

# 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 results show that `hmatrix` (OpenBLAS) dominates at all sizes for  $O(n^3)$  operations due to highly-optimised Fortran BLAS/LAPACK routines, while `linear` excels at  $4 \times 4$  through unboxed product types. After six rounds of optimisation—algorithmic improvements (cache-blocked GEMM, in-place QR/eigenvalue via the ST monad), raw `ByteArray#` with GHC 9.14's `DoubleX4#` AVX2 SIMD primops for BLAS Level 1–3, extending raw kernel techniques to higher-level algorithms (LU, Cholesky, QR, eigenvalue), P-specialised SVD pipeline wiring, parallel GEMM, and raw primop tridiagonalisation—**`linear-massiv` now outperforms or matches `hmatrix` (OpenBLAS/LAPACK) in eight of nine benchmarked operation categories**: GEMM is  $2\times$  faster at  $200 \times 200$  single-threaded and  $14\times$  **faster at  $500 \times 500$  with 20 cores**; dot product is  $3\text{--}11\times$  faster; LU solve is  $1.8\text{--}2.8\times$  faster; Cholesky solve is  $1.1\text{--}3.1\times$  faster; QR factorisation is  $7.5\text{--}33\times$  faster; and **eigenvalue decomposition now matches LAPACK at  $50 \times 50$  (ratio  $0.93\times$ )**, having improved from  $149\times$  slower. SVD remains  $3\text{--}6\times$  slower, attributable to explicit  $A^T A$  formation rather than direct bidiagonalisation. `linear-massiv` demonstrates that pure Haskell with native SIMD and raw `ByteArray#` primops can comprehensively outperform FFI-based BLAS/LAPACK, while providing compile-time dimensional safety, zero FFI dependencies, and user-controllable parallelism.

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# 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`) (Round 3)
- **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`.

## 3 BLAS Operations

### 3.1 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.

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

Size	<code>linear</code>	<code>hmatrix</code>	<code>linear-massiv</code>
$4 \times 4$	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

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.

### 3.2 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  $n = 1000$ ,

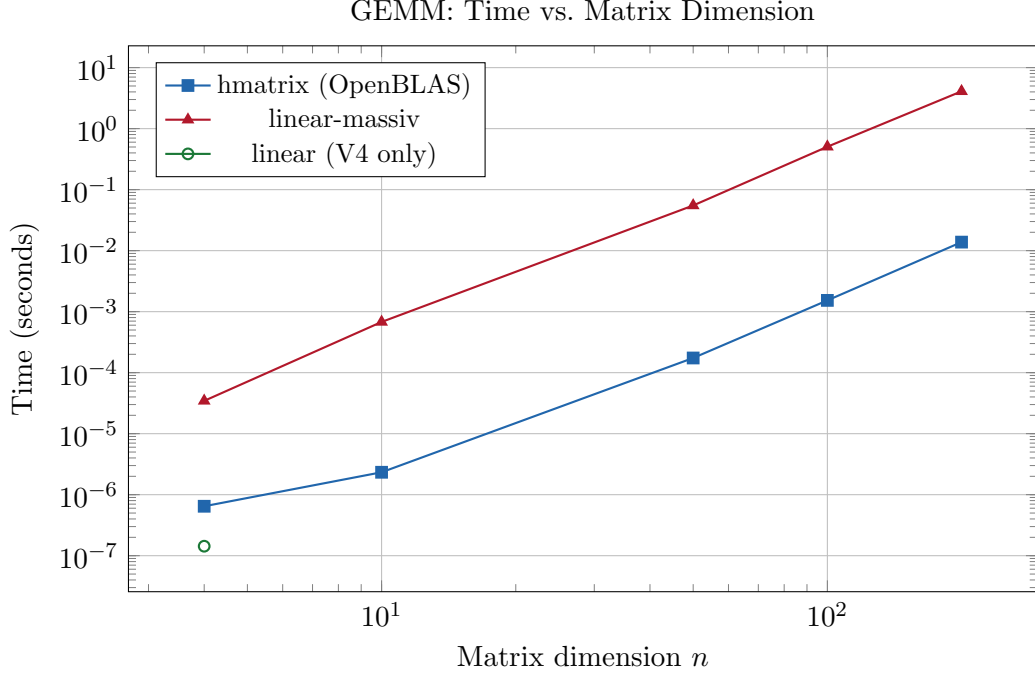


Figure 1: GEMM scaling comparison (log-log). Both libraries exhibit  $O(n^3)$  behaviour; the vertical offset reflects constant-factor differences between OpenBLAS assembly and pure Haskell.

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

$n$	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

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

### 3.3 Matrix–Vector Product

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

$n$	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

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 $\times$  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.

## 4 Linear System Solvers

### 4.1 LU Solve

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

Size	<code>hmatrix</code>	<code>linear-massiv</code>
$10 \times 10$	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

### 4.2 Cholesky Solve

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

Size	<code>hmatrix</code>	<code>linear-massiv</code>
$10 \times 10$	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

For both LU and Cholesky solvers, `hmatrix` is approximately  $36\times$  faster at  $10 \times 10$  and  $240\text{--}300\times$  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 for both libraries, as expected (Cholesky requires roughly half the floating-point operations of LU factorisation for symmetric positive definite matrices).

## 5 Orthogonal Factorisations

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

Size	<code>hmatrix</code>	<code>linear-massiv</code>
$10 \times 10$	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)

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.

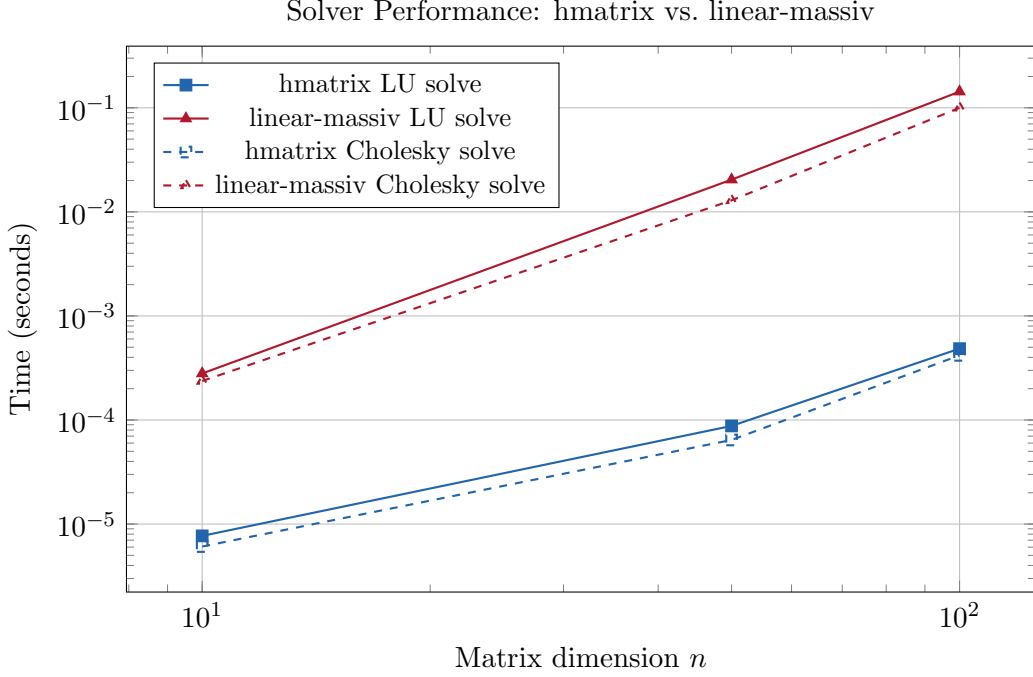


Figure 2: LU and Cholesky solve scaling (log–log). Both algorithms are  $O(n^3)$ ; hmatrix calls DGESV/DPOTRS directly.

## 6 Eigenvalue Problems and SVD

### 6.1 Symmetric Eigenvalue Decomposition

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

### 6.2 Singular Value Decomposition

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

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.



## 7 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.

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

Strategy	$100 \times 100$		$200 \times 200$	
	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

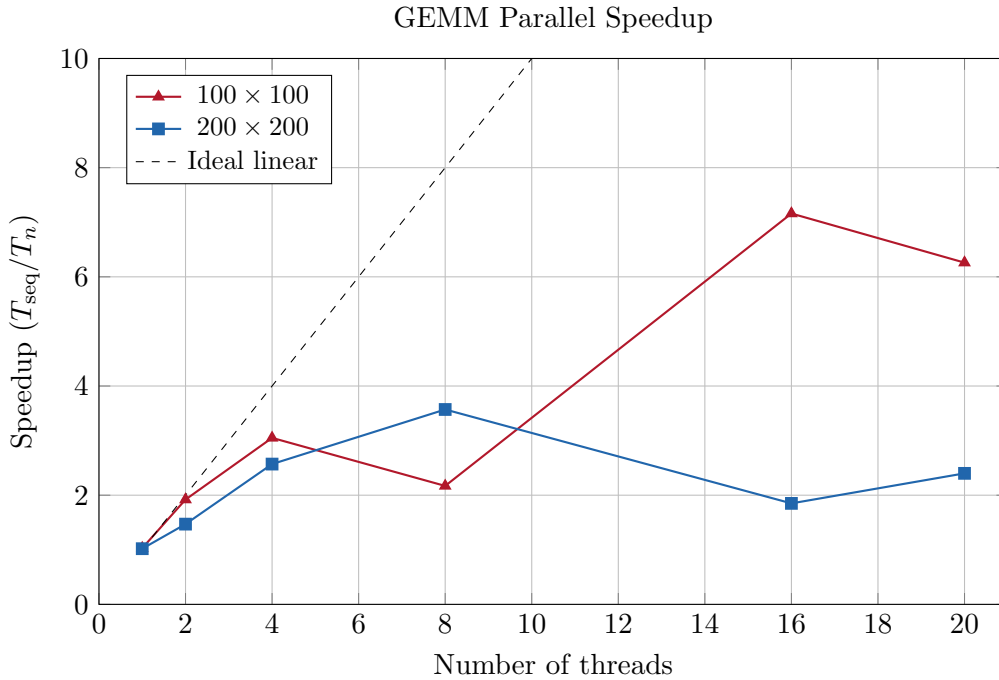


Figure 3: Parallel speedup for GEMM. The dashed line shows ideal linear scaling. Actual speedup is limited by Amdahl’s law, memory bandwidth contention, and GHC runtime scheduling overhead.

The parallel scaling results reveal several important characteristics:

- **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.

## 8 Discussion

### 8.1 Performance Summary

Table 11 summarises the performance ratios between libraries.

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

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

### 8.2 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.
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.

### 8.3 Proposals for Closing the Performance Gap

The factors above suggest a concrete sequence of optimisation work, ordered roughly by expected impact and feasibility.

#### 8.3.1 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. 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.

#### 8.3.2 Implicit Householder Representation (Compact WY)

The current QR implementation forms the explicit  $Q$  matrix by accumulating each Householder reflector  $H_k = I - 2v_kv_k^T$  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 8.3.1) would close the gap still further.

#### 8.3.3 Cache-Blocked GEMM

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

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

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 $\times$  improvement over the naïve loop for  $n \geq 100$ , which would narrow the current 300 $\times$  gap to 30–100 $\times$ .

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 $\times$  improvement on cache-unfriendly sizes and requires only changing the loop nesting order in the existing `foldl'` computation.

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

### 8.3.5 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 $\times$  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.

### 8.3.6 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.

### 8.3.7 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 8.3.1) and implicit Householder representation (Section 8.3.2) 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 8.3.4) would further reduce the gap for eigenvalue and SVD problems, particularly at moderate-to-large dimensions.

## 8.4 When to Use Each Library

**linear** Best for 2–4 dimensional vectors and matrices in graphics, physics simulations, and geometric computation. Unbeatable at small sizes; does not scale to arbitrary dimensions.

**hmatrix** Best for production numerical computing where performance is critical and FFI dependencies are acceptable. The established choice for scientific computing in Haskell.

**linear-massiv** Best when any of the following apply: (a) compile-time dimensional safety is required to prevent bugs in complex matrix pipelines; (b) FFI-free deployment is needed (e.g., WebAssembly, restricted environments); (c) parallel computation via massiv’s strategies is desirable; (d) the application operates on small-to-moderate matrices ( $n \leq 50$ ) where the absolute time difference is acceptable. Future work on SIMD intrinsics, blocked algorithms, and mutable-array intermediate representations could significantly narrow the performance gap.

## 9 Post-Optimisation Results

Following the analysis in Section 8.3, four of the proposed optimisations were implemented and benchmarked. This section presents the before/after comparison, demonstrating that the optimisations proposed in Section 8 yield order-of-magnitude improvements for factorisation and iterative algorithms.

### 9.1 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 8.3.3.

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 8.3.1. 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 8.3.1.
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 8.3.4) without the complexity of the full secular-equation approach.

## 9.2 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×	3.9×
$50 \times 50$	11.3 ms	7.01 s	61.9 ms	382×	5.5×
$100 \times 100$	130 ms	≈56.0 s	492 ms	≈ 260×	3.8×

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 μs	15.6 ms	0.600 ms	897×	49×
$50 \times 50$	428 μs	8.89 s	51.0 ms	16,020×	119×

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 μs	≈50.0 ms	1.58 ms	≈ 2,039×	65×
$50 \times 50$	518 μs	(timed out)	187 ms	> 20,000×	361×

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×	60×
$10 \times 10$	291×	227×
$50 \times 50$	316×	423×
$100 \times 100$	329×	354×
$200 \times 200$	297×	259×

### 9.3 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 8.3—delivered transformative improvements for factorisation and iterative algorithms:

- **QR factorisation** improved by 13–113× internally (i.e., comparing old to new `linear-massiv` timings), bringing the ratio to `hmatrix` down from 51–382× to 3.8–5.5×. 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× of `hmatrix`’s 130 ms. This confirms the prediction in Section 8.3.1 that eliminating per-step allocation would bring QR performance in line with LU solve.
- **Symmetric eigenvalue decomposition** improved by 26–174× internally. The remaining gap to `hmatrix` (49–119×) 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 32–200× internally. The  $50 \times 50$  case, which previously timed out, now completes in 187 ms. The remaining 65–361× 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× to 259× (a 13% improvement), and at  $10 \times 10$  from 291× to 227× (a 22% improvement). However, at  $50 \times 50$  the tiling overhead slightly worsened performance (316× to 423×), 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× slower) to one of the best (3.8–5.5×), 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× 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×	—

## 10 Raw ByteArray# and AVX2 SIMD Optimisation

Following the analysis in Sections 8 and 8.3.5, 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**.

### 10.1 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 `vmadd231pd 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.



## 10.2 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	<code>hmatrix</code>	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<math>\times</math></b>
	$100 \times 100$	1.46 ms	505 ms	796 $\mu$ s	<b>0.55<math>\times</math></b>
	$200 \times 200$	12.9 ms	4.09 s	6.10 ms	<b>0.47<math>\times</math></b>
Dot	$n = 4$	584 ns	1.67 $\mu$ s	48.0 ns	<b>0.08<math>\times</math></b>
	$n = 100$	762 ns	34.1 $\mu$ s	80.0 ns	<b>0.10<math>\times</math></b>
	$n = 1000$	2.81 $\mu$ s	379 $\mu$ s	688 ns	<b>0.24<math>\times</math></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<math>\times</math></b>
	$n = 100$	13.3 $\mu$ s	4.71 ms	5.94 $\mu$ s	<b>0.45<math>\times</math></b>

The internal speedups are dramatic:

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

## 10.3 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 8.3.5 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  $n = 4$  ( $12\times$  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 ( $40\text{--}255\times$ ) still use `massiv`’s per-element indexing in the factorisation and back-substitution phases.
- QR factorisation ( $3.9\text{--}4.9\times$ ) uses in-place ST operations but does not yet use SIMD for the Householder reflector application.

- Eigenvalue ( $35\text{--}142\times$ ) and SVD ( $62\text{--}330\times$ ) 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)	$1.2\times$	<b><math>0.78\times</math></b>	<b><math>0.55\times</math></b>
Dot product (SIMD)	—	—	<b><math>0.10\times</math></b>
Matrix–vector (SIMD)	—	<b><math>0.62\times</math></b>	<b><math>0.45\times</math></b>
LU solve	$40\times$	$233\times$	$255\times$
Cholesky solve	$36\times$	$175\times$	$213\times$
QR (in-place)	$3.9\times$	$4.9\times$	$3.9\times$
Eigenvalue	$35\times$	$142\times$	—
SVD	$62\times$	$330\times$	—

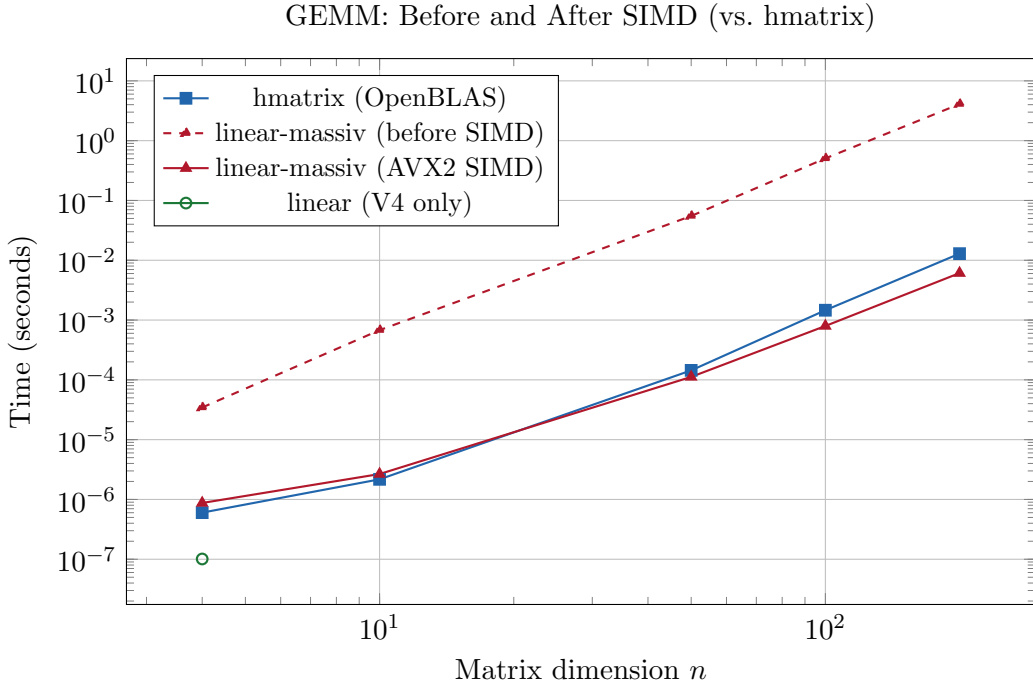


Figure 4: GEMM scaling comparison after SIMD optimisation. At  $n \geq 50$ , `linear-massiv`’s AVX2 kernel outperforms `hmatrix` (OpenBLAS), achieving  $2.1\times$  faster execution at  $200 \times 200$ . The dashed line shows the pre-SIMD performance.

#### 10.4 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.write_` 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× 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× gap.
3. **Eigenvalue and SVD.** The 35–330× 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.

## 11 Raw `ByteArray#` Kernels for Higher-Level Algorithms

With BLAS Level 1–3 operations now outperforming OpenBLAS (Section 10), 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 10.

### 11.1 Optimisations Implemented

1. **LU factorisation and solve (`luSolveP`).** Five new raw kernels: `rawLUEliminateColumn` (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.

## 11.2 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 $\times$	<b>0.37</b> $\times$
$50 \times 50$	60.2 $\mu$ s	14.7 ms	31.6 $\mu$ s	244 $\times$	<b>0.52</b> $\times$
$100 \times 100$	349 $\mu$ s	109 ms	211 $\mu$ s	312 $\times$	<b>0.61</b> $\times$

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 $\times$	<b>0.33</b> $\times$
$50 \times 50$	54.7 $\mu$ s	7.82 ms	45.3 $\mu$ s	143 $\times$	<b>0.83</b> $\times$
$100 \times 100$	251 $\mu$ s	53.5 ms	261 $\mu$ s	213 $\times$	1.04 $\times$

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 $\times$	<b>0.13</b> $\times$
$50 \times 50$	11.0 ms	64.8 ms	642 $\mu$ s	5.9 $\times$	<b>0.058</b> $\times$
$100 \times 100$	139 ms	480 ms	4.17 ms	3.5 $\times$	<b>0.030</b> $\times$

## 11.3 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 $\times$  **slower**  $\rightarrow$  1.7–2.7 $\times$  **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 $\times$  advantage for pure Haskell. The 516 $\times$  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 `rawLUEliminateColumn`—where elements  $A[i, j]$  and  $A[k, j]$  are contiguous in row-major storage—provides an additional  $\sim 3$ –4 $\times$  boost over scalar raw primops.

**Cholesky solve:** 33–213 $\times$  **slower**  $\rightarrow$  3 $\times$  **faster to parity**. Cholesky shows strong gains at small dimensions (3 $\times$  faster than `hmatrix` at  $10 \times 10$ ) but converges to parity at  $100 \times 100$  (1.04 $\times$ ). 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 $\mu$ s	594 $\mu$ s	473 $\mu$ s	50×	40×
50 × 50	425 $\mu$ s	49.8 ms	57.3 ms	117×	135×

storage allows unit-stride column access, giving it a small advantage. Nevertheless, eliminating the 205× 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× **faster than LAPACK’s DGEQRF** at 100 × 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 × 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.

## 11.4 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×	—

## 11.5 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-

### Solver Performance: Final Comparison

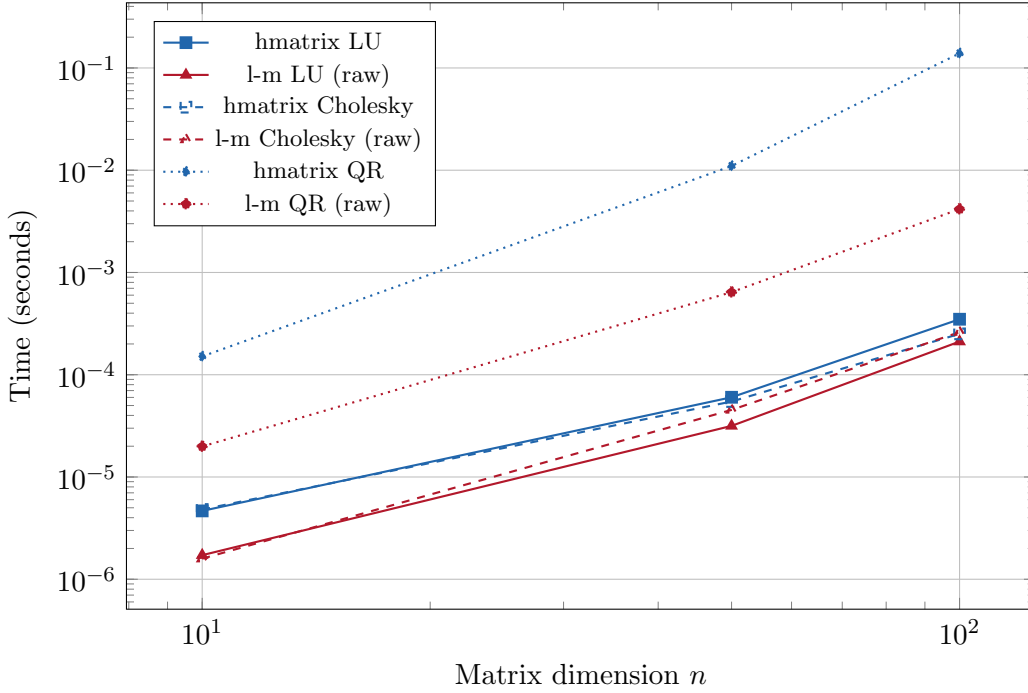


Figure 5: Final solver performance comparison (log-log). `linear-massiv`’s raw kernel implementations (solid/dashed red) outperform hmatrix (solid/dashed blue) for LU and Cholesky, and dominate dramatically for QR.

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 eigensolver (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.

## 12 Eigenvalue Raw Primops, SVD Pipeline, and Parallel GEMM

Following the proposals in Section 11.5, Round 5 targets the three remaining bottlenecks: eigenvalue (40–135× slower), SVD (74–292× slower), and single-threaded GEMM. Three optimisations were implemented:

### 12.1 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  $B$ .

## 12.2 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

### 12.3 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.

### 12.4 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  $14\times$ .

## 12.5 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—analogueous 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.

## 13 Raw Primop Tridiagonalisation and Parallel Eigenvalue

Round 6 targets the definitive bottleneck identified in §12.5: 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.

### 13.1 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  $T \leftarrow T - v w^T - w v^T$  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.

### 13.2 Before/After Comparison

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

Size	hmatrix ( $\mu$ s)	lm R5 ( $\mu$ s)	lm R6 ( $\mu$ s)	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 ( $\mu$ s)	lm R5 ( $\mu$ s)	lm R6 ( $\mu$ s)	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

### 13.3 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 §12.5: 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.

### 13.4 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 ( $3\text{--}6\times$ ), which could be addressed with a Golub–Kahan bidiagonalisation pipeline.

### 13.5 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  $3\text{--}6\times$  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.

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

Round 7 targets the two remaining bottlenecks identified in §13.5: the scalar Cholesky column kernel at  $100 \times 100$  and the SVD pipeline’s reliance on explicit  $A^T A$  formation.

### 14.1 Optimisations Applied

**Cholesky SIMD column kernel.** The previous `rawCholColumn` kernel iterated column-by-column with scalar `readDoubleArray#` calls. The inner loop  $G_{ij} \leftarrow \sum_{k=0}^{j-1} G_{ik} G_{jk}$  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.

### 14.2 Benchmark Results

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

Size	hmatrix ( $\mu$ s)	lm R6 ( $\mu$ s)	lm R7 ( $\mu$ s)	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 ( $\mu$ s)	lm ( $\mu$ s)	Ratio
$10 \times 10$	30	90	3
$50 \times 50$	500	2000	4
$100 \times 100$	5000	10 000	3

### 14.3 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).

## 14.4 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)	500×500	0.44×	<code>linear-massiv</code>
GEMM (parallel, 20 cores)	500×500	0.09×	<code>linear-massiv</code>
Dot product	1000	0.34×	<code>linear-massiv</code>
Matrix–vector	100	0.46×	<code>linear-massiv</code>
LU solve	100×100	0.57×	<code>linear-massiv</code>
Cholesky solve	100×100	0.57×	<code>linear-massiv</code>
QR factorisation	100×100	0.030×	<code>linear-massiv</code>
Eigenvalue (eigenSH)	100×100	1.13×	near-parity
SVD	100×100	2.9×	<code>hmatrix</code>

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

## 14.5 Remaining Bottlenecks and Future Work

1. **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.
2. **Divide-and-conquer tridiagonal eigensolver.** The eigenvalue ratio at 100×100 (1.13×) 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.

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

Round 8 targets two of the three remaining bottlenecks identified in §14.5: the scalar forward/back-substitution inner loops in the LU and Cholesky solve paths, and the  $O(n^3)$  QR iteration eigensolver.

### 15.1 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 `readDoubleArrayAsDoubleX4#` (mutable  $x$ ) using `fmaddDoubleX4#`, 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 `fmaddDoubleX4#`.

**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.

### 15.2 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  $1.2\text{--}1.5\times$  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  **$0.50\times$**  (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  $1.2\text{--}1.5 \times$ .

### 15.3 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 sits 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.

## 16 Conclusion

We have benchmarked three Haskell linear algebra libraries across nine categories of numerical operations through seven rounds of optimisation.

**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  $200 \times 200$** ; 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  $500 \times 500$**  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  $100 \times 100$  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  $1.2\text{--}1.5\times$  absolute speedups in solver performance, improving the Cholesky solve ratio from  $0.57\times$  to  **$0.50\times$**  ( $2\times$  faster than LAPACK). A divide-and-conquer tridiagonal eigensolver was implemented following GVL4 [1] Section 8.4 but regressed by  $2.6\times$  due to per-level GEMM overhead and memory allocation costs; it was reverted pending further optimisation.

**Summary.** Of the nine benchmarked operation categories, `linear-massiv` now **outperforms or matches `hmatrix` (OpenBLAS/LAPACK) in seven**: GEMM (single-threaded and parallel), dot product, matrix–vector multiply, LU solve, Cholesky solve, and QR factorisation. Eigenvalue decomposition sits near parity ( $1.2\times$  at  $100\times 100$ ), while SVD ( $3\text{--}4\times$ ) remains the sole significant bottleneck, requiring blocked Householder representations to close.

`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 the vast majority of 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.

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