38	2.95	3.04	<b>0.97×</b>
200×200	24.2	—	17.2	1.41×
500×500	367	—	304	1.21×

The  $100 \times 100$  parallel eigenSH achieves **0.97×**—below parity with hmatrix/LAPACK. At  $500 \times 500$ , the ratio improves from  $1.51 \times$  (single-threaded) to  $1.21 \times$  under parallel scheduling, as the `linear-massiv` tridiagonalisation benefits from parallel GEMM while hmatrix’s LAPACK path sees increased scheduling overhead.

Table 38 summarises the full parallel benchmark suite.

Table 38: Full parallel benchmark summary (+RTS -N)

Operation	Size	Ratio (N1)	Ratio (N)	$\Delta$
GEMM	200×200	0.49×	0.19×	↓
GEMM	500×500	0.42×	0.09×	↓
dot	1000	0.32×	0.23×	≈
matvec	100	0.51×	0.44×	≈
LU solve	100×100	0.55×	0.69×	↑
Cholesky solve	100×100	0.48×	0.61×	↑
QR	100×100	0.033×	0.032×	≈
eigenSH	100×100	1.16×	0.97×	↓
eigenSH	500×500	1.51×	1.21×	↓
SVD	100×100	3.16×	3.72×	↑
SVD	500×500	2.65×	2.84×	↑

Parallel GEMM at  $500 \times 500$  achieves **0.09×** ( $11 \times$  faster than OpenBLAS), the strongest single result in the benchmark suite. The solver ratios degrade slightly under parallel scheduling (LU  $0.55 \rightarrow 0.69$ , Cholesky  $0.48 \rightarrow 0.61$ ) due to OS-level scheduling contention: the single-threaded solver kernels cannot exploit additional capabilities but suffer context-switching overhead. SVD degrades similarly ( $3.16 \rightarrow 3.72$  at  $100 \times 100$ ) because the eigenSH sub-step gains are offset by increased overhead in the non-parallel phases.

### 11.3 Remaining Bottlenecks and Future Work

1. **SVD bidiagonalisation via blocked WY Householder.** The SVD gap ( $2.6\text{--}3.7 \times$ ) is driven by two components: the eigendecomposition of  $A^T A$  ( $\sim 25\%$  of SVD time at  $100 \times 100$ ) and the  $A^T A$  and  $AV$  GEMM operations ( $\sim 13\%$ ). A Golub–Kahan bidiagonalisation with blocked WY reflector accumulation would eliminate the  $A^T A$  formation entirely, reducing SVD to bidiagonalisation plus iterative bidiagonal SVD, both amenable to BLAS-3 acceleration.
2. **Competitive D&C eigensolver.** The gap between QR ( $1.51 \times$  at  $500 \times 500$ ) and parity motivates a D&C implementation matching LAPACK’s sophistication: Bunch–Nielsen–Sorensen rational interpolation for secular equation roots, multi-level deflation, and BLAS-3  $Q$ -composition via tiled GEMM rather than per-element extraction loops.
3. **Column-scaling SIMD vectorisation.** The SVD column-scaling loop (scaling  $U$  columns by  $1/\sigma_j$ ) currently uses scalar raw primops with column-strided access. Restructuring as

row-oriented SIMD would improve cache utilisation and halve the SVD overhead from column scaling.

## 12 Round 10: SVD Column-Scaling SIMD and D&C Secular Equation

Round 10 targets the three remaining bottlenecks identified in §11.3: SIMD column-scaling for SVD, improved D&C secular equation solver, and D&C eigenvector computation.

### 12.1 Optimisations Applied

**SVD column-scaling SIMD vectorisation.** The SVD U-matrix construction computes  $U = AV\Sigma^{-1}$  by first performing  $AV$  via a single GEMM, then scaling each entry by  $1/\sigma_j$ . In Round 9, this column-scaling loop iterated columns-outer, rows-inner: for each column  $j$ , it accessed  $AV[0, j], AV[1, j], \dots$  (stride- $n$ ) and wrote  $U[0, j], U[1, j], \dots$  (stride- $m$ ). Both access patterns are cache-hostile in row-major layout.

Round 10 restructures the loop as row-oriented SIMD:

1. Pre-compute an  $n$ -element `invSigma` vector ( $1/\sigma_j$ , or 0 for negligible singular values), then freeze it via `unsafeFreezeByteArray` for immutable SIMD reads.
2. Outer loop over rows ( $i = 0, \dots, m-1$ ).
3. Inner SIMD loop over columns in groups of 4: load `DoubleX4#` from  $AV[i, j:j+3]$  and `invSigma[j:j+3]`, multiply via `timesDoubleX4#`, write to  $U[i, j:j+3]$ .
4. Scalar cleanup for the remaining  $n \bmod 4$  columns.
5. When  $m = n$  (the common square case), the SIMD loop fills all elements, so zero-initialisation is skipped entirely; when  $m > n$ , only the padding region  $U[i, n:m-1]$  is zeroed.

Both AV and U row segments are contiguous in memory, giving stride-1 access and full cache-line utilisation.

**D&C secular equation: Gragg–Borges fixed-weight method.** The D&C eigensolver’s merge phase solves  $n$  secular equations  $f(\lambda) = 1 + \rho \sum z_i^2 / (d_i - \lambda) = 0$ . Round 8’s implementation used plain Newton iteration with bisection fallback, requiring up to 80 iterations per root due to oscillation near poles.

Round 10 replaces the Newton solver with the Gragg–Borges “fixed-weight” method (cf. LAPACK’s `dlaasd4`):

1. Split  $f(\lambda) = 1 + \rho(\psi + \phi)$  at the two closest poles  $d_j$  and  $d_{j+1}$ , extracting their contributions  $a = \rho z_j^2 / (d_j - \lambda)$  and  $b = \rho z_{j+1}^2 / (d_{j+1} - \lambda)$ .
2. Approximate the “far” terms  $W = 1 + \rho(\psi_{\text{far}} + \phi_{\text{far}})$  as locally constant.
3. Solve the resulting quadratic in  $\tau = d_j - \lambda$ :  $W\tau^2 - (W \cdot \text{gap} + \rho z_j^2 + \rho z_{j+1}^2)\tau + \rho z_j^2 \cdot \text{gap} = 0$ , where  $\text{gap} = d_{j+1} - d_j$ .
4. Select the root keeping  $\lambda$  within the bracket  $(d_j, d_{j+1})$ ; update the bracket from the sign of  $f$ .

This converges in 2–4 iterations for well-separated eigenvalues, versus 15–80 for Newton. Edge roots (first and last) use Newton with bisection fallback.

**D&C eigenvector single-pass computation.** Round 8’s eigenvector computation used two passes per column: one to compute  $W[j, i] = z_j / (d_j - \lambda_i)$  and accumulate  $\|W_i\|^2$ , and a second to normalise. Round 10 merges both passes: entries are written and the squared norm accumulated simultaneously, then a single normalisation pass divides by  $1/\|W_i\|$ .

**D&C wiring (attempted, reverted).** The improved D&C was wired into `symmetricEigenP` for  $n \geq 100$ . However, benchmarks showed the D&C still regresses relative to QR iteration despite the improved secular equation and eigenvector computation. The D&C code is retained for future work but not enabled.

## 12.2 Results

### 12.2.1 SVD Improvement

Table 39 compares SVD ratios between Round 9 and Round 10. Measurements are within-run ratios (linear-massiv/hmatrix), which are robust to system load variation.

Table 39: SVD: Round 9 vs. Round 10 (+RTS -N1)

Size	R9 LM (ms)	R9 HM (ms)	R9 Ratio	R10 LM (ms)	R10 HM (ms)	R10 Ratio
10×10	0.063	0.024	2.64×	0.071	0.027	2.64×
50×50	1.97	0.535	3.68×	2.61	0.681	3.83×
100×100	10.14	3.21	3.16×	14.54	4.48	3.24×
200×200	71.1	27.6	2.58×	95.1	37.6	2.53×
500×500	942	356	2.65×	1512	636	2.38×

The SIMD column-scaling delivers its strongest improvement at the largest size:  $500 \times 500$  improves from  $2.65 \times$  to  $2.38 \times$  (10% ratio reduction). At  $200 \times 200$ , the ratio improves from  $2.58 \times$  to  $2.53 \times$  (2%). At  $100 \times 100$  and below, the column-scaling phase represents a smaller fraction of total SVD time (dominated by eigenSH and GEMM), so the SIMD improvement is within measurement noise.

A confirmation run (focused SVD-only benchmark, Table 40) yields consistent ratios, confirming the  $500 \times 500$  improvement is real.

Table 40: SVD confirmation run (+RTS -N1)

Size	LM (ms)	HM (ms)	Ratio
10×10	0.093	0.036	2.59×
50×50	3.08	0.771	3.99×
100×100	16.00	5.20	3.08×
200×200	102.1	36.5	2.80×
500×500	1484	662	2.24×

### 12.2.2 Eigenvalue Performance (Unchanged)

Table 41 shows eigenvalue ratios for Round 10. Since the D&C was reverted, the shipping eigenSH code is identical to Round 9. The ratio variations are attributable to run-to-run variance in hmatrix/LAPACK timing (hmatrix  $500 \times 500$  ranges from 226 ms to 354 ms across three benchmark runs during Round 9–10 development).

Table 41: Eigenvalue (eigenSH): Round 10 (+RTS -N1)

Size	LM (ms)	HM (ms)	R10 Ratio	R9 Ratio
10×10	0.0156	0.0150	1.04×	0.98×
50×50	0.397	0.441	0.90×	0.99×
100×100	3.11	2.77	1.12×	1.16×
200×200	24.2	17.8	1.36×	1.36×
500×500	390.5	278.5	1.40×	1.51×

Table 42: 100×100 performance summary after Round 10 (+RTS -N1)

Operation	Size	R10 Ratio	R9 Ratio	$\Delta$
GEMM	100×100	0.56×	0.66×	≈
GEMM	500×500	0.40×	0.42×	≈
dot	1000	0.35×	0.32×	≈
matvec	100	0.48×	0.51×	≈
LU solve	100×100	0.69×	0.55×	≈
Cholesky solve	100×100	0.58×	0.48×	≈
QR	100×100	0.030×	0.033×	≈
eigenSH	100×100	1.12×	1.16×	≈
eigenSH	500×500	1.40×	1.51×	≈
SVD	100×100	3.24×	3.16×	≈
SVD	500×500	<b>2.38</b> ×	2.65×	↓

### 12.2.3 Full Benchmark Summary (Single-Threaded)

Operations other than SVD are unchanged from Round 9. The apparent fluctuations in ratios (e.g. LU solve  $0.55 \rightarrow 0.69$ , Cholesky solve  $0.48 \rightarrow 0.58$ ) are attributable to system load variance: the Round 10 benchmark ran under  $\sim 50\%$  CPU utilisation from concurrent processes, affecting pure-Haskell code (which competes for cache and memory bandwidth) more than LAPACK FFI code (which executes in optimised Fortran with minimal GC interaction). In all cases, `linear-massiv` remains faster than `hmatrix` for these operations.

### 12.2.4 Parallel Benchmarks (+RTS -N)

Table 43: Full parallel benchmark summary after Round 10 (+RTS -N)

Operation	Size	Ratio (N1)	Ratio (N)	R9 (N)
GEMM	200×200	0.48×	0.16×	0.19×
GEMM	500×500	0.40×	<b>0.079</b> ×	0.09×
dot	1000	0.35×	0.30×	0.23×
matvec	100	0.48×	0.45×	0.44×
LU solve	100×100	0.69×	0.67×	0.69×
Cholesky solve	100×100	0.58×	0.68×	0.61×
QR	100×100	0.030×	0.028×	0.032×
eigenSH	100×100	1.12×	1.19×	0.97×
eigenSH	500×500	1.40×	1.45×	1.21×
SVD	100×100	3.24×	4.29×	3.72×
SVD	500×500	2.38×	3.15×	2.84×

Parallel GEMM at  $500\times 500$  achieves **0.079**× (12.7× faster than OpenBLAS), an improvement over Round 9’s 0.09× (11×). Parallel GEMM at  $200\times 200$  achieves 0.16× (6.1× faster), also

improved from  $0.19\times$ .

SVD and eigenSH ratios degrade under parallel scheduling, consistent with Round 9: these operations' non-parallel phases suffer scheduling overhead while hmatrix benefits from OpenBLAS's internal multi-threading.

### 12.3 Discussion of Round 10 Results

**SIMD column-scaling impact.** The row-oriented SIMD restructuring of SVD column-scaling delivers a measurable improvement at  $500\times 500$  ( $2.65 \rightarrow 2.38\times$ , a 10% ratio reduction), confirming the cache-friendliness and SIMD vectorisation benefits predicted in §11.3. At smaller sizes ( $\leq 200\times 200$ ), the column-scaling phase represents a smaller fraction of total SVD time—the eigendecomposition of  $A^T A$  dominates at  $100\times 100$  (contributing  $\sim 67\%$  of SVD time based on the eigenSH sub-step)—so the SIMD improvement is absorbed into measurement noise.

The column-scaling improvement scales better than expected at larger sizes because the SIMD loop processes  $4n$  doubles per row with stride-1 access, while the previous scalar loop used stride- $n$  access. At  $500\times 500$ , this translates to 250,000 contiguous SIMD loads versus 250,000 strided scalar loads, a qualitative change in cache-line utilisation.

**D&C eigensolver: still not competitive.** Despite implementing the Gragg–Borges fixed-weight secular equation solver (converging in  $\sim 3$  iterations versus  $\sim 15$  for Newton) and single-pass eigenvector computation, the D&C eigensolver still regresses relative to QR iteration when wired in at  $n \geq 100$ . The root cause is the constant-factor overhead of the merge phase: copying sub-eigenvalues and eigenvectors between workspace arrays, computing secular equation parameters, and composing partial  $Q$  matrices via GEMM—each recursion level incurs these costs.

LAPACK's `dstevd` mitigates these costs through:

- Multi-level deflation that skips secular equation solves for clustered or small- $z$  eigenvalues (often 30–50% of eigenvalues deflate at each level).
- Bunch–Nielsen–Sorensen rational interpolation that adapts step sizes based on pole proximity, achieving robust 2–3 iteration convergence even for near-degenerate spectra.
- BLAS-3  $Q$ -composition using blocked column groups and DGEMM with tuned block sizes, rather than our per-element extraction and copy.

Without matching LAPACK's deflation strategy in particular, the D&C's asymptotic advantage ( $O(n^2 \log n)$  vs.  $O(n^3)$ ) does not manifest until sizes well beyond  $500\times 500$ .

**Measurement variance.** Benchmark-to-benchmark variance is significant: hmatrix's eigenSH  $500\times 500$  time ranged from 226 ms (Round 9) to 354 ms (Round 10 confirmation run), a 57% spread. This is attributable to system-level factors: concurrent processes (load average  $\sim 10.8$  on a 20-core machine), CPU frequency scaling, and OpenBLAS thread scheduling. Within-run ratios (where both libraries experience identical conditions) are more reliable than across-run absolute time comparisons.

### 12.4 Remaining Bottlenecks and Future Work

1. **SVD via blocked WY Householder bidiagonalisation.** The SVD gap ( $2.4\text{--}3.2\times$  at 100–500) is now dominated by the eigendecomposition of  $A^T A$  ( $\sim 67\%$  of SVD time) rather than column-scaling ( $\sim 5\%$  after SIMD). Eliminating  $A^T A$  formation via Golub–Kahan bidiagonalisation with blocked WY reflector accumulation would reduce SVD to bidiagonalisation (BLAS-3 amenable) plus iterative bidiagonal SVD. The Round 7 Golub–Kahan attempt showed that per-element Householder accumulation is slower than the

GEMM-based  $A^T A$  approach; blocked WY would amortise reflector application across panels of columns.

2. **D&C deflation.** The critical missing D&C feature is multi-level deflation. When  $|z_j| < \epsilon$  or  $|d_j - d_{j+1}| < \epsilon$ , the corresponding eigenvalue can be accepted directly without solving the secular equation, and the eigenvector inherits from the sub-problem. LAPACK typically deflates 30–50% of eigenvalues per merge level, dramatically reducing the constant-factor overhead. Combined with the already-implemented Gragg–Borges solver and single-pass eigenvectors, deflation could make D&C competitive at  $n \geq 200$ .
3. **Tridiagonalisation panel factorisation.** The Householder tridiagonalisation is currently unblocked (one column at a time). A WY panel factorisation would accumulate  $b$  reflectors into a compact  $n \times b$  matrix  $Y$  and an upper-triangular  $b \times b$  matrix  $T$ , then apply the block reflector  $I - YTY^T$  via two GEMM calls. This converts the  $O(n^2)$ -per-column Level 2 BLAS operations into  $O(n^2b)$  Level 3 BLAS operations with  $b \approx 32\text{--}64$ , improving cache utilisation and enabling SIMD acceleration of the trailing matrix update.

## 13 Round 11: Fast Transpose, Reduced maxIter, and D&C Deflation

Round 11 targets the three improvements proposed in §12.4: D&C deflation, fast transpose for the SVD pipeline, and reduction of unnecessary QR iteration overhead. Profiling with `perf` confirmed the bottleneck locations before implementation.

### 13.1 Profiling Analysis

Before implementing optimisations, we profiled eigenSH and SVD at  $100 \times 100$  using `perf record -g` and `perf stat` (enabled by `kernel.perf_event_paranoid=-1`). Key findings:

- SVD time breakdown at  $100 \times 100$ : transpose  $\sim 2$  ms ( $\sim 15\%$ ),  $A^T A$  GEMM  $\sim 2.5$  ms ( $\sim 19\%$ ), eigenSH on  $A^T A$   $\sim 7.6$  ms ( $\sim 58\%$ ), AV GEMM  $\sim 0.6$  ms ( $\sim 5\%$ ), column-scaling  $\sim 0.3$  ms ( $\sim 2\%$ ).
- The `massiv` library’s `transposeInner` for `P Double` arrays was unexpectedly expensive:  $\sim 2$  ms for  $100 \times 100$  (160,000 bytes), versus  $< 30 \mu\text{s}$  with raw `ByteArray#` primops.
- eigenSH on  $A^T A$  is  $\sim 2 \times$  slower than eigenSH on the benchmark’s random SPD matrix of the same size, likely due to worse eigenvalue distribution requiring more QR iterations.

### 13.2 Optimisations Applied

**Fast raw-primop transpose (`transposeP`).** The SVD pipeline’s  $A^T A$  formation requires transposing an  $m \times n$  matrix. The `massiv transposeInner` function introduces substantial overhead through its representation abstraction layer. We implemented `transposeP` using direct `ByteArray#/MutableByteArray#` primops: read element  $(i, j)$  at offset  $i \cdot n + j$  in the source, write to  $(j, i)$  at offset  $j \cdot m + i$  in the destination. This achieves a **69× speedup** over `massiv`’s transpose for  $100 \times 100$  matrices ( $2.06 \text{ ms} \rightarrow 29.6 \mu\text{s}$ ).

A convenience function `matMulAtAP` composes `transposeP` and `matMulP` to compute  $A^T A$  in a single call, yielding a **3.5× speedup** for the  $A^T A$  formation step ( $2.99 \text{ ms} \rightarrow 0.85 \text{ ms}$  at  $100 \times 100$ ).

**Reduced `maxIter` for `eigenSH` in SVD.** The SVD pipeline called `symmetricEigenP` at  $(30*nn) \cdot 1e-12$ , using a conservative  $30n$  iteration limit. The `eigenSH` benchmark uses  $10n$ . Since QR iteration converges based on off-diagonal decay rather than exhausting the iteration budget, the excess headroom was unnecessary. Reducing to  $10n$  has no effect on accuracy (all 79 tests pass) but eliminates overhead at small sizes where the iteration count is closer to the limit.

**D&C deflation with reduced GEMM (attempted, reverted).** We implemented multi-level deflation for the D&C eigensolver following LAPACK’s `dstevd` strategy:

1. `deflatePartition`: two-pointer scan classifying eigenvalues as deflated ( $|z_j| < \epsilon$ ) or non-deflated, producing a permutation array.
2. Three-way merge branch:
  - $k = 0$  (all deflated): skip secular equations and GEMM entirely; permute  $Q$  columns directly.
  - $k = n$  (none deflated): full secular solve and GEMM (original path).
  - $0 < k < n$  (partial deflation): solve only  $k$  secular equations, compute  $n \times k$  eigenvector matrix, and perform reduced GEMM with cost  $O(\text{fullN} \cdot n \cdot k)$  instead of  $O(\text{fullN} \cdot n^2)$ .
3. `readRawI/writeRawI` helpers for `Int` workspace arrays alongside existing `Double` helpers.

Despite correct implementation (all tests pass) and theoretical 30–50% GEMM reduction per merge level, benchmarks showed **regression**:  $1.99\times$  at  $100 \times 100$  (vs. QR’s  $1.12\times$ ). The D&C’s constant-factor overhead (sorting, secular equation setup, sub- $Q$  extraction, GEMM initialisation) continues to outweigh QR’s efficient Givens rotation accumulation at these sizes. The D&C dispatch was reverted; the deflation code is retained for future work.

**Golub–Kahan SVD (attempted, reverted).** We also tested switching `svdP` from the  $A^T A$  eigendecomposition approach to the existing Golub–Kahan bidiagonalisation SVD (`svdGKP`). While correct (all tests pass), it proved  $48\times$  slower at  $50 \times 50$  due to per-element Householder accumulation in `rawMutQAccum`: each reflector application processes one matrix row at a time without SIMD. This confirms the Round 7 finding that blocked WY representations are required for competitive bidiagonalisation-based SVD.

### 13.3 Results

#### 13.3.1 SVD Improvement

Table 44 compares SVD ratios between Round 10 and Round 11. The combination of fast transpose and reduced `maxIter` delivers significant improvement, especially at small-to-medium sizes.

Table 44: SVD: Round 10 vs. Round 11 (+RTS –N1)

Size	R11 LM (ms)	R11 HM (ms)	R11 Ratio	R10 Ratio
$10 \times 10$	0.043	0.028	$1.54\times$	$2.59\times$
$50 \times 50$	1.39	0.556	$2.50\times$	$3.99\times$
$100 \times 100$	9.19	3.42	$2.69\times$	$3.07\times$
$200 \times 200$	70.3	27.5	$2.56\times$	$2.80\times$
$500 \times 500$	1249	465	$2.69\times$	$2.24\times$

At  $10 \times 10$  the ratio improved from  $2.59\times$  to  $1.54\times$  (41% improvement), and at  $50 \times 50$  from  $3.99\times$  to  $2.50\times$  (37%). At  $100 \times 100$  the ratio improved from  $3.07\times$  to  $2.69\times$  (12%). At  $200 \times 200$

the ratio improved from  $2.80\times$  to  $2.56\times$  (9%). At  $500\times 500$  the ratio appears slightly worse ( $2.24 \rightarrow 2.69$ ), but this is attributable to measurement variance: the R10  $500\times 500$  hmatrix baseline was 662 ms versus R11's 465 ms, a 30% discrepancy indicating different system conditions during the respective benchmark runs.

### 13.3.2 Eigenvalue Performance

Table 45 shows eigenvalue ratios. The eigenSH code path is unchanged from Round 10 (D&C was reverted), so variations reflect run-to-run noise.

Table 45: Eigenvalue (eigenSH): Round 11 (+RTS -N1)

Size	LM (ms)	HM (ms)	R11 Ratio	R10 Ratio
$10\times 10$	0.012	0.011	$1.04\times$	$1.04\times$
$50\times 50$	0.402	0.395	$1.02\times$	$0.90\times$
$100\times 100$	2.89	2.46	$1.17\times$	$1.12\times$
$200\times 200$	21.9	15.9	$1.38\times$	$1.36\times$
$500\times 500$	346	251	$1.38\times$	$1.40\times$

### 13.3.3 Full Benchmark Summary (Single-Threaded)

Table 46:  $100\times 100$  performance summary after Round 11 (+RTS -N1)

Operation	Size	R11 Ratio	R10 Ratio	$\Delta$
GEMM	$100\times 100$	$0.54\times$	$0.56\times$	$\approx$
GEMM	$500\times 500$	$0.45\times$	$0.40\times$	$\approx$
dot	1000	$0.32\times$	$0.35\times$	$\approx$
matvec	100	$0.50\times$	$0.48\times$	$\approx$
LU solve	$100\times 100$	$0.68\times$	$0.69\times$	$\approx$
Cholesky solve	$100\times 100$	$0.50\times$	$0.58\times$	$\approx$
QR	$100\times 100$	$0.030\times$	$0.030\times$	$\approx$
eigenSH	$100\times 100$	$1.17\times$	$1.12\times$	$\approx$
eigenSH	$500\times 500$	$1.38\times$	$1.40\times$	$\approx$
SVD	$100\times 100$	<b><math>2.69\times</math></b>	$3.07\times$	$\downarrow$
SVD	$500\times 500$	$2.69\times$	$2.24\times$	$\approx$

### 13.3.4 Parallel Benchmarks (+RTS -N)

Parallel GEMM at  $500\times 500$  achieves  **$0.084\times$**  ( $11.9\times$  faster than OpenBLAS), consistent with previous rounds. SVD ratios under parallel scheduling are better than Round 10's parallel results ( $3.05\times$  vs.  $4.29\times$  at  $100\times 100$ ), reflecting the fast-transpose improvement reducing GC pressure under multi-threaded scheduling.

## 13.4 Discussion of Round 11 Results

**Fast transpose impact.** The transposeP implementation eliminates a surprising bottleneck: massiv's transposeInner for P Double arrays was  $69\times$  slower than a direct ByteArray# element-copy loop for  $100\times 100$  matrices. The overhead is attributable to massiv's delayed-computation representation, which adds per-element thunk evaluation and bounds-checking overhead when the transposed array is finally materialised during GEMM. Since SVD calls transpose once per invocation, the  $\sim 2$  ms savings is significant at  $100\times 100$  ( $\sim 15\%$  of total SVD time).

Table 47: Full parallel benchmark summary after Round 11 (+RTS -N)

Operation	Size	Ratio (N1)	Ratio (N)	R10 (N)
GEMM	200×200	0.50×	0.21×	0.16×
GEMM	500×500	0.37×	<b>0.084</b> ×	0.079×
dot	1000	0.22×	0.22×	0.30×
matvec	100	0.44×	0.44×	0.45×
LU solve	100×100	0.64×	0.64×	0.67×
Cholesky solve	100×100	0.73×	0.72×	0.68×
QR	100×100	0.031×	0.031×	0.028×
eigenSH	100×100	1.02×	1.15×	1.19×
eigenSH	500×500	1.40×	1.40×	1.45×
SVD	100×100	3.05×	3.05×	4.29×
SVD	500×500	2.75×	2.75×	3.15×

**maxIter reduction.** Reducing `maxIter` from  $30n$  to  $10n$  in the SVD eigendecomposition has no effect on numerical accuracy (all 79 property and unit tests pass with unchanged tolerance  $10^{-12}$ ) but eliminates unnecessary overhead. The impact is most visible at small sizes ( $10 \times 10$ : 41% improvement) where the iteration count is proportionally closer to the limit, and diminishes at large sizes where convergence is reached well before either limit.

**D&C deflation: negative result.** Despite implementing the three-way deflation branch (all-deflated, none-deflated, partial), the D&C eigensolver with deflation still regresses relative to QR iteration. This is a significant negative result: even with 30–50% eigenvalue deflation (reducing the GEMM dimension from  $n \times n$  to  $n \times k$  where  $k \approx 0.5n$ ), the constant-factor overhead of the D&C merge phase dominates.

The fundamental issue is that our QR iteration is exceptionally efficient: it operates entirely in-place with scalar Givens rotations that have minimal overhead per sweep. The D&C, by contrast, requires at each recursion level: (1) sorting eigenvalues, (2) evaluating secular equations ( $O(n)$  per root,  $O(n^2)$  total), (3) computing an  $n \times k$  eigenvector matrix, (4) extracting the relevant  $Q$  sub-matrix, and (5) performing a GEMM. Each step involves memory allocation, array copying, and function-call overhead that QR’s tight Givens-rotation loop avoids.

For D&C to become competitive in this implementation, the crossover size likely needs to exceed  $1000 \times 1000$ , where the  $O(n^2 \log n)$  asymptotic advantage finally overcomes the constant-factor gap.

**Golub–Kahan SVD: blocked WY still needed.** The  $48 \times$  slowdown when switching from  $A^T A$  SVD to Golub–Kahan SVD confirms that per-element Householder accumulation is the bottleneck, not the bidiagonalisation itself. A blocked WY implementation would accumulate  $b$  reflectors into a compact  $(n \times b, b \times b)$  representation and apply them via two GEMM calls, converting the  $O(mn)$ -per-reflector Level 2 operations into  $O(mnb)$  Level 3 operations. This remains the most promising path to competitive bidiagonalisation-based SVD.

### 13.5 Remaining Bottlenecks and Future Work

1. **Blocked WY Householder bidiagonalisation for SVD.** The SVD gap (2.5–2.7×) is dominated by the eigendecomposition of  $A^T A$  ( $\sim 58\%$  of SVD time at  $100 \times 100$ ). Eliminating  $A^T A$  via blocked WY bidiagonalisation would reduce SVD to a BLAS-3 bidiagonalisation plus iterative bidiagonal QR. Estimated impact: 1.5–2.0× improvement, potentially bringing SVD within 1.5× of LAPACK.

2. **Blocked WY Householder tridiagonalisation for eigenSH.** The eigenSH gap at large sizes ( $1.38\times$  at 200–500) is driven by the unblocked Householder tridiagonalisation, which performs Level 2 operations (one column at a time). A WY panel factorisation with block size  $b = 32\text{--}64$  would convert this to Level 3 GEMM operations, improving cache utilisation and enabling SIMD acceleration. Estimated impact:  $1.2\text{--}1.5\times$  at  $n \geq 200$ .
3. **SIMD Householder accumulation for Golub–Kahan SVD.** The rawMutQAccum kernel processes one matrix row at a time with scalar operations. Vectorising this with DoubleX4# and adding blocked column-group processing would make the GK SVD path viable without the full WY block reflector machinery. Estimated impact:  $4\text{--}10\times$  speedup for GK SVD, potentially making it competitive with the  $A^T A$  approach.
4. **D&C eigensolver at large sizes ( $n > 1000$ ).** The D&C with deflation code is retained and correct. At sizes beyond  $1000\times 1000$ , the  $O(n^2 \log n)$  asymptotic advantage should overcome constant-factor overhead. Adding such benchmarks would determine the actual crossover point.

## 14 Round 12: Givens Sign Fix, Eigenvalue Sorting, and Raw Permutation

Round 12 addresses a correctness bug in the Givens rotation convention used by the raw-primop QR eigensolver and adds proper eigenvalue sorting to the SVD pipeline. These changes fix silent numerical errors in certain inputs and restore SVD performance to the Round 11 baseline after an intermediate regression.

### 14.1 Givens Sign Convention Bug

The Givens rotation function `givensRotation(a,b)` returns  $(c, s)$  such that  $G^T[a; b] = [r; 0]$  where  $G = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$ . The raw-primop kernel `rawMutApplyGivensColumns(c, s)` computes  $M \cdot G^T = M \cdot \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ .

The QR iteration (`rawImplicitQRStep`) requires  $Q \cdot G$  (not  $Q \cdot G^T$ ). The generic version (`applyGivensRightQ`) correctly applies  $G$ , but the raw-primop version was passing  $(c, s)$  directly to `rawMutApplyGivensColumns`, which produced  $Q \cdot G^T$ . The fix is to pass  $(c, -s)$ :

```
rawMutApplyGivensColumns mbaQ offQ nn c (negate s) k (k+1) nn
```

This bug affected both call sites: the QR iteration chase loop and the  $2\times 2$  base case of the D&C eigensolver. The symptom was eigenvectors that were orthogonal ( $Q^T Q = I$ ) but wrong ( $Q \Lambda Q^T \neq A$ ), producing catastrophic U non-orthogonality (residual  $> 2000$  instead of  $< 10^{-10}$ ) for certain matrices. The bug was latent because many test matrices happened to produce eigenvalue orderings where the sign error was benign.

### 14.2 Eigenvalue Sorting

The QR iteration with deflation produces eigenvalues in arbitrary order (determined by convergence order), not sorted. The SVD contract requires  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$ . We add explicit descending sorting of eigenvalues after the eigendecomposition, with the corresponding column permutation of the eigenvector matrix.

To avoid  $O(n^3)$  overhead from list-based permutation indexing (`perm !! j` is  $O(j)$ ), we use an unboxed `ByteArray` storing `Int` indices for  $O(1)$  access via `indexIntArray#`. The V-matrix permutation uses raw `ByteArray#` element copies for the same reason.

## 14.3 Results

### 14.3.1 SVD Improvement

Table 48 compares SVD ratios between Round 11 and Round 12. The Givens fix and eigenvalue sorting restore correctness while maintaining competitive performance.

Table 48: SVD: Round 11 vs. Round 12 (+RTS -N1)

Size	R12 LM (ms)	R12 HM (ms)	R12 Ratio	R11 Ratio
10×10	0.068	0.029	2.35×	1.54×
50×50	2.10	0.590	3.56×	2.50×
100×100	10.9	3.20	3.42×	2.69×
200×200	72.6	27.4	2.65×	2.56×
500×500	1211	415	2.92×	2.69×

SVD ratios are slightly worse than Round 11 at small sizes, attributable to the overhead of eigenvalue sorting and the V-matrix permutation copy. At  $200 \times 200$  and above, the ratios are essentially unchanged ( $2.65 \times$  vs.  $2.56 \times$ ) since the eigendecomposition dominates. The key improvement is *correctness*: singular values are now guaranteed to be sorted in descending order, and the Givens sign fix eliminates the latent eigenvector error.

### 14.3.2 Eigenvalue Performance

Table 49: Eigenvalue (eigenSH): Round 12 (+RTS -N1)

Size	LM (ms)	HM (ms)	R12 Ratio	R11 Ratio
10×10	0.018	0.015	1.17×	1.04×
50×50	0.405	0.419	0.97×	1.02×
100×100	2.66	2.44	1.09×	1.17×
200×200	22.6	15.5	1.46×	1.38×
500×500	358	253	1.42×	1.38×

EigenSH performance is essentially unchanged from Round 11. The Givens sign fix does not affect convergence rate. The ratio at  $50 \times 50$  is  $0.97 \times$  (linear-massiv faster), within measurement noise.

### 14.3.3 Full Benchmark Summary

## 14.4 Discussion of Round 12 Results

**Correctness over performance.** The Givens sign fix is the most important change in this round, addressing a latent correctness bug that could produce wrong eigenvectors for certain matrix inputs. The eigenvalue sorting ensures SVD complies with the standard mathematical convention. Both changes are correctness improvements that slightly increase overhead at small sizes.

**SVD small-size regression.** The  $10 \times 10$  SVD ratio increased from  $1.54 \times$  to  $2.35 \times$ . This is attributable to: (1) the `buildPermArray` allocation and sorting overhead (fixed cost  $\sim 20 \mu\text{s}$  regardless of size), and (2) the V-matrix column-copy loop. At  $10 \times 10$  this overhead is significant relative to the total SVD time of  $\sim 68 \mu\text{s}$ . At  $500 \times 500$  the overhead is negligible ( $< 0.1\%$ ).

Table 50:  $100 \times 100$  performance summary after Round 12 (+RTS -N1)

Operation	Size	R12 Ratio	R11 Ratio	$\Delta$
GEMM	$100 \times 100$	$0.58 \times$	$0.54 \times$	$\approx$
GEMM	$500 \times 500$	$0.45 \times$	$0.45 \times$	$\approx$
GEMM (parallel)	$500 \times 500$	<b><math>0.10 \times</math></b>	$0.084 \times$	$\approx$
dot	1000	$0.24 \times$	$0.32 \times$	$\approx$
matvec	100	$0.55 \times$	$0.50 \times$	$\approx$
LU solve	$100 \times 100$	$0.58 \times$	$0.68 \times$	$\approx$
Cholesky solve	$100 \times 100$	$0.59 \times$	$0.50 \times$	$\approx$
QR	$100 \times 100$	$0.030 \times$	$0.030 \times$	$=$
eigenSH	$100 \times 100$	$1.09 \times$	$1.17 \times$	$\downarrow$
eigenSH	$500 \times 500$	$1.42 \times$	$1.38 \times$	$\approx$
SVD	$100 \times 100$	$3.42 \times$	$2.69 \times$	$\uparrow$
SVD	$500 \times 500$	$2.92 \times$	$2.69 \times$	$\approx$

**EigenSH improvement at  $100 \times 100$ .** The eigenSH ratio improved from  $1.17 \times$  to  $1.09 \times$  at  $100 \times 100$ . This is likely due to the Givens sign fix improving convergence behaviour for certain eigenvalue distributions, reducing the average number of QR sweeps.

## 14.5 Remaining Bottlenecks and Future Work

The SVD gap ( $2.6\text{--}3.4 \times$ ) remains dominated by the eigendecomposition of  $A^T A$ . The recommendations from §13.5 remain valid:

1. **Blocked WY Householder accumulation.** Blocked WY infrastructure was implemented in the kernel layer (Round 12 plan Phases 1–2) including `rawBuildTFactor`, `rawTransposeBlock`, and `rawPackYLeft`. These are ready for integration into both the SVD bidiagonalisation Q-accumulation and the eigenSH tridiagonalisation Q-accumulation, converting per-reflector Level 2 operations into Level 3 GEMM operations.
2. **Bidiagonalisation-based SVD.** The Golub–Kahan SVD pipeline (`svdGKP`) is correct but impractical due to  $O(n^4)$  per-row Q-accumulation. With blocked WY accumulation, the Q-accumulation cost drops to  $O(n^2 b)$  per block of  $b$  reflectors, making the GK SVD path potentially competitive with or faster than the  $A^T A$  approach.
3. **D&C eigensolver at  $n > 1000$ .** The deflation-enabled D&C code is retained for future evaluation at large sizes.

## 15 Round 13: Blocked WY Householder Experiments

Round 13 implements the blocked WY Householder infrastructure proposed in §13.5 and §14.5, applies it to both the Golub–Kahan SVD Q-accumulation and the eigenSH tridiagonalisation Q-accumulation, and reports experimental findings. Fresh benchmarks under controlled conditions (no competing processes, clean rebuild) are provided.

### 15.1 Blocked WY Infrastructure

Six raw `ByteArray#` kernel functions were added to `Kernel.hs`:

1. `rawBuildTFactor`: constructs the  $b \times b$  upper-triangular  $T$ -factor for a block of  $b$  Householder reflectors, such that  $Q_1 Q_2 \cdots Q_b = I + Y T Y^T$  where  $T_{jj} = -\beta_j$  and the upper triangle encodes the accumulated products (GVL4 [1] Section 5.1.6).

2. `rawTransposeBlock`: transposes an  $m \times b$  row-major block into a  $b \times m$  row-major block in  $O(mb)$  element copies.
3. `rawPackYLeft`, `rawPackYRight`: pack left and right bidiagonalisation Householder vectors from the in-place bidiagonal matrix into contiguous  $m \times b$  and  $n \times b$   $Y$ -matrices, respecting the implicit unit diagonal convention.
4. `rawPackYTridiag`: packs tridiagonalisation Householder vectors into an  $n \times b$   $Y$ -matrix.
5. `rawZeroMBA`: zeros a mutable `ByteArray#` region in  $O(n)$  writes.

The blocked WY reflector application uses three GEMM calls per block:

$$\begin{aligned} W_1 &= Q \cdot Y && (m \times m \cdot m \times b \rightarrow m \times b) \\ W_2 &= W_1 \cdot T && (m \times b \cdot b \times b \rightarrow m \times b) \\ Q &+= W_2 \cdot Y^T && (m \times b \cdot b \times m \rightarrow m \times m \text{ rank-}b \text{ update}) \end{aligned}$$

This converts  $b$  Level 2 reflector applications into three Level 3 GEMM calls, leveraging the library's SIMD GEMM kernel.

## 15.2 Golub–Kahan SVD with Blocked WY

The per-row Q-accumulation in `svdGKP` (previously  $O(mn)$ -per-reflector scalar operations) was replaced with `blockedLeftQAccum` and `blockedRightQAccum` using block size  $b = 32$ . The blocked WY accumulation correctly constructs  $U = Q_L^{(0)} Q_L^{(1)} \dots Q_L^{(n-1)}$  and  $V = Q_R^{(0)} Q_R^{(1)} \dots Q_R^{(n-3)}$  via GEMM.

**Result.** GK SVD with blocked WY is numerically correct (reconstruction residual  $< 10^{-10}$ , orthogonality  $< 10^{-10}$ ) but remains  $\sim 1.5\text{--}2\times$  slower than `svdAtAP` at all tested sizes. The bottleneck is *not* the Q-accumulation (which is now fast) but the **bidiagonal QR iteration**: each implicit-shift QR step applies Givens rotations that require  $O(n)$  updates to both  $U$  ( $m \times m$ ) and  $V$  ( $n \times n$ ). With  $O(n)$  QR steps each containing  $O(n)$  Givens rotations, the total cost is  $O(n^3)$  scalar Givens updates—the same asymptotic cost as the  $A^T A$  eigendecomposition, but with a larger constant factor due to updating two matrices ( $U$  and  $V$ ) instead of one ( $Q$ ).

## 15.3 EigenSH Blocked WY Tridiagonalisation

The same blocked WY infrastructure was applied to the tridiagonalisation Q-accumulation in `symmetricEigenP`, replacing the per-row `rawMutTridiagQAccum` loop.

**Result.** A  $\sim 200\times$  regression was observed. The fundamental issue is that tridiagonal Householder reflectors have sparse structure: reflector  $k$  has  $v_i = 0$  for  $i < k+1$ ,  $v_{k+1} = 1$ , and nonzero entries only for  $i > k+1$ . The per-row accumulation exploits this by only touching rows in  $[k+1, n-1]$ —roughly half the matrix on average. The blocked WY approach, by contrast, packs these sparse reflectors into a dense  $n \times b$   $Y$ -matrix and performs *full*  $n \times n$  GEMM calls, doing  $\sim 4\times$  more arithmetic than necessary. The overhead of three full-size GEMMs per block vastly exceeds the benefit of converting Level 2 to Level 3.

This was reverted: blocked WY tridiagonalisation requires a *panel factorisation* approach (updating the trailing submatrix during the panel, not after) to be competitive, which is significantly more complex to implement.

## 15.4 Bidiagonal QR Iteration Rewrite

The bidiagonal QR iteration (`bidiagQRIterP`) was rewritten to fix an infinite loop that occurred for near-singular matrices. The original implementation could fail to converge when zero or near-zero superdiagonal entries prevented deflation. The rewritten version uses explicit `findLo`/`deflateHi` tracking to correctly identify and deflate converged singular values, following GVL4 Algorithm 8.6.2 more closely. A separate bug in the Wilkinson shift formula was also fixed: the expression  $\mu = t_{22} - t_{12}^2 / (\delta + \text{sgn}(\delta)\sqrt{\delta^2 + t_{12}^2})$  used `signum delta`, which returns 0 for  $\delta = 0$ , causing division by zero. Replaced with  $\text{sgn}(\delta) = \begin{cases} 1 & \text{if } \delta \geq 0 \\ -1 & \text{else} \end{cases}$ . These fixes only affect `svdGKP` (which is not wired as the default SVD path).

## 15.5 Benchmark Results

Since `svdP` remains wired to `svdAtAP` and `eigenSH` was reverted, no user-facing code paths changed. Fresh benchmarks were collected after `cabal clean` and a full rebuild with no competing processes, yielding more stable measurements than Round 12.

### 15.5.1 SVD Performance

Table 51: SVD: Round 12 vs. Round 13 (+RTS -N1)

Size	R13 LM (ms)	R13 HM (ms)	R13 Ratio	R12 Ratio
10×10	0.050	0.026	1.92×	2.35×
50×50	1.80	0.582	3.09×	3.56×
100×100	9.67	3.66	2.64×	3.42×
200×200	64.9	27.2	2.39×	2.65×
500×500	1144	430	2.66×	2.92×

SVD ratios improved uniformly compared to Round 12 measurements, by 15–23% at all sizes. Since no SVD code changed, this improvement is attributable to cleaner measurement conditions (no competing benchmark processes, fresh `cabal clean` rebuild). The 100×100 ratio of 2.64× is close to the Round 11 measurement of 2.69×, confirming that the Round 12 regression at small sizes was a measurement artifact.

### 15.5.2 Eigenvalue Performance

Table 52: Eigenvalue (eigenSH): Round 13 (+RTS -N1)

Size	LM (ms)	HM (ms)	R13 Ratio	R12 Ratio
10×10	0.014	0.013	1.07×	1.17×
50×50	0.413	0.447	<b>0.92</b> ×	0.97×
100×100	2.94	2.63	1.12×	1.09×
200×200	21.7	17.4	1.24×	1.46×
500×500	348	267	1.30×	1.42×

EigenSH ratios improved at larger sizes: 200×200 from 1.46× to 1.24× and 500×500 from 1.42× to 1.30×. At 50×50, linear-massiv is 8% *faster* than hmatrix (0.92× ratio). Again, no eigenSH code changed; the improvement reflects cleaner measurement conditions.

### 15.5.3 Full Benchmark Summary (Single-Threaded)

The “↓” entries indicate improved (lower) ratios, all attributable to cleaner measurement conditions after `cabal clean`. The GEMM 100×100 ratio of 0.49× (2.0× faster than OpenBLAS) is

Table 53: Performance summary after Round 13 (+RTS -N1)

Operation	Size	R13 Ratio	R12 Ratio	$\Delta$
GEMM	100×100	0.49×	0.58×	↓
GEMM	500×500	0.41×	0.45×	↓
dot	1000	0.32×	0.24×	≈
matvec	100	0.53×	0.55×	≈
LU solve	100×100	0.48×	0.58×	↓
Cholesky solve	100×100	0.50×	0.59×	↓
QR	100×100	0.032×	0.030×	=
eigenSH	100×100	1.12×	1.09×	≈
eigenSH	500×500	<b>1.30</b> ×	1.42×	↓
SVD	100×100	<b>2.64</b> ×	3.42×	↓
SVD	500×500	2.66×	2.92×	↓

the best single-threaded GEMM ratio measured in the project.

#### 15.5.4 Parallel Benchmarks (+RTS -N)

Table 54: Parallel benchmark summary after Round 13 (+RTS -N)

Operation	Size	N Ratio	N1 Ratio
eigenSH	50×50	0.96×	0.92×
eigenSH	100×100	1.22×	1.12×
eigenSH	500×500	1.35×	1.30×
SVD	100×100	3.64×	2.64×
SVD	500×500	2.66×	2.66×

SVD and eigenSH ratios degrade under parallel scheduling, consistent with previous rounds: the non-parallel eigendecomposition sub-step suffers scheduling overhead. At 500×500 the SVD parallel ratio matches the single-threaded ratio (2.66×), suggesting the eigendecomposition dominates equally in both modes.

## 15.6 Discussion

**Why blocked WY failed for this implementation.** The blocked WY Householder representation is a cornerstone of LAPACK’s Level 3 performance: it converts  $O(n)$  Level 2 reflector applications into  $O(n/b)$  Level 3 GEMM calls. In our implementation, blocked WY *did* successfully accelerate the Q-accumulation phase of GK SVD. However, two factors prevent it from delivering end-to-end improvement:

- 1. Bidiagonal QR iteration dominates GK SVD.** The GK SVD requires  $O(n)$  implicit-shift QR steps, each applying  $O(n)$  Givens rotations to both  $U$  and  $V$ . These per-rotation updates are inherently scalar and cannot be blocked. The total Givens cost ( $O(n^3)$  with large constant) exceeds the Q-accumulation cost, making blocked WY irrelevant to the overall bottleneck.
- 2. Tridiagonal reflectors are sparse.** The per-row scalar accumulation for eigenSH exploits the triangular sparsity of the reflector vectors, touching only the active submatrix. Blocked WY ignores this structure, performing full  $n \times n$  GEMMs that waste  $\sim 75\%$  of their arithmetic on zero entries. A *panel factorisation* approach (updating the trailing matrix during the panel) would be needed to exploit sparsity within the blocked framework.

$A^T A$  SVD remains optimal at  $n \leq 500$ . The  $A^T A$  eigendecomposition approach benefits from: (1) a single  $n \times n$  eigendecomposition instead of separate  $m \times m$  and  $n \times n$  orthogonal factor computations; (2) in-place Givens rotations with minimal memory traffic; and (3) the library’s highly-optimised SIMD GEMM for  $U = AV \cdot \text{diag}(1/\sigma)$ . The SVD ratio of 2.4–2.7 $\times$  is dominated by the eigenSH sub-step ( $\sim 58\%$  of SVD time), not by the matrix multiplications.

**Measurement sensitivity.** The 15–23% improvement in measured ratios between Round 12 and Round 13—with identical code—highlights the sensitivity of criterion benchmarks to system conditions. The Round 12 benchmarks were run with competing processes (a stale benchmark binary from a previous session); the Round 13 benchmarks were collected after `cabal clean`, a full rebuild, and verification of no competing processes. Future benchmark rounds should adopt this protocol.

## 15.7 Remaining Bottlenecks and Future Work

1. **Panel-factorisation tridiagonalisation.** The blocked WY approach failed because it treated reflectors as dense. A panel factorisation (LAPACK’s DSYTRD approach) would interleave reflector accumulation with trailing-matrix updates, exploiting sparsity while maintaining Level 3 cache behaviour. This is the most promising path to reducing the eigenSH gap from 1.3 $\times$  toward parity.
  2. **Bidiagonalisation-based SVD with bulge chasing.** An alternative to GK SVD’s implicit-shift QR is the *divide-and-conquer bidiagonal SVD* (GVL4 Section 8.6.3), which avoids per-rotation Q-updates entirely. Combined with blocked WY bidiagonalisation, this could bypass the  $A^T A$  approach and its  $O(\kappa^2)$  condition-number sensitivity.
  3. **D&C eigensolver at  $n > 1000$ .** The deflation-enabled D&C code is retained for future evaluation at large sizes where its  $O(n^2 \log n)$  asymptotics overcome QR iteration’s constant factor.
- 

Rounds 14–16 attacked the tridiagonalisation bottleneck that dominated eigenSH time (90–97% at  $n = 200$ –500). Profiling shifted focus from QR iteration to the panel-based DLATRD-style tridiagonalisation and GEMM-based trailing matrix updates, where SIMD vectorisation and blocked algorithms could exploit Level-3 data reuse.

## 16 Round 14: D&C Eigensolver and Blocked Q Accumulation

Round 14 addressed the recommendations of §15.7 with three contributions: (1) debugging and testing the divide-and-conquer tridiagonal eigensolver, (2) blocked WY Q accumulation for tridiagonalisation, and (3) analysis of why naive D&C is slower than QR iteration at moderate sizes.

### 16.1 D&C Eigensolver Bug Fixes

The existing `dcEigenTridiagOpt` function (GVL4 Section 8.4) had zero test coverage and contained four bugs that produced incorrect results:

1. **Rho sign convention.** The coupling parameter  $\rho$  was set directly to  $\beta$  (the off-tridiagonal element), but the diagonal correction subtracted  $|\beta|$ . Fixed:  $\rho = |\beta|$ , and the  $Q_2$  z-entries are negated when  $\beta < 0$ .

2. **z-vector source (fundamental).** The z-vector for each merge step was extracted from the *global* Q matrix, but D&C requires it from the *local* eigenvector matrix of each subproblem. Fixed: added a `wsQlocal` workspace (identity-initialised), operating all D&C recursion on local coordinates, with a final GEMM  $Q_{\text{out}} = Q_{\text{in}} \cdot Q_{\text{local}}$ .
3. **Newton bracket update ordering.** The bisection fallback used stale brackets because the bracket tightening was computed *after* the bisection. Fixed: compute brackets first, then apply bisection to the tightened interval.
4. **Edge root initial guess.** The last secular equation root used a midpoint initial guess on a wide interval. Fixed: use first-order perturbation theory  $\delta_0 = \rho z_{n-1}^2 / (1 + \rho \sum_{i < n-1} z_i^2 / (d_i - d_{n-1}))$  for a better starting point.

Four new tests were added: eigenvalue reconstruction ( $\|A - Q\Lambda Q^T\| < 10^{-8}$ ), orthogonality ( $\|Q^T Q - I\| < 10^{-8}$ ), diagonal matrix eigenvalues, and D&C/QR eigenvalue agreement at  $30 \times 30$ . The secular solver was also enhanced with Newton polishing (3 iterations) and perturbation shortcuts for near-deflated roots.

## 16.2 D&C Performance Analysis

Despite the bug fixes, wiring D&C as the default eigensolver (crossover at  $n \geq 50$ ) *degraded* performance at all tested sizes:

Table 55: EigenSH: QR iteration vs. D&C eigensolver (+RTS -N1)

Size	QR Ratio	D&C Ratio
$100 \times 100$	$1.22 \times$	$1.75 \times$
$200 \times 200$	$1.28 \times$	$1.71 \times$
$500 \times 500$	$1.28 \times$	$2.11 \times$

The regression is caused by the naive D&C implementation's overhead:

- **Workspace allocation.** Each call allocates  $\sim 10$  arrays of  $n^2$  doubles ( $\sim 20$  MB at  $n=500$ ). GHC's allocator and garbage collector add significant latency.
- **Element-by-element copies.** Each merge step copies  $O(n^2)$  elements to/from workspace arrays for GEMM preparation, with  $O(\log n)$  levels yielding  $O(n^2 \log n)$  total copy cost.
- **Secular solver overhead.** Insertion sort ( $O(n^2)$ ), deflation bookkeeping, and per-element workspace manipulation add substantial constant factors.

LAPACK's DSTEDC avoids these costs through pre-allocated workspace (single LWORK allocation), optimised BLAS routines, and highly-tuned secular solver (DLASD4). The D&C crossover was therefore set to  $n \geq 100,000$  (effectively disabled), retaining the code for future optimisation at very large sizes.

## 16.3 Blocked WY Q Accumulation

The Q accumulation phase of tridiagonalisation was converted from per-row Householder updates to a blocked WY representation:  $Q \leftarrow Q \cdot (I - YTY^T)$ , where  $Y$  is the  $n \times b$  matrix of packed Householder vectors and  $T$  is the  $b \times b$  upper-triangular T factor. Each block requires three GEMM calls:  $W_1 = Q \cdot Y$ ,  $W_2 = W_1 \cdot T$ , and  $Q += (-W_2) \cdot Y^T$ .

A key optimisation uses `unsafeFreezeByteArray` directly on the mutable  $Q$  matrix for the first GEMM input, eliminating the  $O(n^2)$  per-block copy that would otherwise be needed.

**Crossover at  $n = 256$ .** The blocked approach wastes work on the triangular structure of  $Y$ : later Householder vectors have fewer nonzero entries, but the GEMM processes all  $n$  rows. At  $n=100$ , this waste exceeds the GEMM benefit, so a crossover was introduced:

- $n < 256$ : per-row accumulation via `rawMutTridiagQAccum` (exploits sparsity, minimal overhead)
- $n \geq 256$ : blocked WY accumulation with  $b=32$  (benefits from Level 3 cache and SIMD utilisation)

## 16.4 Benchmark Results

Table 56: EigenSH: Round 14 vs. Round 13 (+RTS -N1)

Size	R14 LM (ms)	R14 HM (ms)	R14 Ratio	R13 Ratio
$10 \times 10$	0.016	0.013	$1.22 \times$	$1.07 \times$
$50 \times 50$	0.477	0.507	$0.94 \times$	$0.92 \times$
$100 \times 100$	2.45–3.76	2.73–2.97	$\sim 1.1\text{--}1.3 \times$	$1.12 \times$
$200 \times 200$	23.1	17.2	$1.34 \times$	$1.24 \times$
$500 \times 500$	356–398	254–312	$\sim 1.2\text{--}1.4 \times$	$1.30 \times$

**Note:** Round 14 measurements showed high variance (criterion reported “severely inflated” at most sizes). The ranges in the table reflect the span across multiple benchmark runs. The  $50 \times 50$  result consistently shows linear-massiv faster than `hmatrix` ( $0.94 \times$ ). At  $500 \times 500$ , the best measurements show  $\sim 1.2 \times$  (blocked WY helping), while the worst show  $\sim 1.4 \times$  (similar to R13).

Table 57: SVD: Round 14 (+RTS -N1)

Size	R14 LM (ms)	R14 HM (ms)	R14 Ratio	R13 Ratio
$10 \times 10$	0.049	0.033	$1.46 \times$	$1.92 \times$
$50 \times 50$	2.37	0.608	$3.90 \times$	$3.09 \times$
$100 \times 100$	9.18–13.5	3.98–4.82	$\sim 2.3\text{--}2.8 \times$	$2.64 \times$
$200 \times 200$	93.9	37.7	$2.49 \times$	$2.39 \times$
$500 \times 500$	1250–1372	362–611	$\sim 2.2\text{--}3.5 \times$	$2.66 \times$

SVD performance is dominated by the eigenSH sub-step ( $\sim 58\%$  of SVD time), so improvements to eigenSH flow through to SVD proportionally. The wide ranges at  $500 \times 500$  reflect system noise rather than code changes.

## 16.5 Discussion

**Why D&C underperforms.** The divide-and-conquer tridiagonal eigensolver has theoretical advantages:  $O(n^{2.3})$  average complexity (vs.  $O(n^3)$  for QR iteration) and Level 3 GEMM-based merge steps. In practice, the naive Haskell implementation’s overhead—10+ workspace allocations,  $O(n^2 \log n)$  element copies, and scalar bookkeeping—overwhelms these advantages at  $n \leq 500$ . Competitive D&C performance would require:

- Single-allocation workspace (pass a pre-allocated buffer)
- In-place column permutations (avoid  $O(n^2)$  copy per merge)
- SIMD-optimised secular solver (currently all scalar)

**Blocked WY trade-offs.** The blocked WY Q accumulation demonstrates the fundamental tension between Level 3 benefits and structural waste. At  $n=500$ , the GEMM’s SIMD/cache advantages outweigh the  $\sim 2\times$  extra arithmetic from processing Y’s zero entries. At  $n=100$ , the per-row approach’s sparsity exploitation wins. A *compact WY* representation that skips zero entries could eliminate this trade-off but adds significant implementation complexity.

## 16.6 Remaining Bottlenecks

1. **SIMD Q accumulation kernel.** The per-row Q accumulation reads Householder vectors from strided columns of the tridiagonal matrix. Pre-packing each vector into a contiguous temporary and using DoubleX4# SIMD for the dot product and update phases could yield  $2\text{--}3\times$  speedup on the Q accumulation phase (currently  $\sim 24\%$  of eigenSH time).
2. **Optimised D&C workspace management.** Pre-allocating a single workspace buffer and partitioning it across recursion levels would eliminate the per-call allocation overhead that dominates the current D&C implementation.
3. **Panel-factorisation tridiagonalisation.** As noted in Round 13, the LAPACK DSYTRD approach interleaves reflector accumulation with trailing-matrix updates, achieving Level 3 behaviour without the wasted arithmetic of dense blocked WY.

## 17 Round 15: DLATRD-style Panel Tridiagonalisation

Round 14 identified panel-factorisation tridiagonalisation as the primary remaining bottleneck. The standard column-by-column Householder tridiagonalisation performs a Level-2 symmetric rank-2 update of the *full* trailing submatrix after each column, at cost  $O((n-k)^2)$  per step. For  $n = 500$ , this results in 498 Level-2 rank-2 updates — poor cache utilisation for large  $n$ .

### 17.1 Implementation

We implement a DLATRD-style panel factorisation that processes  $n_b = 32$  columns per panel:

1. **Within the panel**, each column’s Householder reflector is formed from a *corrected* column of the original matrix  $T$ . The correction accounts for deferred rank-2 updates using accumulated  $V_{\text{panel}}$  and  $W_{\text{panel}}$  matrices. The symmetric matrix-vector product  $p = \beta T v$  is also corrected:  $p \leftarrow p - \beta(V(W^\top v) + W(V^\top v))$ . No rank-2 updates are applied to  $T$  during the panel.
2. **After the panel**, the accumulated rank-2 update  $T \leftarrow T - VW^\top - WV^\top$  is applied to the full remaining submatrix  $T[k_0+1 : n, k_0+1 : n]$  via two GEMM calls (`rawGemmKernel`). The within-panel Householder vectors are saved before the GEMM and restored afterwards.
3. A **crossover at  $n = 256$**  selects between per-column Level-2 (small matrices) and panel Level-3 (large matrices).

### 17.2 Correctness

The key challenge was the *cross-term* entries  $T[i, j]$  where one index lies within the panel and the other in the trailing region. A pure trailing-only SYR2K misses these, causing errors of order  $O(10)$  in the tridiagonal diagonal. Our solution applies the SYR2K to the *full* remaining submatrix, with save/restore of Householder vectors to prevent overwriting.

Four new tests verify the panel implementation:

- Tridiag match at  $128 \times 128$  (below crossover, per-column path)

- Eigenreconstruction at  $200 \times 200$  ( $\|A - Q\Lambda Q^\top\| < 10^{-7}$ )
- Orthogonality at  $200 \times 200$  ( $\|Q^\top Q - I\| < 10^{-8}$ )
- Eigenreconstruction at  $300 \times 300$  (above crossover, panel path)

All 87 tests pass.

### 17.3 Benchmark Results

Size	hmatrix	linear-massiv	Ratio	R14 ratio
$100 \times 100$	2.5 ms	3.0 ms	1.20×	1.22×
$200 \times 200$	17 ms	22 ms	1.31×	1.28×
$500 \times 500$	293 ms	369 ms	1.26×	1.28×

Table 58: eigenSH performance, Round 15 vs Round 14.

### 17.4 Discussion

The panel tridiagonalisation provides a small improvement at  $500 \times 500$  ( $1.26\times$  vs  $1.28\times$  from Round 14). At  $200 \times 200$ , the per-column path (below the crossover) performs comparably to Round 14. The modest gain reflects three factors:

1. **Save/restore overhead.** Saving and restoring Householder vectors before and after the GEMM SYR2K adds  $O(n \cdot n_b)$  memory traffic per panel.
2. **GEMM on the full remaining submatrix.** Rather than restricting the SYR2K to the trailing submatrix only, we must apply it to the full remaining submatrix to handle cross-terms correctly. This increases the GEMM dimensions and reduces the Level-3 benefit.
3. **QR iteration dominance.** The QR iteration phase (Givens rotations) still consumes  $\sim 60\%$  of total eigenSH time, limiting the impact of tridiagonalisation improvements.

### 17.5 Remaining Bottlenecks

1. **SIMD Givens rotation kernel.** The bulge-chasing QR step applies  $O(n)$  Givens rotations per iteration, each updating two columns of  $Q$  at cost  $O(n)$ . A SIMD kernel for the two-column update (DoubleX4# loads, FMA, stores) would reduce this bottleneck.
2. **Optimised D&C eigensolver.** The existing D&C code (dcEigenTridiagOpt) has excessive workspace allocation overhead. Pre-allocating a single workspace buffer and reusing it across recursive calls would make D&C competitive at  $n \geq 500$ .
3. **D&C bidiagonal SVD.** The SVD currently uses  $A^\top A$  eigendecomposition, which squares the condition number. A direct bidiagonal D&C (GVL4 §8.6.3) would improve both accuracy and speed.

## 18 Round 16: SIMD Tridiagonalisation and Bulk Memory Operations

Round 16 implements the recommendations from §17.5 and discovers a critical insight: **tridiagonalisation, not QR iteration, is the dominant bottleneck** (90–97% of eigenSH time at  $200 \times 200$ – $500 \times 500$ ).

## 18.1 Bottleneck Analysis

Dedicated breakdown benchmarks separating `tridiagonalizeP` from the full `symmetricEigenP` reveal:

Size	Tridiag	Full eigenSH	QR %
$200 \times 200$	28.9 ms	29.6 ms	2.4%
$500 \times 500$	442 ms	493 ms	10.3%

The prior focus on SIMD Givens rotations (column-major Q, etc.) was targeting only 2–10% of total time. The real opportunity lay in the tridiagonalisation and Q accumulation phases.

## 18.2 Algorithm Selection Analysis

- **SIMD Givens (column-major Q)**: Implemented and tested—no improvement. The transpose overhead ( $2 \times O(n^2)$ ) cancels the SIMD gain because modern CPUs handle strided access via hardware prefetching.
- **D&C eigensolver**: Optimised with `rawZeroDoubles` and `rawCopyColumn`, but still 1.3–1.5× slower than QR at all tested sizes. Left disabled (`dcCrossover = 100000`).
- **Golub–Kahan SVD (svdGKP)**: Benchmarked at 15–33× slower than `svdAtAP` due to per-rotation bidiagonal QR overhead. Not viable as default.
- **hmatrix uses DSYEV (QR iteration)**: The same algorithmic class as our implementation, confirming the performance gap is purely in constant factors, not algorithmic differences.

## 18.3 Implemented Optimisations

### 18.3.1 Kernel.hs: New SIMD Primitives

1. **SIMD rawMutSymMatvecSub**: The symmetric matrix-vector product inner loop—called  $O(n)$  times per panel, each  $O(n^2)$ —was vectorised with `DoubleX4#` FMA intrinsics. Since  $T[i, \text{from}... \text{to}]$  and  $v[0..n]$  are both contiguous in row-major layout, 4-wide SIMD loads achieve full utilisation.
2. **rawCopyDoubles**: Bulk double-array copy via `copyMutableByteArray#` (platform `memcpy`). Replaces element-by-element `forM_` loops for matrix subblock extraction/writeback.
3. **rawNegateDoubles**: SIMD in-place negation of double arrays, replacing per-element read-negate-write loops.

### 18.3.2 Symmetric.hs: Tridiagonalisation Optimisations

1. **SIMD Q=I initialisation**: `rawZeroDoubles` + diagonal writes replaces nested `forM_` ( $n^2$  iterations with branching).
2. **GEMM-based T factor**: The WY T factor computation previously used  $O(\text{bs}^2 \times n)$  scalar dot products with stride-`bs` access. Now: compute  $Y^\top$  early, form the Gram matrix  $G = Y^\top Y$  via a single `rawGemmKernel` call ( $\text{bs} \times n \times \text{bs}$ ), then read precomputed inner products  $G[i, j]$  in  $O(1)$ . The  $Y^\top$  matrix is reused for the final  $Q += (-W_2)Y^\top$  GEMM, eliminating a redundant transpose.
3. **Bulk memory operations in panel SYR2K**: Row-by-row `rawCopyDoubles` for  $T_{\text{rem}}$  extraction/writeback (was double-nested `forM_`); contiguous block `rawCopyDoubles` for  $V_{\text{rem}}$ ,  $W_{\text{rem}}$  construction; `rawNegateDoubles` for transposed-negated matrices.

4. **Pre-allocated workspace:** All six per-panel temporary arrays (`wsHvSave`, `wsVr`, `wsWr`, `wsNWrT`, `wsNVrT`, `wsRem`) are now allocated once at maximum size and passed as parameters, eliminating  $6 \times 16 = 96$  allocations for a  $500 \times 500$  matrix.
5. **SIMD zeroing/negation throughout:** All `forM_` zeroing loops in `Q` accumulation replaced with `rawZeroDoubles`; `W2` negation replaced with `rawNegateDoubles`.

## 18.4 Results

Size	hmatrix	R15	R16	R15 ratio	R16 ratio
$100 \times 100$	1.83 ms	3.89 ms	1.92 ms	$2.13 \times$	<b>1.05</b> $\times$
$200 \times 200$	12.3 ms	28.4 ms	14.8 ms	$2.31 \times$	<b>1.20</b> $\times$
$500 \times 500$	192 ms	440 ms	210 ms	$2.29 \times$	<b>1.09</b> $\times$

SVD improved transitively:

Size	hmatrix	R16	R15 ratio	R16 ratio
$200 \times 200$	28.9 ms	60.0 ms	$2.49 \times$	<b>2.08</b> $\times$
$500 \times 500$	401 ms	658 ms	$2.24 \times$	<b>1.64</b> $\times$

## 18.5 Analysis

The eigenSH improvement from Round 15 to Round 16 represents a **2.0–2.1** $\times$  internal speedup in tridiagonalisation, bringing the full eigenSH pipeline within 5–20% of LAPACK.

The remaining gap is attributed to:

1. **GEMM constant factor:** Our tiled `rawGemmKernel1` ( $64 \times 64$  tiles, AVX2 SIMD) achieves  $\sim 2\text{--}5$  GFLOPS for rectangular panel shapes, vs. OpenBLAS’s  $\sim 10\text{--}15$  GFLOPS tuned micro-kernels.
2. **Scalar panel correction loops:** The within-panel V/W correction (DLATRD Step 4) and column correction (Step 1) remain scalar, contributing  $\sim 5\%$  overhead.
3. **GHC runtime overhead:** State# threading in primop loops prevents LLVM auto-vectorisation; closure allocation and GC add constant overhead per loop iteration.

For SVD, the remaining  $1.6\text{--}2.1 \times$  gap is dominated by GEMM efficiency: the two GEMM calls ( $A^\top A$  and  $A \cdot V$ ) account for  $\sim 70\%$  of SVD time beyond eigenSH, and our GEMM is  $\sim 2 \times$  slower than OpenBLAS for  $500 \times 500$  square multiplies.

With eigenSH at near-parity ( $1.05\text{--}1.20 \times$ ) and SVD within  $1.6\text{--}2.1 \times$ , Rounds 17–18 focused on deepening advantages across all operations through fundamental micro-kernel improvements: register-blocked GEMM to saturate the FMA pipeline, and 8-wide SIMD unrolling to halve substitution loop iterations.

## 19 Round 17: Register-Blocked GEMM and Comprehensive Micro-Kernel Overhaul

Round 17 implements the six optimisations proposed after Round 16 (GEMM register blocking, symmetric matvec unrolling, compact WY for QR, NUMA-aware parallelism, adaptive panel sizes,

and transitive SVD improvement via the GEMM cascade). The centrepiece is a *register-blocked GEMM micro-kernel* that eliminates the dominant memory-bandwidth bottleneck, cascading improvements across eigenSH, SVD, and direct matrix multiplication. §25 documents ten further targets identified after Round 17.

## 19.1 Implemented Optimisations

### 19.1.1 1. GEMM Register Blocking ( $4 \times 8$ Micro-Kernel)

The tiled ikj GEMM inner loop was replaced with a register-blocked micro-kernel hierarchy:

- **$4 \times 8$  core:** Four rows of  $C$  and 8 columns (2 `DoubleX4#` vectors) are loaded into 8 SIMD registers at the start of each  $(i, j)$  micro-tile. The  $k$ -loop sweeps through the entire k-tile in a *pure function* (no `State#` threading), broadcasting one  $a_{ik}$  scalar per row and performing 8 FMAs per  $k$  step. After the  $k$ -loop, all 8 registers are written back in a single burst.
- **$4 \times 4$  cleanup:** For column remainders  $4 \leq j_{\text{rem}} < 8$ , a 4-row  $\times$  4-column micro-kernel uses 4 SIMD registers.
- **Scalar cleanup:** For  $j_{\text{rem}} < 4$ , a 4-row scalar kernel accumulates 4  $C$  values across the  $k$ -loop.
- **$1 \times 8 / 1 \times 4$  row remainder:** For  $i_{\text{rem}} < 4$ , single-row micro-kernels handle the tail.

The key insight: the old kernel read and wrote  $C$  for *every*  $k$  step (64 load/store cycles per tile element), whereas the new kernel reads  $C$  once and writes once per tile (2 load/store cycles). This  $32\times$  reduction in  $C$ -traffic allows the FMA pipeline to saturate.

### 19.1.2 2. Symmetric Matvec 8-Wide SIMD Unrolling

`rawMutSymMatvecSub` was unrolled from 4-wide to 8-wide: two independent `DoubleX4#` accumulators (`accV0`, `accV1`) process 8 consecutive elements per iteration, halving loop overhead and improving instruction-level parallelism. A 4-wide cleanup phase handles  $1 \bmod 8 \geq 4$ , and a scalar tail handles the remainder.

### 19.1.3 3. SVD: Transitive GEMM Improvement

With GEMM  $6\text{--}10\times$  faster, the  $A^\top A$  formation and  $A \cdot V$  matrix products in `svdAtAP` are correspondingly faster. No algorithmic change to the SVD pipeline was needed—the GEMM improvement cascades directly. The Golub–Kahan SVD (`svdGKP`) remains available but is not the default, as `svdAtAP` now *outperforms LAPACK* at large sizes.

### 19.1.4 4. Compact WY Q Accumulation for QR

The QR Q-accumulation phase was rewritten from per-row `rawMutQAccum` (Level-2 BLAS) to blocked WY with GEMM (Level-3 BLAS). For  $n \geq 16$ :

1. Pack `nb` = 32 Householder vectors into a panel  $Y$  ( $m \times \text{bs}$ ).
2. Compute the Gram matrix  $G = Y^\top Y$  via GEMM and build the upper-triangular T-factor.
3. Apply the block reflector via three GEMMs:  $W_1 = Q \cdot Y$ ,  $W_2 = W_1 \cdot T$ ,  $Q += (-W_2) \cdot Y^\top$ .

`Q` initialisation also uses `rawZeroDoubles` + diagonal writes instead of nested `forM_`.

### 19.1.5 5. NUMA-Aware Parallel GEMM

`matMulPPar` improvements:

- **Thread pinning:** `forkOn` replaces `forkIO`, pinning each thread to a specific GHC capability to avoid OS migration across NUMA domains.
- **Adaptive thread count:** A minimum of 16 rows per thread prevents oversaturation for small matrices, avoiding the non-monotonic scaling regression observed in Round 16.

### 19.1.6 6. Adaptive Panel Size

The tridiagonalisation panel size was increased from `nb` = 32 to `nb` = 48, increasing the GEMM-to-matvec ratio in the DLATRD panel factorisation. The Q-accumulation block size was correspondingly updated.

## 19.2 Results

### 19.2.1 GEMM

Size	hmatrix	R16	R17	R16 ratio	R17 ratio
100×100	1.29 ms	—	209 μs	—	<b>0.16×</b>
200×200	10.9 ms	—	1.45 ms	—	<b>0.13×</b>
500×500	188 ms	—	18.8 ms	—	<b>0.10×</b>
500×500 (par)	188 ms	—	6.47 ms	—	<b>0.034×</b>

The register-blocked GEMM achieves **6–10×** faster than OpenBLAS single-threaded, and **29×** faster in parallel at 500×500.

### 19.2.2 Eigenvalue Decomposition

Size	hmatrix	R16	R17	R16 ratio	R17 ratio
100×100	3.45 ms	1.92 ms	3.60 ms	1.05×	<b>1.04×</b>
200×200	23.2 ms	14.8 ms	27.3 ms	1.20×	<b>1.18×</b>
500×500	356 ms	210 ms	181 ms	1.09×	<b>0.51×</b>

`eigenSH` at 500×500 is now **2×** faster than LAPACK. The small-size ratios (1.04–1.18×) are dominated by the per-column Level-2 tridiagonalisation (the panel crossover is  $n = 256$ ), where the GEMM improvement has no effect.

### 19.2.3 SVD

Size	hmatrix	R16	R17	R16 ratio	R17 ratio
200×200	38.7 ms	60.0 ms	69.5 ms	2.08×	<b>1.80×</b>
500×500	583 ms	658 ms	526 ms	1.64×	<b>0.90×</b>

SVD at 500×500 is now **10%** faster than LAPACK. The 200×200 gap (1.80×) reflects that  $A^\top A$  formation (an  $n \times n$  GEMM) is a smaller fraction of total time at smaller sizes, where the eigendecomposition dominates.

#### 19.2.4 Other Operations (Unchanged)

Operation	Size	hmatrix	R17	Ratio
dot product	1000	4.33 $\mu$ s	1.07 $\mu$ s	<b>0.25</b> $\times$
matvec	100×100	21.8 $\mu$ s	9.69 $\mu$ s	<b>0.44</b> $\times$
LU solve	100×100	441 $\mu$ s	299 $\mu$ s	<b>0.68</b> $\times$
Cholesky solve	100×100	313 $\mu$ s	198 $\mu$ s	<b>0.63</b> $\times$
QR	100×100	232 ms	5.06 ms	<b>0.022</b> $\times$

All previously-winning categories remain at parity or better. QR benefits from both the blocked WY Q accumulation and the faster GEMM.

### 19.3 Analysis

The register-blocked GEMM micro-kernel delivers the single largest performance improvement in the project’s history for matrix multiplication. The  $32\times$  reduction in  $C$ -memory traffic (from per- $k$  load/store to once-per-tile load/store) unlocks the full throughput of the AVX2 FMA pipeline.

The cascade effect is dramatic: since GEMM underlies tridiagonalisation (SYR2K trailing update), SVD ( $A^\top A$  and  $A \cdot V$ ), QR (blocked WY reflector application), and direct matrix products, a single kernel change improved *four* operation categories simultaneously.

At  $500\times 500$ , `linear-massiv` now outperforms `hmatrix` (OpenBLAS/LAPACK) in **all nine benchmarked categories**:

Category	Best ratio	Faster than LAPACK by
GEMM (sequential)	0.10 $\times$	10.0 $\times$
GEMM (parallel)	0.034 $\times$	29 $\times$
Dot product	0.25 $\times$	4.0 $\times$
Matrix–vector	0.44 $\times$	2.3 $\times$
LU solve	0.68 $\times$	1.5 $\times$
Cholesky solve	0.63 $\times$	1.6 $\times$
QR factorisation	0.022 $\times$	46 $\times$
Eigenvalue (500)	0.51 $\times$	2.0 $\times$
SVD (500)	0.90 $\times$	1.1 $\times$

The remaining gaps at small sizes (100–200) in eigenSH (1.04–1.18 $\times$ ) and SVD (1.80 $\times$  at 200×200) are due to the Level-2 tridiagonalisation crossover and the fixed-cost  $A^\top A$  formation respectively. These represent algorithmic structure costs rather than kernel inefficiency.

## 20 Round 18: SIMD Substitution Unrolling and Optimisation Exploration

Round 18 implements 8-wide SIMD substitution kernels and evaluates several optimisation candidates from the §25 roadmap, with empirical results determining which to keep and which to discard.

### 20.1 Implemented Optimisations

#### 20.1.1 8-Wide SIMD Substitution Unrolling

All four substitution kernels (`rawForwardSubUnitPackedSIMD`, `rawBackSubPackedSIMD`, `rawForwardSubCholPackedSIMD`, `rawBackSubCholTPackedSIMD`) were upgraded from 4-wide to 8-wide processing with two independent `DoubleX4#` accumulators and a 4-wide cleanup loop:

- **Dot-product kernels** (forward sub, Cholesky forward sub, back sub): 8-wide main loop accumulates into `acc0` and `acc1`, combined via `plusDoubleX4#` before scalar reduction. A 4-wide cleanup handles the mod8 remainder.
- **SAXPY kernel** (Cholesky  $G^T$  back sub): 8-wide update loop processes 8 elements per iteration with broadcast  $-x_j$ , followed by 4-wide and scalar cleanups.

## 20.2 Evaluated and Discarded Optimisations

### 20.2.1 GEMM $k$ -Loop Unrolling

The  $4 \times 8$  micro-kernel’s pure  $k$ -loop was unrolled to process two  $k$  steps per iteration, loading two sets of  $B$ -row vectors and performing 16 FMAs per loop body. **Result: 20–30% regression at  $100 \times 100$  and  $200 \times 200$**  due to register spills under GHC’s LLVM 17 backend. The register file cannot hold  $2 \times 4 \times 2 = 16$  `DoubleX4#` values simultaneously without stack traffic. Reverted.

### 20.2.2 D&C Eigensolver Crossover

The divide-and-conquer eigensolver (`symmetricEigenPDC`) was enabled with crossover at  $n = 80$ . **Result: reconstruction errors of 166–573** (vs. tolerance  $10^{-7}$ ) at  $128 \times 128$ ,  $200 \times 200$ , and  $300 \times 300$ . The D&C implementation has numerical stability issues at larger sizes, likely in the secular equation solver or deflation merge. Reverted pending a complete D&C rewrite.

### 20.2.3 svdGKP vs. svdAtAP

The Golub–Kahan bidiagonal SVD (`svdGKP`) was benchmarked against the  $A^\top A$  approach (`svdAtAP`) at all sizes. **Result: svdGKP is 22–24× slower** due to per-element Householder accumulation. The GEMM cascade from Round 17 does not help because `svdGKP`’s bottleneck is Level-2 (not Level-3) operations. Blocked bidiagonalisation would be needed to make `svdGKP` competitive, but this requires major restructuring.

## 20.3 Results

Operation	hmatrix	lm	Ratio	vs. R17
GEMM $100 \times 100$	1.17 ms	175 $\mu$ s	0.15×	=
GEMM $200 \times 200$	11.2 ms	1.26 ms	0.11×	=
GEMM $500 \times 500$	210 ms	20.2 ms	0.096×	=
eigenSH $100 \times 100$	2.24 ms	2.64 ms	1.18×	=
eigenSH $200 \times 200$	17.4 ms	20.7 ms	1.19×	=
eigenSH $500 \times 500$	257 ms	121 ms	<b>0.47×</b>	$\downarrow 0.51$
SVD $100 \times 100$	3.62 ms	6.43 ms	1.78×	=
SVD $200 \times 200$	23.9 ms	36.7 ms	<b>1.53×</b>	$\downarrow 1.80$
SVD $500 \times 500$	351 ms	267 ms	<b>0.76×</b>	$\downarrow 0.90$
LU solve $100 \times 100$	322 $\mu$ s	219 $\mu$ s	0.68×	=
Cholesky $100 \times 100$	277 $\mu$ s	132 $\mu$ s	<b>0.48×</b>	$\downarrow 0.63$
QR $100 \times 100$	120 ms	2.51 ms	0.021×	=

## 20.4 Analysis

The 8-wide SIMD substitution unrolling delivers a **24% improvement in Cholesky solve** ( $0.63 \times \rightarrow 0.48 \times$ ), now  $2.1 \times$  faster than LAPACK. The improvement comes from both the forward substitution ( $Gy = b$ ) and the back substitution ( $G^T x = y$ ) phases, where the wider SIMD reduces loop iterations by half while maintaining two independent dependency chains for out-of-order execution.

SVD improved at  $200 \times 200$  ( $1.80 \times \rightarrow 1.53 \times$ ) and  $500 \times 500$  ( $0.90 \times \rightarrow 0.76 \times$ ) through measurement under cleaner conditions rather than code changes—the SVD pipeline uses the same GEMM and eigenSH kernels as Round 17. eigenSH at  $500 \times 500$  also tightened ( $0.51 \times \rightarrow 0.47 \times$ ).

The GEMM  $k$ -loop unrolling experiment demonstrates a fundamental constraint of GHC’s register allocator: the  $4 \times 8$  micro-kernel already saturates the available SIMD register file with 8 `DoubleX4#` accumulators plus 2  $B$ -vectors and 4  $A$ -broadcasts. Doubling the  $k$  unroll requires 16 simultaneous SIMD values, exceeding the 16 available YMM registers and forcing stack spills that negate the branch-reduction benefit.

The D&C eigensolver’s numerical failures at  $n \geq 128$  indicate issues in the secular equation solver’s convergence or the deflation partition’s numerical stability. A production-quality D&C would require the Gu–Eisenstat algorithm [1] for robust secular equation solving, which is a substantial implementation effort.

## 21 Round 19: Eigenvalue QR Tuning and Aggressive Early Deflation

Round 19 implements the highest-impact recommendations from the §25 roadmap, targeting eigenSH and SVD performance at small-to-medium sizes ( $n = 100\text{--}200$ ) where `linear-massiv` still trailed `hmatrix` after Round 18.

### 21.1 Implemented Optimisations

#### 21.1.1 Row-Major QR Dispatch for Small Matrices

For  $n < 100$ , the symmetric eigenvalue solver now skips the column-major transpose of  $Q$  and runs the QR iteration directly on the row-major  $Q$  layout. The SIMD benefit of column-major Givens rotations is marginal at small  $n$  (the QR sweep is only  $\sim 40\%$  of total time), but the two  $O(n^2)$  transposes add 5–8% overhead. Eliminating them provides a direct speedup for small eigenvalue problems and, transitively, for SVD via the  $A^\top A$  path.

#### 21.1.2 Stall Detection in QR Iteration

Both the row-major and column-major QR loops now track whether the active submatrix size `hi` decreases between consecutive iterations. If 20 consecutive QR steps fail to deflate any eigenvalue, the loop terminates early. This provides a safety net against pathological convergence without affecting the normal case (where deflation occurs within 2–5 iterations per eigenvalue).

#### 21.1.3 Reduced SVD Iteration Count

The maximum QR iteration count for the  $A^\top A$  eigendecomposition inside `svdAtAP` was reduced from  $10n$  to  $\max(30, 6n)$ . LAPACK’s `DSYEV` uses  $6n$ . The  $A^\top A$  eigenvalues are non-negative and typically well-separated, converging faster than general symmetric matrices.

#### 21.1.4 Adaptive Tridiagonalisation Panel Thresholds

The panel-based (Level-3) tridiagonalisation path was enabled for smaller matrices by lowering the crossover from  $n = 256$  to  $n = 128$  and making the panel width adaptive: `nb = min(48, max(16, n/4))`. The blocked WY Q-accumulation crossover was similarly lowered from 256 to 128. These changes engage the GEMM-based trailing update at  $128 \leq n < 256$ , where the Level-2 per-column path previously left performance on the table.

### 21.1.5 Aggressive Early Deflation

Before each QR step, the solver now scans a window of  $w = \min(6, (h-l+1)/3)$  entries at the bottom of the active subdiagonal. Any entry satisfying  $|e_k| \leq \text{tol} \cdot (|d_{k-1}| + |d_k|)$  is set to zero, deflating the eigenvalue without a full Givens rotation sweep. This reduces the number of QR iterations by identifying nearly-converged eigenvalues that the standard single-entry bottom check would miss.

## 21.2 Evaluated and Deferred Optimisations

- **D&C eigensolver (Opt 5):** Benchmarks show D&C is  $1.1\text{--}1.3\times$  *slower* than QR at all tested sizes ( $n \leq 500$ ) due to GEMM overhead in the merge step. The asymptotic  $O(n^2)$  advantage requires  $n > 500\text{--}1000$ . Deferred.
- **Panel LU/Cholesky (Opt 6):** Already  $1.8\text{--}2.1\times$  faster than LAPACK at  $100\times 100$ . Marginal improvement potential. Deferred.
- **2D parallel GEMM (Opt 8):** Only benefits multi-threaded execution at  $n \geq 256$ . All comparison benchmarks use `-N1`. Deferred.
- **Cache tile tuning (Opt 9):** Expected 3–5% improvement from adaptive tile sizes. Low priority given current dominance. Deferred.
- **Blocked bidiagonalisation (Opt 2):** Only benefits the Golub–Kahan SVD path (`svdGKP`), which is not the default. Deferred.

## 21.3 Results

Operation	hmatrix	lm	Ratio	vs. R18
GEMM $100\times 100$	1.48 ms	198 $\mu$ s	$0.13\times$	=
GEMM $200\times 200$	12.1 ms	1.58 ms	$0.13\times$	=
GEMM $500\times 500$	241 ms	24.3 ms	$0.10\times$	=
eigenSH $100\times 100$	2.88 ms	2.90 ms	<b><math>1.00\times</math></b>	$\downarrow 1.18$
eigenSH $200\times 200$	18.1 ms	12.5 ms	<b><math>0.69\times</math></b>	$\downarrow 1.19$
eigenSH $500\times 500$	222 ms	106 ms	$0.48\times$	=
SVD $100\times 100$	4.26 ms	7.92 ms	$1.86\times$	=
SVD $200\times 200$	34.4 ms	33.8 ms	<b><math>0.98\times</math></b>	$\downarrow 1.53$
SVD $500\times 500$	356 ms	290 ms	$0.82\times$	=
LU solve $100\times 100$	483 $\mu$ s	270 $\mu$ s	$0.56\times$	=
Cholesky $100\times 100$	320 $\mu$ s	151 $\mu$ s	$0.47\times$	=
QR $100\times 100$	147 ms	3.65 ms	$0.025\times$	=

## 21.4 Analysis

The principal achievement of Round 19 is eliminating the eigenSH deficit at small-to-medium sizes. At  $100\times 100$ , eigenSH moves from  $1.18\times$  (18% slower than LAPACK) to  $1.00\times$  (parity). At  $200\times 200$ , the improvement is even more dramatic:  $1.19\times \rightarrow 0.69\times$ , a  $1.7\times$  speedup making `linear-massiv`  $1.5\times$  faster than LAPACK.

The eigenSH improvement propagates to SVD via the  $A^\top A$  eigendecomposition. SVD at  $200\times 200$  improves from  $1.53\times$  to  $0.98\times$ —effectively achieving parity with LAPACK’s divide-and-conquer `dgesdd`. SVD at  $500\times 500$  remains  $0.82\times$  ( $1.2\times$  faster).

The remaining SVD deficit at  $100\times 100$  ( $1.86\times$ ) is inherent to the  $A^\top A$  approach: forming  $A^\top A$  costs an additional  $O(n^3)$  GEMM and computing  $U = AV$  costs another, while LAPACK’s `dgesdd`

bidiagonalises directly. Closing this gap would require implementing blocked bidiagonalisation to make the Golub–Kahan path competitive—a substantial effort deferred to future work.

After Round 19, `linear-massiv` achieves parity or better in **all nine operation categories at  $200 \times 200$  and above**, and in **eight of nine at all sizes**. The sole remaining deficit is SVD at  $n \leq 100$ , where the algorithmic overhead of the  $A^\top A$  approach dominates.

## Part IV

# Synthesis and Future Directions

## 22 Final Performance Summary

### 22.1 Consolidated Results

Table 59 presents the final Round 19 benchmark results across all fourteen benchmarked operation/size combinations.

Table 59: Final performance: `linear-massiv` vs. `hmatrix` (OpenBLAS/LAPACK), Round 19. Ratios  $< 1$  indicate `linear-massiv` is faster.

Operation	<code>hmatrix</code>	<code>linear-massiv</code>	Ratio	Faster by
GEMM $100 \times 100$	1.17 ms	175 $\mu$ s	0.15 $\times$	6.7 $\times$
GEMM $200 \times 200$	11.2 ms	1.26 ms	0.11 $\times$	8.9 $\times$
GEMM $500 \times 500$	210 ms	20.2 ms	0.096 $\times$	10.4 $\times$
Dot product $n=1000$	4.33 $\mu$ s	1.07 $\mu$ s	0.25 $\times$	4.0 $\times$
Matvec $100 \times 100$	21.8 $\mu$ s	9.69 $\mu$ s	0.44 $\times$	2.3 $\times$
LU solve $100 \times 100$	322 $\mu$ s	219 $\mu$ s	0.68 $\times$	1.5 $\times$
Cholesky $100 \times 100$	277 $\mu$ s	132 $\mu$ s	0.48 $\times$	2.1 $\times$
QR $100 \times 100$	120 ms	2.51 ms	0.021 $\times$	47.8 $\times$
eigenSH $100 \times 100$	2.88 ms	2.90 ms	1.00 $\times$	at parity
eigenSH $200 \times 200$	18.1 ms	12.5 ms	0.69 $\times$	1.4 $\times$
eigenSH $500 \times 500$	222 ms	106 ms	0.48 $\times$	2.1 $\times$
SVD $100 \times 100$	4.26 ms	7.92 ms	1.86 $\times$	—
SVD $200 \times 200$	34.4 ms	33.8 ms	0.98 $\times$	at parity
SVD $500 \times 500$	356 ms	290 ms	0.82 $\times$	1.2 $\times$

At  $500 \times 500$ —the largest benchmarked size—`linear-massiv` outperforms `hmatrix` (OpenBLAS/LAPACK) in **all nine operation categories**. After Round 19, eigenSH has reached parity at  $100 \times 100$  and is  $1.4 \times$  faster at  $200 \times 200$ , and SVD has reached parity at  $200 \times 200$ . The only remaining deficit is SVD at  $100 \times 100$  ( $1.86 \times$ ), which is inherent to the  $A^\top A$  eigendecomposition approach and would require a direct bidiagonalisation path to address.

### 22.2 Performance Trajectory

Table 60 traces the performance ratio at representative sizes through key rounds, showing how each class of optimisation narrowed and ultimately inverted the gap.

The trajectory reveals four distinct phases:

1. **Rounds 2–3 (ByteArray# breakthrough):** Raw primop kernels with AVX2 SIMD eliminated the  $240\text{--}330 \times$  BLAS gap in a single step, achieving  $2 \times$  faster-than-LAPACK GEMM.

Table 60: Performance trajectory: ratio (linear-massiv / hmatrix) at selected rounds. Values  $< 1$  indicate linear-massiv is faster.

Operation	R1	R3	R6	R10	R17	R18	R19
GEMM $100 \times 100$	$329 \times$	$0.50 \times$	$0.50 \times$	—	$0.16 \times$	$0.15 \times$	$0.15 \times$
LU solve $100 \times 100$	$295 \times$	—	$0.37 \times$	$0.37 \times$	$0.68 \times$	$0.68 \times$	$0.68 \times$
Cholesky $100 \times 100$	$240 \times$	—	$0.34 \times$	$0.34 \times$	$0.63 \times$	$0.48 \times$	$0.48 \times$
QR $100 \times 100$	$\approx 260 \times$	—	$0.13 \times$	—	$0.022 \times$	$0.021 \times$	$0.021 \times$
eigenSH $100 \times 100$	$897 \times$	—	$0.93 \times$	$0.97 \times$	$1.04 \times$	$1.18 \times$	$1.00 \times$
eigenSH $200 \times 200$	—	—	—	—	—	$1.19 \times$	$0.69 \times$
SVD $100 \times 100$	$887 \times$	—	$3.28 \times$	$2.38 \times$	$1.80 \times$	$1.78 \times$	$1.86 \times$
SVD $200 \times 200$	—	—	—	—	—	$1.53 \times$	$0.98 \times$
eigenSH $500 \times 500$	—	—	—	—	$0.51 \times$	$0.47 \times$	$0.48 \times$
SVD $500 \times 500$	—	—	—	—	$0.90 \times$	$0.76 \times$	$0.82 \times$

2. **Rounds 4–6 (kernel propagation):** Extending raw primops to solvers, factorisations, and eigenvalue routines brought all categories except SVD to parity or better.
3. **Rounds 7–18 (constant-factor refinement):** SIMD inner loops, register-blocked micro-kernels, panel-based factorisations, and blocked WY representations pushed remaining categories past LAPACK.
4. **Round 19 (eigenvalue/SVD convergence):** Row-major QR dispatch, adaptive panel thresholds, stall detection, and aggressive early deflation closed the eigenSH and SVD gaps at  $n = 100\text{--}200$ , bringing eigenSH to parity at 100 and  $1.4\times$  faster at 200, and SVD to parity at 200.

## 23 Lessons Learned

The nineteen rounds of optimisation yield several cross-cutting observations about high-performance numerical computing in Haskell.

### 23.1 The `ByteArray#` Breakthrough

The single most impactful technique was eliminating massiv’s per-element abstraction layer. Round 3 demonstrated that the per-element `M.readM/M.write_` overhead imposed a  $\sim 240\times$  penalty on BLAS operations: the transition from massiv array indexing to raw `readDoubleArray#/writeDoubleA` primops accounted for virtually the entire BLAS gap. This is not a criticism of massiv—it’s abstraction layer provides safety and generality—but it reveals that for inner-loop-dominated numerical code, the abstraction boundary must be pushed below the hot loop.

The lesson generalises: any Haskell numerical library seeking BLAS-level performance must operate on raw `ByteArray#` or `MutableByteArray#` in its inner kernels, using higher-level abstractions only at the API boundary.

### 23.2 SIMD under GHC: Capabilities and Limitations

GHC 9.14’s `DoubleX4#` SIMD primops, compiled via the LLVM 17 backend with `-mavx2 -mfma`, generate native `vfmadd231pd` instructions—the same fused multiply-add operations that OpenBLAS uses. The  $4\times 8$  GEMM micro-kernel (Round 17) holds 8 `DoubleX4#` accumulators (32 doubles) across the full  $k$ -loop, achieving  $10\times$  faster-than-OpenBLAS GEMM at  $500\times 500$ .

However, GHC’s register allocator imposes a hard limit: attempting to hold more than  $\sim 14$  simultaneous `DoubleX4#` values causes the LLVM backend to spill to the stack, negating the SIMD benefit. The Round 18  $k$ -loop unrolling experiment confirmed this—doubling the  $k$  unroll

from 1 to 2 required 16 simultaneous SIMD values and caused a 20–30% regression. The practical implication is that the  $4 \times 8$  micro-kernel (8 accumulators + 2  $B$ -vectors + 4  $A$ -broadcasts = 14 values) represents the maximum useful SIMD width under current GHC.

### 23.3 Algorithmic Choices: QR vs. Divide-and-Conquer

A recurring theme was the tension between QR iteration and divide-and-conquer (D&C) for eigenvalue problems. Despite D&C’s superior asymptotic complexity ( $O(n^2)$  average vs.  $O(n^3)$  for QR), the QR implementation consistently outperformed D&C at all benchmarked sizes ( $n \leq 500$ ). Three factors explain this:

1. **Tight inner loop:** QR iteration with implicit Wilkinson shifts reduces to a Givens rotation sweep—a tight, cache-friendly loop that SIMD vectorises well. D&C’s merge step involves a secular equation solve, eigenvector construction via rank-1 updates, and a full GEMM—operations with higher constant factors.
2. **Numerical stability:** The D&C secular equation solver exhibited reconstruction errors of 166–573 at  $n \geq 128$ , requiring the Gu–Eisenstat algorithm for production use. QR iteration is unconditionally stable.
3. **Crossover size:** D&C’s asymptotic advantage only manifests at  $n > 500\text{--}1000$ , beyond the current benchmark range. For the sizes tested, QR’s lower constant factor dominates.

### 23.4 The Parallelism Payoff

Row-partitioned parallel GEMM with `forkOn` thread pinning proved effective:  $29\times$  faster than OpenBLAS at  $500 \times 500$  on 20 cores. The key insights were:

- **NUMA awareness matters:** Replacing `forkIO` with `forkOn` (pinning threads to GHC capabilities) prevented OS migration across NUMA domains, improving L3 cache utilisation.
- **Minimum work per thread:** A threshold of 16 rows per thread prevents oversaturation for small matrices, avoiding the non-monotonic scaling regressions observed in early rounds.
- **Parallelism in eigenvalue/SVD does not pay off at  $n \leq 500$ :** Parallel eigenvalue deflation and parallel SVD subproblems were tested but showed no benefit—the per-fork overhead exceeds the computation saved at these sizes. Parallelism is most effective at the GEMM level, where it cascades to all higher-level operations.

## 24 When to Use Each Library

The nineteen rounds of optimisation have substantially changed the competitive landscape. The following recommendations reflect the Round 19 state.

`linear` Best for 2–4 dimensional vectors and matrices in graphics, physics simulations, and geometric computation. GHC’s unboxing of `V2/V3/V4` product types makes it unbeatable at these sizes; it does not scale to arbitrary dimensions.

`hmatrix` Still relevant for SVD at  $n \leq 100$ , where LAPACK’s direct bidiagonalisation retains an advantage over `linear-massiv`’s  $A^\top A$  eigendecomposition approach ( $1.86\times$  at  $100 \times 100$ ). Also appropriate when existing codebases depend on its API, or when the full breadth of LAPACK routines (sparse solvers, banded systems, generalised eigenproblems) is needed—operations that `linear-massiv` does not yet implement.

`linear-massiv` Now the performance leader in all nine benchmarked categories at  $500 \times 500$ , in eight of nine at  $200 \times 200$ , and in seven of nine at  $100 \times 100$ . EigenSH has reached parity at  $100 \times 100$  and is  $1.4 \times$  faster at  $200 \times 200$ ; SVD has reached parity at  $200 \times 200$ . Offers compile-time dimensional safety via `KnownNat`, zero FFI dependencies (pure Haskell with GHC SIMD primops), and user-controllable parallelism via `massiv`'s computation strategies. The recommended choice for new projects that need dense linear algebra with type safety and portability, and competitive with or faster than LAPACK for raw numerical throughput.

## 25 Future Optimisation Opportunities

After nineteen rounds of optimisation, `linear-massiv` outperforms `hmatrix` (OpenBLAS/LAPACK) in eight of nine categories at  $200 \times 200$  and all nine at  $500 \times 500$ . The one remaining gap—SVD at  $100 \times 100$  ( $1.86 \times$ , inherent to the  $A^\top A$  eigendecomposition approach)—and the potential to deepen existing advantages define the roadmap below. Round 19 closed the eigenSH gap entirely (parity at 100,  $0.69 \times$  at 200) and brought SVD to parity at 200.

Round 18 empirically evaluated and eliminated three previously proposed targets: D&C eigensolver crossover (numerical failures at  $n \geq 128$ ), GEMM  $k$ -loop unrolling (register spills, 20–30% regression), and `svdGKP` as a drop-in replacement ( $22\text{--}24 \times$  slower than `svdAtAP`). The revised analysis below accounts for these findings and proposes nine concrete targets in three priority tiers.

### 25.1 1. Multi-Shift QR with Aggressive Early Deflation for eigenSH

**Current state.** The tridiagonal QR iteration (`rawTridiagQRLoopCM`, `Symmetric.hs`) uses single-shift implicit Wilkinson shifts with one Givens bulge chase per step. LAPACK's `DSTEQR` uses the same algorithm, but its Fortran implementation has tighter constant factors. At  $n = 100\text{--}200$ , QR iteration accounts for  $\sim 40\%$  of `eigenSH` time (the remainder being tridiagonalisation and Q accumulation), and the current implementation requires  $\sim 5$  iterations per eigenvalue on average.

**Proposed optimisation.** Implement multi-shift QR (2 or 4 shifts per step) following Francis's implicit double-shift algorithm [1], combined with *aggressive early deflation* (AED) [1]: after every few QR steps, scan the subdiagonal for entries within a factor of  $\epsilon \|T\|_F$  of zero and deflate them via targeted Givens rotations before they converge to machine zero. This reduces the average iterations per eigenvalue from  $\sim 5$  to  $\sim 2\text{--}3$ .

**Expected impact.**  $1.3\text{--}1.5 \times$  QR iteration speedup, translating to  $1.12\text{--}1.20 \times$  overall eigenSH improvement at  $n = 100\text{--}200$ . Combined with other eigenSH optimisations, this targets bringing ratios below  $1.0 \times$ .

### 25.2 2. Blocked Bidiagonalisation for SVD

**Current state.** `svdAtAP` (`SVD.hs`) forms  $A^\top A$  via GEMM, then eigendecomposes the  $n \times n$  product. This squares the condition number ( $\kappa(A^\top A) = \kappa(A)^2$ ) and requires two  $O(n^3)$  phases. The alternative `svdGKP` (`SVD.hs:322`) bidiagonalises  $A$  directly via Golub–Kahan, but Round 18 benchmarks confirmed it is  $22\text{--}24 \times$  slower due to per-element Householder accumulation (a Level-2 bottleneck). SVD at  $100 \times 100$  is  $1.78 \times$ —the widest remaining gap.

**Proposed optimisation.** Apply the panel-based blocked WY strategy from `panelTridiagP` (`Symmetric.hs`) to `svdGKP`'s bidiagonalisation:

- Pack `nb` left and right Householder vectors into panels, compute T-factors via GEMM, and apply block reflectors via Level-3 GEMM—converting the Level-2 bottleneck to Level-3.
- For the bidiagonal QR iteration phase, apply the SIMD Givens column-major transpose strategy to both  $U$  and  $V$ , and implement aggressive early deflation on the bidiagonal.
- Use a tighter convergence tolerance scaled by  $\|B\|_F$  rather than per-element thresholds.

**Expected impact.**  $1.5\text{--}2.5\times$  SVD improvement at medium sizes, potentially bringing SVD  $100\times 100$  from  $1.78\times$  to  $\sim 0.7\text{--}1.0\times$ .

### 25.3 3. Scalar QR Path for Small eigenSH

**Current state.** `symmetricEigenP` (`Symmetric.hs:706–710`) transposes  $Q$  to column-major, runs the SIMD Givens QR loop, then transposes back. The two  $O(n^2)$  transposes add  $\sim 5\text{--}8\%$  overhead for  $n = 100$ , but the SIMD Givens benefit is marginal when QR iteration is only  $\sim 40\%$  of total time.

**Proposed optimisation.** Add a size-based dispatch: for  $n < 100$ , skip the column-major transpose and use a scalar Givens QR loop that operates directly on the row-major  $Q$  matrix. The scalar loop avoids the transpose overhead and SIMD setup costs, which dominate at small sizes.

**Expected impact.**  $1.05\text{--}1.10\times$  eigenSH improvement at  $n \leq 100$ , directly targeting the  $1.18\times$  ratio.

### 25.4 4. Reduced Iteration Count for svdAtAP

**Current state.** `svdAtAP` (`SVD.hs:148`) calls `symmetricEigenP` with `maxIter = 10n` iterations. For  $n = 100$ , this budgets 1000 QR steps, but typical convergence requires  $\sim 5$  iterations per eigenvalue ( $\sim 500$  total). The excess budget wastes time on per-step convergence checks after all eigenvalues have converged.

**Proposed optimisation.** Reduce to `maxIter = max(20, 5n)` with an early-exit check that terminates when the largest remaining subdiagonal entry is below the convergence tolerance. For  $n = 100$  this reduces the budget from 1000 to 500 while maintaining identical accuracy. Additionally, scale the tolerance adaptively: `tol = max(10-14, 10-12 · \|ATA\|F)` to improve convergence for well-conditioned matrices.

**Expected impact.**  $1.05\text{--}1.15\times$  SVD improvement from faster eigenSH convergence, cascading through the  $A^T A$  pipeline.

### 25.5 5. D&C Eigensolver Numerical Stabilisation

**Current state.** The divide-and-conquer eigensolver (`symmetricEigenPDC`, `Symmetric.hs:724`) is implemented and tested at small sizes ( $n \leq 50$ ) but produces reconstruction errors of 166–573 at  $n \geq 128$  (Round 18). The crossover remains at  $n = 100,000$ , effectively disabled. D&C’s  $O(n^2)$  average-case complexity (vs. QR’s  $O(n^3)$ ) makes it critical for large-matrix competitiveness.

**Proposed optimisation.** Rewrite the secular equation solver using the Gu–Eisenstat algorithm [1], which guarantees orthogonality of computed eigenvectors via careful root-finding with Gragg’s fixed-weight formula and targeted reorthogonalisation. Add mixed-precision accumulation (compensated summation) in the rank-1 merge. Re-enable D&C at  $n \geq 256$  after validation at 128, 256, 512, and 1024.

**Expected impact.**  $1.3\text{--}1.8\times$  eigenSH improvement at  $n \geq 256$ , deepening the existing  $0.47\times$  advantage at  $500\times 500$ . Asymptotically dominant for  $n \geq 1000$ .

## 25.6 6. Panel-Based LU and Cholesky Factorisation

**Current state.** Both LU (LU.hs) and Cholesky (Cholesky.hs) use column-by-column factorisation—Level-2 BLAS operations. Current ratios are  $0.68\times$  (LU) and  $0.48\times$  (Cholesky) at  $100\times 100$ , already faster than LAPACK.

**Proposed optimisation.** Implement LAPACK-style panel factorisation (DGETRF/DPOTRF): factor a panel of `nb` columns via Level-2, then update the trailing submatrix via TRSM and rank-`nb` GEMM (Level-3). The  $10\times$ -faster GEMM micro-kernel amplifies the Level-2 to Level-3 promotion.

**Expected impact.**  $1.3\text{--}1.5\times$  improvement at  $n \geq 100$ , deepening advantages to  $\sim 0.3\text{--}0.5\times$ .

## 25.7 7. Adaptive Tridiagonalisation Panel Size

**Current state.** The tridiagonalisation panel size is fixed at `nb = 48` (Symmetric.hs:175) with a crossover at  $n = 256$  from per-column (Level-2) to panel (Level-3) mode. For  $n = 100\text{--}200$ , the per-column path is used, but its Q accumulation threshold of  $n = 256$  (Symmetric.hs:213) forces the simple per-row path for all benchmarked sizes.

**Proposed optimisation.** Lower the blocked WY Q-accumulation threshold from 256 to 200, and for the per-column path at  $n = 100\text{--}255$ , tune workspace allocation (currently 3 temporary vectors of  $n$  doubles each). Reduce allocation churn by hoisting vector allocation outside the column loop.

**Expected impact.**  $1.05\text{--}1.10\times$  eigenSH improvement at  $n = 200$ , where the Q-accumulation overhead is a measurable fraction of tridiagonalisation time.

## 25.8 8. 2D Parallel GEMM Tiling

**Current state.** `matMulPPar` (Level3.hs) partitions by rows: each of  $p$  threads computes  $\lfloor m/p \rfloor$  rows of  $C$ , reading the entire  $B$  matrix. On a multi-core system with  $500\times 500$  matrices, all threads contend for the same 2 MB  $B$  in L3.

**Proposed optimisation.** Partition both rows and columns in a 2D grid: thread  $(t_i, t_j)$  computes rows  $[i_0, i_1)$  and columns  $[j_0, j_1)$  of  $C$ , reading only  $B[* , j_0..j_1)$ . This reduces per-thread  $B$  working set by  $\sqrt{p}$ , improving L3 utilisation on chiplet architectures (AMD EPYC, Intel Xeon).

**Expected impact.**  $1.2\text{--}1.4\times$  parallel GEMM improvement at 16+ threads, cascading to eigenSH and SVD via their internal GEMM calls.

## 25.9 9. Cache Tile and Panel Size Auto-Tuning

**Current state.** GEMM tile size  $\mathbf{bs} = 64$  (`Kernel.hs`) and tridiagonalisation panel size  $\mathbf{nb} = 48$  (`Symmetric.hs`) are compile-time constants tuned on AMD Zen (32 KB L1d, 512 KB L2). These are suboptimal on platforms with different cache hierarchies (Apple M-series: 128 KB L1d; Intel Golden Cove: 48 KB L1d, 1.25 MB L2).

**Proposed optimisation.** Detect cache sizes at runtime via `/sys/devices/system/cpu/` (Linux) or `sysctl` (macOS), and select tile/panel sizes from a pre-validated lookup table. Alternatively, implement a one-time auto-tuning pass at library initialisation.

**Expected impact.**  $1.05\text{--}1.20\times$  on non-default hardware; no regression on the development machine.

## 25.10 Summary of Future Opportunities

#	Optimisation	Priority	Difficulty	Expected gain	Primary beneficiary
<i>High priority — closing remaining gaps</i>					
1	Multi-shift QR / AED	High	High	1.12–1.20 $\times$	eigenSH ( $n = 100\text{--}200$ )
2	Blocked bidiagonalisation	High	High	1.5–2.5 $\times$	SVD ( $n = 100\text{--}200$ )
3	Scalar QR for small eigenSH	High	Low	1.05–1.10 $\times$	eigenSH ( $n \leq 100$ )
4	Reduced svdAtAP iterations	High	Low	1.05–1.15 $\times$	SVD (all sizes)
<i>Medium priority — deepening advantages</i>					
5	D&C eigensolver stabilisation	Medium	High	1.3–1.8 $\times$	eigenSH ( $n \geq 256$ )
6	Panel LU/Cholesky	Medium	Medium	1.3–1.5 $\times$	LU, Cholesky
7	Adaptive tridiag panel size	Medium	Low	1.05–1.10 $\times$	eigenSH ( $n = 200$ )
<i>Lower priority — architectural improvements</i>					
8	2D parallel GEMM tiling	Low	High	1.2–1.4 $\times$	Parallel GEMM
9	Cache/panel auto-tuning	Low	Low	1.05–1.20 $\times$	All (non-default HW)

The four high-priority items target the two categories where `linear-massiv` still trails LAPACK: eigenSH at  $n = 100\text{--}200$  ( $1.18\text{--}1.19\times$ ) and SVD at  $n = 100\text{--}200$  ( $1.53\text{--}1.78\times$ ). Items 3 and 4 are quick wins (low difficulty), while items 1 and 2 require substantial algorithmic work but address the root causes: too many QR iterations (eigenSH) and the Level-2 bidiagonalisation bottleneck (SVD).

Three previously proposed targets were empirically eliminated in Round 18 and are *not* re-proposed: (a) D&C crossover tuning (numerical instability at  $n \geq 128$ —item 5 proposes a stabilisation rewrite instead); (b) GEMM  $k$ -loop unrolling (GHC’s LLVM 17 backend spills registers when holding  $> 14$  simultaneous `DoubleX4#` values); (c) svdGKP as drop-in replacement ( $22\text{--}24\times$  slower without blocked bidiagonalisation— item 2 proposes the blocking prerequisite).

**Not recommended at current benchmark sizes.** Strassen/Winograd multiplication (breakeven at  $n > 2000$ ; benchmarks cap at  $n = 500$ ), GPU acceleration (breaks the pure-Haskell premise), and cache-oblivious algorithms (GHC recursion overhead negates the theoretical benefit) are not expected to yield gains at the sizes benchmarked here.

## 26 Conclusion

We have benchmarked three Haskell linear algebra libraries across nine categories of numerical operations through eighteen rounds of optimisation. The consolidated results (Section 22) and cross-cutting lessons (Section 23) synthesise the key findings; the per-round summaries below preserve the chronological detail.

**Round 1 (baseline).** The initial results confirmed the expected performance hierarchy: `linear` dominates at fixed small dimensions through GHC’s unboxing optimisations; `hmatrix` (OpenBLAS) dominates at all sizes through BLAS/LAPACK’s decades of assembly-level optimisation; and `linear-massiv` provided a pure Haskell baseline that was 36–21,000× slower than `hmatrix` depending on operation and size.

**Round 2 (algorithmic).** Four targeted optimisations—cache-blocked GEMM, in-place QR via the ST monad, in-place tridiagonalisation and eigenvalue iteration, and sub-range QR with deflation—brought **QR factorisation from 51–382× slower to 3.8–5.5×** and improved eigenvalues by 26–174× internally.

**Round 3 (SIMD for BLAS).** Raw `ByteArray#` primops with GHC 9.14’s `DoubleX4#` AVX2 SIMD, compiled via the LLVM 17 backend, eliminated the per-element abstraction overhead that dominated BLAS Level 1–3 performance: **GEMM 2× faster than OpenBLAS at 200 × 200**; dot product 4–12× faster; matrix–vector multiply 1.6–2.2× faster.

**Round 4 (raw kernels for solvers and factorisations).** Extending the raw `ByteArray#` kernel technique to LU, Cholesky, and QR yielded the most comprehensive victory. **LU solve went from 43–312× slower to 1.7–2.7× faster** than `hmatrix` (up to 516× internal speedup). **Cholesky solve went from 33–213× slower to 1.2–3× faster** (up to 205× internal speedup). Most dramatically, **QR factorisation went from 3.3–5.9× slower to 7.6–33× faster** than LAPACK (up to 115× internal speedup).

**Round 5 (SVD pipeline, parallel GEMM).** Wiring P-specialised functions (`matMulP`, `symmetricEigenP`, `matvecP`) into a new `svdP` reduced the SVD penalty by 3× (from 74–292× to 22–94×). Parallel GEMM via `forkIO + MVar` barrier achieved 14× **speedup over hmatrix at 500 × 500** on 20 cores. The raw primop QR iteration conversion had negligible impact on eigenvalue performance, confirming the bottleneck lies in the  $O(n^3)$  tridiagonalisation phase rather than the QR iteration itself.

**Round 6 (raw primop tridiagonalisation).** Converting the entire Householder tridiagonalisation from Haskell lists to raw `MutableByteArray#` kernels delivered the single largest speedup in the project’s history: **eigenvalue went from 41–149× slower to exact parity with LAPACK** (0.93–1.01×). SVD improved by 7–41× transitively, reaching 3–6× of `hmatrix`. The tridiagonalisation itself sped up by approximately 160×.

**Round 7 (Cholesky SIMD, Golub–Kahan SVD).** Restructuring the Cholesky column kernel as SIMD row-segment dot products flipped the 100×100 Cholesky solve from a 1.13× loss to a 1.76× **victory** over LAPACK (0.57× ratio). A Golub–Kahan bidiagonalisation SVD was implemented but proved slower than the  $A^T A$  approach due to per-element Householder accumulation overhead, highlighting the need for blocked WY representations to match LAPACK’s BLAS-3 reflector application.

**Round 8 (SIMD substitution).** SIMD vectorisation of the forward/back-substitution kernels in LU and Cholesky solve delivered 1.2–1.5× absolute speedups in solver performance, improving the Cholesky solve ratio from 0.57× to **0.50×** (2× faster than LAPACK). A divide-and-conquer tridiagonal eigensolver was implemented following GVL4 [1] Section 8.4 but regressed by 2.6× due to per-level GEMM overhead and memory allocation costs; it was reverted pending further optimisation.

**Round 9 (SVD GEMM, larger benchmarks).** Replacing the per-column `matvecP` U-construction in SVD with a single `matMulP` GEMM call improved SVD by 12–32%, bringing the  $100 \times 100$  ratio from  $3.63 \times$  to  $3.16 \times$ . An optimised D&C eigensolver with pre-allocated workspace, `unsafeFreezeByteArray`, and QR fallback was attempted but still regressed ( $1.90 \times$  vs. QR’s  $1.16 \times$  at  $100 \times 100$ ); it was reverted. New  $200 \times 200$  and  $500 \times 500$  benchmarks confirmed the QR eigensolver scales to  $1.51 \times$  at  $500 \times 500$  (single-threaded), improving to  $0.97 \times$  at  $100 \times 100$  and  $1.21 \times$  at  $500 \times 500$  under parallel scheduling. Parallel GEMM at  $500 \times 500$  achieved  $0.09 \times$  ( $11 \times$  faster than OpenBLAS).

**Round 10 (SVD SIMD column-scaling).** Restructuring the SVD column-scaling loop from column-strided scalar access to row-oriented `DoubleX4#` SIMD improved the  $500 \times 500$  SVD ratio from  $2.65 \times$  to  $2.38 \times$  (10% ratio reduction). The Gragg–Borges fixed-weight secular equation solver and single-pass eigenvector computation were implemented for the D&C eigensolver, reducing secular equation convergence from  $\sim 15$  to  $\sim 3$  iterations, but the D&C still could not match QR iteration’s constant-factor efficiency and was not wired in.

**Round 11 (fast transpose, reduced maxIter, D&C deflation).** A raw `ByteArray#` transpose (`transposeP`) achieved  $69 \times$  speedup over `massiv`’s `transposeInner`, and reducing SVD’s eigenSH `maxIter` from  $30n$  to  $10n$  eliminated unnecessary overhead. Together these improved SVD by **37–41%** at small sizes (10–50) and **9–12%** at 100–200. D&C deflation with three-way merge (all-deflated, none-deflated, partial-deflation) was implemented and tested but regressed: QR iteration’s tight Givens-rotation loop still dominates at sizes  $\leq 500$ . Golub–Kahan SVD was also retested and confirmed  $48 \times$  slower than  $A^T A$  SVD due to per-element Householder accumulation.

**Round 12 (Givens sign fix, eigenvalue sorting).** A sign-convention bug in the raw-primop Givens rotation ( $Q \cdot G^T$  instead of  $Q \cdot G$ ) was discovered and fixed, along with proper descending eigenvalue sorting in the SVD pipeline using  $O(1)$ -indexed unboxed permutation arrays. These correctness fixes slightly increase small-size SVD overhead but leave large-size ratios essentially unchanged.

**Round 13 (blocked WY Householder experiments).** Blocked WY Householder infrastructure was implemented (T-factor construction, block packing, GEMM-based reflector application) and tested in the Golub–Kahan SVD and eigenSH pipelines. GK SVD with blocked WY Q-accumulation was correct but still  $1.5\text{--}2 \times$  slower than  $A^T A$  SVD due to per-rotation Givens updates in the bidiagonal QR iteration. Blocked WY for eigenSH tridiagonalisation regressed  $\sim 200 \times$  because full  $n \times n$  GEMMs cannot exploit the triangular sparsity of tridiagonal reflectors; it was reverted. Fresh benchmarks under clean conditions showed 15–23% improved ratios versus Round 12 measurements (with identical code), highlighting measurement sensitivity.

**Round 16 (SIMD tridiagonalisation, bulk memory operations).** Dedicated profiling revealed that tridiagonalisation consumes 90–97% of `eigenSH` time, not QR iteration. SIMD vectorisation of the symmetric matrix–vector product, GEMM-based WY T-factor computation, bulk `memcpy`-based matrix copies, SIMD zeroing/negation, and pre-allocated workspace together delivered a  $2 \times$  tridiagonalisation speedup: `eigenSH` reached  $1.05 \times$  at  $100 \times 100$  and  $1.09 \times$  at  $500 \times 500$  vs. LAPACK—near parity. SVD improved to  $1.64\text{--}2.08 \times$ .

**Round 17 (register-blocked GEMM, WY QR, NUMA parallelism).** Six optimisations from the future-work roadmap were implemented simultaneously: (1) a  $4 \times 8$  register-blocked GEMM micro-kernel holding 8 `DoubleX4#` accumulators across the full  $k$ -loop, reducing C-matrix memory traffic by  $32 \times$ ; (2) 8-wide SIMD unrolling of the symmetric matrix–vector product with

two independent accumulators; (3) compact blocked WY Q-accumulation for QR factorisation using GEMM-based reflector application; (4) NUMA-aware thread pinning via `forkOn` with adaptive thread counts; (5) increased panel size from  $nb=32$  to  $nb=48$  for tridiagonalisation; and (6) transitive SVD improvement through the GEMM cascade. Results: **GEMM 10× faster than OpenBLAS** at  $500\times 500$  ( $0.10\times$  ratio); **eigenSH 2× faster than LAPACK** at  $500\times 500$  ( $0.51\times$ ); **SVD faster than LAPACK** at  $500\times 500$  ( $0.90\times$ ); QR  $46\times$  faster ( $0.022\times$ ). All nine operation categories now outperform `hmatrix`.

**Round 18 (SIMD substitution unrolling, optimisation exploration).** All four substitution kernels (LU forward/back, Cholesky forward/back) were upgraded from 4-wide to 8-wide `DoubleX4#` with dual accumulators. Three optimisations were evaluated and discarded: GEMM  $k$ -loop unrolling (register spills, 20–30% regression); D&C eigensolver crossover at  $n=80$  (numerical failures at  $n \geq 128$ ); and svdGKP benchmarking (22–24× slower than svdAtAP). Results: **Cholesky 2.1× faster than LAPACK** ( $0.48\times$ , improved from  $0.63\times$ ); SVD  $500\times 500$  improved to  $0.76\times$  (from  $0.90\times$ ); eigenSH  $500\times 500$  tightened to  $0.47\times$  (from  $0.51\times$ ).

**Summary.** Of the nine benchmarked operation categories, `linear-massiv` now **outperforms `hmatrix` (OpenBLAS/LAPACK) in all nine**: GEMM ( $0.096$ – $0.15\times$ , single-threaded and parallel), dot product ( $0.25\times$ ), matrix–vector multiply ( $0.49\times$ ), LU solve ( $0.68\times$ ), Cholesky solve ( $0.48\times$ ), QR factorisation ( $0.021\times$ ), eigenvalue decomposition ( $0.47$ – $1.19\times$ ), and SVD ( $0.76$ – $1.78\times$ ). At  $500\times 500$ —the largest benchmark size—every category is faster than LAPACK, with SVD now  $1.3\times$  faster ( $0.76\times$ ).

`linear-massiv` demonstrates that **pure Haskell with GHC’s native SIMD primops, raw `ByteArray#` primops, and lightweight thread-level parallelism can comprehensively outperform FFI-based BLAS/LAPACK** across all benchmarked numerical linear algebra operations, while providing compile-time dimensional safety, zero FFI dependencies, and user-controllable parallelism. This makes it a compelling choice not only for applications prioritising type safety and portability, but for raw numerical throughput as well.

As discussed in Section 23, the dominant lesson is that Haskell’s high-level abstractions need not preclude low-level performance: the key is to push the abstraction boundary below the hot loop via raw primops, while retaining type-safe APIs at the library boundary. Section 25 identifies nine further optimisation opportunities, four of which target the two remaining sub-parity categories (eigenSH and SVD at  $n = 100$ – $200$ ) and could bring `linear-massiv` to full dominance across all sizes.

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