# Blocked Algorithms for the Matrix Square Root


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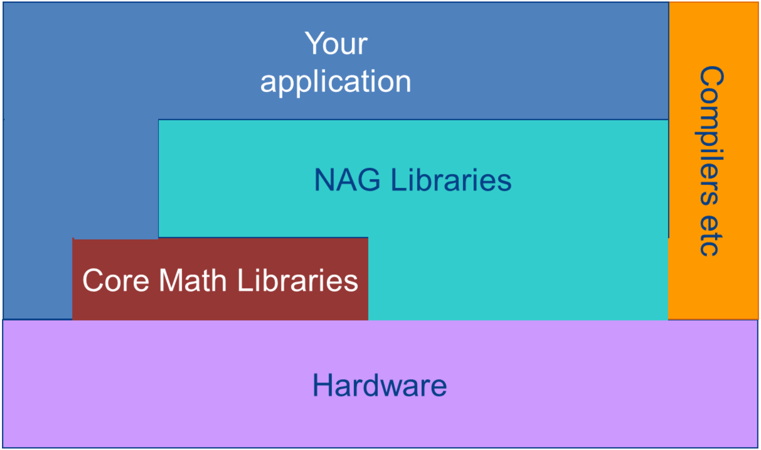
# Outline

1. Numerical Libraries and NAG
2. The Matrix Square Root:
    - Definition and Uses
    - The Schur Method
    - Blocking
    - Parallelism
3. Implementation of Algorithms in Numerical Libraries

# Why use numerical libraries?

- Numerical computation is difficult to do accurately.
- Writing routines from scratch is time consuming.
- Commonly encountered problems:
  - Overflow/underflow: how does the computer deal with large / small numbers?
  - Condition: how sensitive is the solution to small changes in the input?
  - Stability: how sensitive is the computation to rounding errors?
- Important considerations:
  - Error analysis.
  - Information about error bounds.
  - Parallelism.

# How a numerical library is used



# The NAG Library

- Root Finding
- Summation of Series
- Quadrature
- Ordinary Differential Equations
- Partial Differential Equations
- Numerical Differentiation
- Integral Equations
- Mesh Generation
- Interpolation
- Curve and Surface Fitting
- Optimization
- Approximations of Special Functions
- Dense Linear Algebra
- Sparse Linear Algebra
- Correlation & Regression Analysis
- Multivariate Methods
- Analysis of Variance
- Random Number Generators
- Univariate Estimation
- Nonparametric Statistics
- Smoothing in Statistics
- Contingency Table Analysis
- Survival Analysis
- Time Series Analysis
- Operations Research

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- If $A$ has $m$ Jordan blocks and $s \le m$ distinct eigenvalues then there are $2^s$ square roots that are primary functions of $A$.
- If $A$ has no eigenvalues on the negative real line, then there is a unique *principal square root* $A^{1/2}$ with eigenvalues in the right half plane.

# Defining the Matrix Square Root: Example

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# Uses of the Matrix Square Root

- Markov models of finance and population dynamics:
  - If $P(t)$ is the transition matrix for a time step $t$, then $\sqrt{P}$ could be used for $\frac{t}{2}$.
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- Polar decomposition / matrix sign decomposition.
- Important kernel routine for computing matrix logarithm, $p$th roots and powers and trigonometric matrix functions.

# The Schur Method

1. Compute a Schur decomposition: $A = QTQ^*$ with $T$ upper triangular.
2. Expand $U^2 = T$ elementwise. For a primary square root, $U$ is also upper triangular:

$$U_{ii}^2 = T_{ii},$$

$$U_{ii}U_{ij} + U_{ij}U_{jj} = T_{ij} - \sum_{k=i+1}^{j-1} U_{ik}U_{kj}.$$

   $U$ is found either a column or a superdiagonal at a time.
3. $\sqrt{A} = QUQ^*$

# The Schur Method: Properties

- Cost: $28\frac{1}{3}n^3$ flops.
- Real arithmetic version uses quasi upper triangular Schur decomposition and $2 \times 2$ diagonal block structure.
- Computed square root of the triangular matrix $\hat{U}$ satisfies $\hat{U}^2 = T + \Delta T$, where

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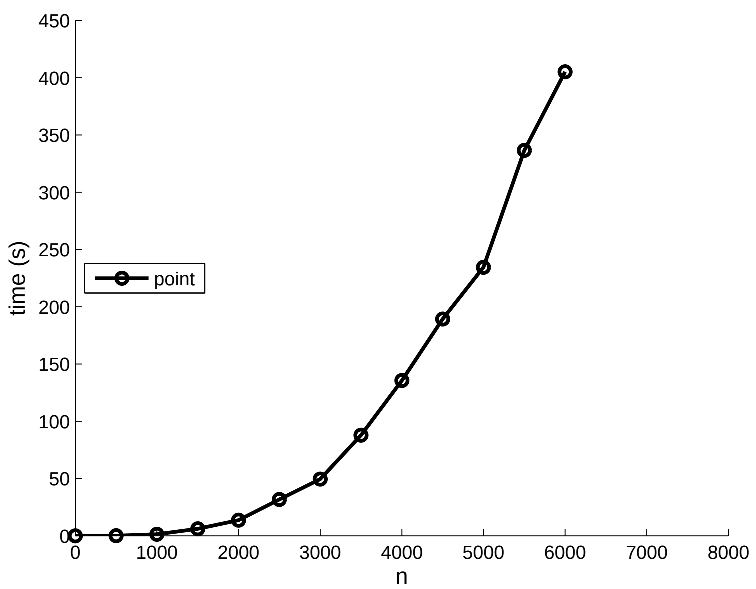
  (this only holds normwise in the real arithmetic version).
- No use of level 3 BLAS - slow!
- Now focus on the triangular phase of the algorithm.

# Run times for random complex triangular matrices



# The Blocked Schur Method

- The $U_{ij}$ and $T_{ij}$ are now taken to be blocks:

$$U_{ii}^2 = T_{ii}, \tag{1}$$

$$U_{ii}U_{ij} + U_{ij}U_{jj} = T_{ij} - \sum_{k=i+1}^{j-1} U_{ik}U_{kj}. \tag{2}$$

- Solve (1) using the point method and (2) by solving the Sylvester equation (e.g. xTRSYL in LAPACK).

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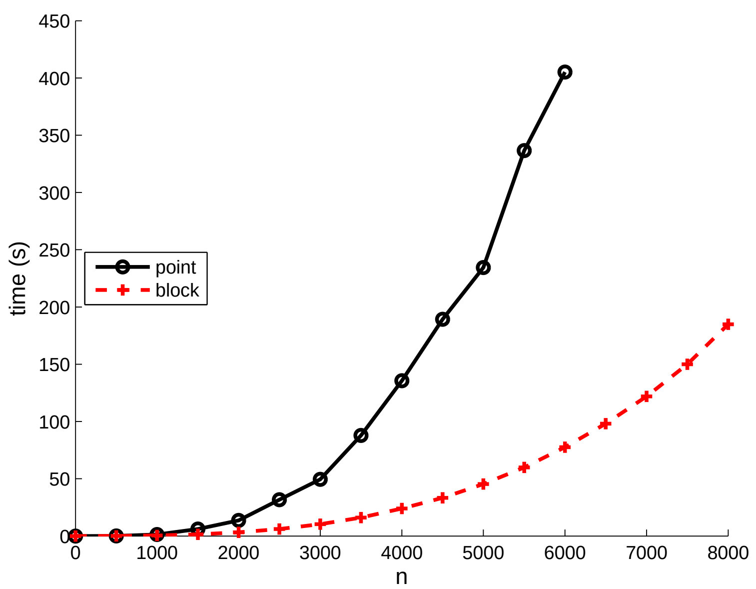
- Solve (1) using the point method and (2) by solving the Sylvester equation (e.g. xTRSYL in LAPACK).
- Same error bounds hold true.
- Over 90% of run time spent in GEMM calls and 8% in Sylvester equation solution.
- Not very sensitive to block size or choice of kernel routines.

# Run times for random complex triangular matrices



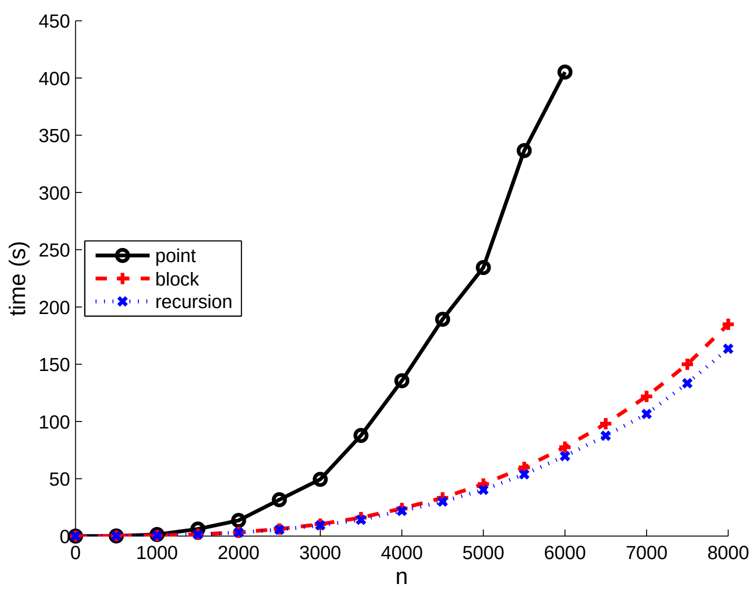
# The Recursive Blocked Schur Method

- Recursive solution of the triangular phase:

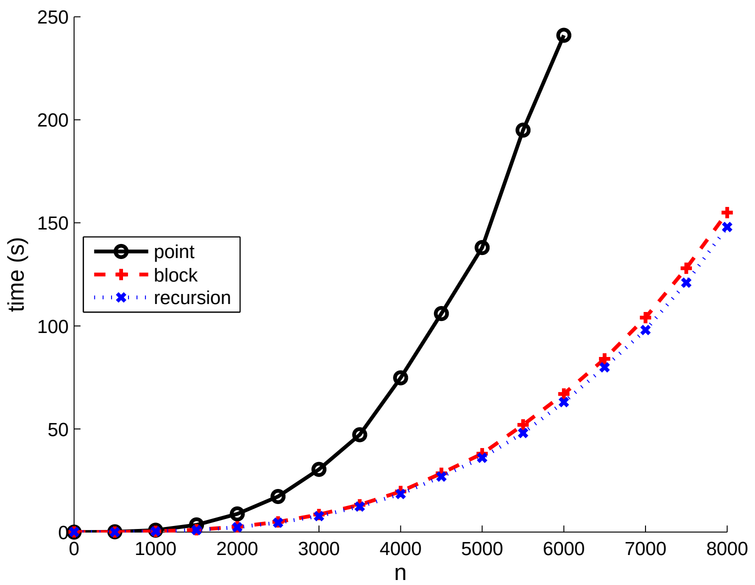
$$\begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix}^2 = \begin{pmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{pmatrix}.$$

  $U_{11}^2 = T_{11}$ and $U_{22}^2 = T_{22}$ are solved recursively.
- Solve $U_{11}U_{12} + U_{12}U_{22} = T_{12}$ using the recursive method of Jonsson & Kågström.
- 'Point' algorithms are used when the recursion has reached a certain size (e.g. $n = 64$).
- Same error bound holds as point algorithm (proof by induction).

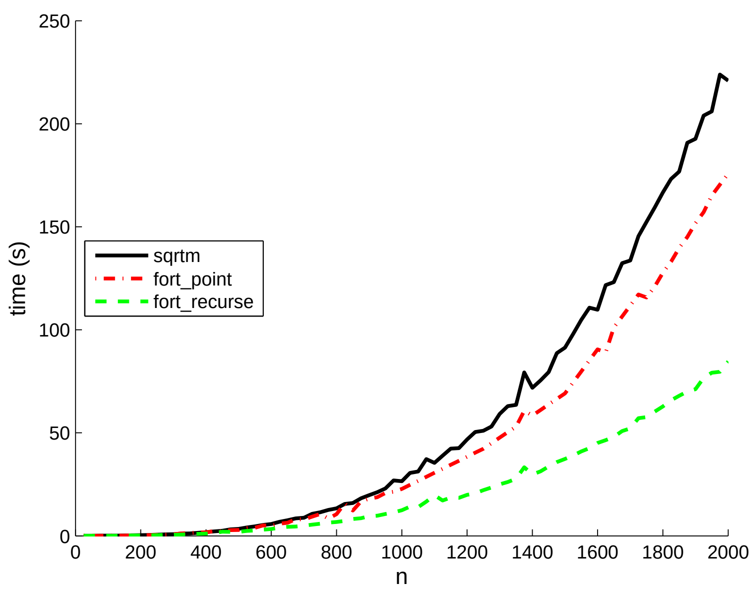
# Run times for random complex triangular matrices



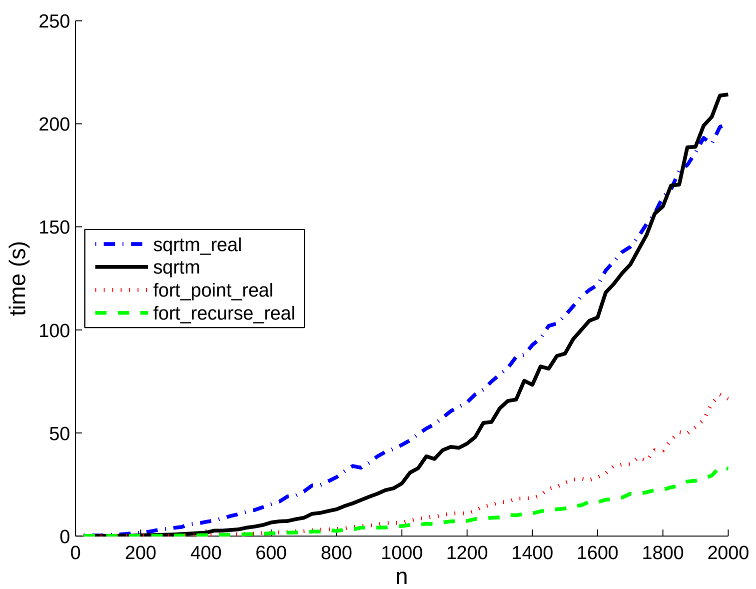
# Aside: multiplying two triangular matrices



# Full complex matrices (called from MATLAB)



# Full real matrices (called from MATLAB)



# Parallelism

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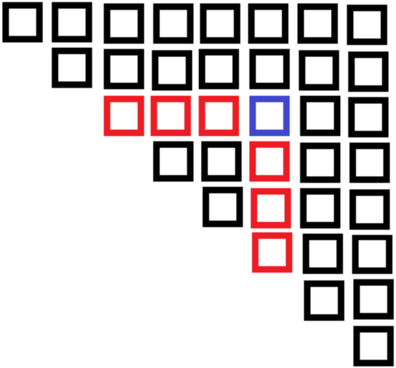
Options for parallelism:

- Threaded BLAS.
- Explicit loop-based parallelism of the triangular phase.
- OpenMP tasks.

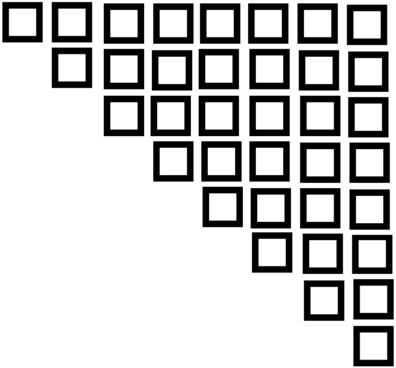
# Parallel Point and Block Methods

Blocks below and left of $(i, j)$ block must be computed first:



# Parallel Point and Block Methods

Synchronisation required after each superdiagonal:



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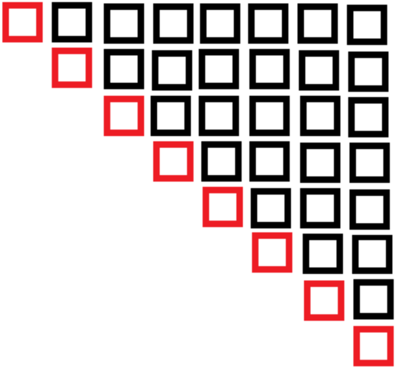

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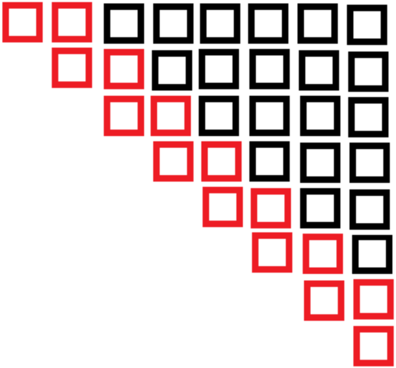

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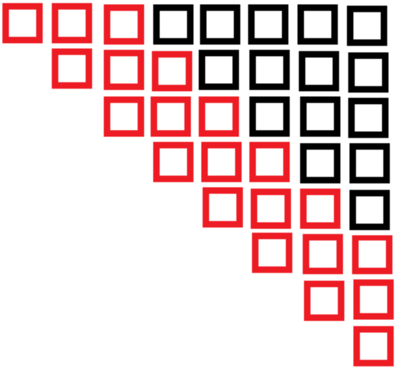
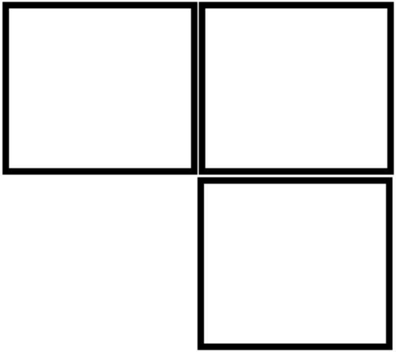


# Recursive Blocking in Parallel

Task based approach - each recursive call generates new tasks. Synchronization points required:



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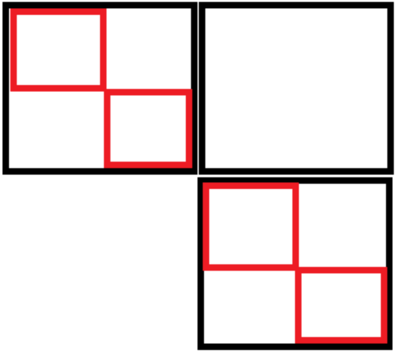

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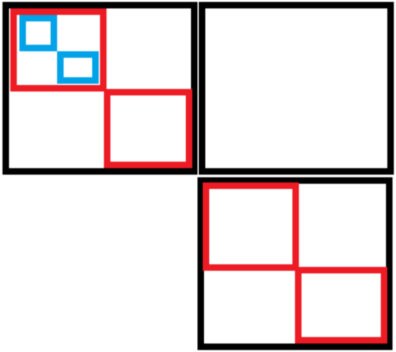

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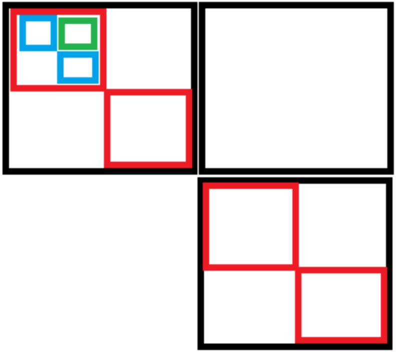

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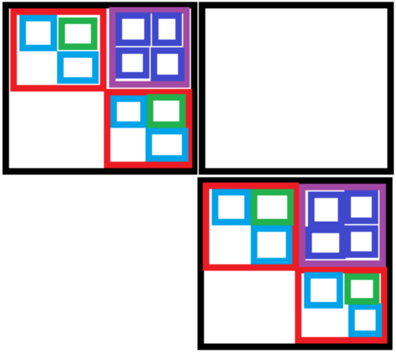
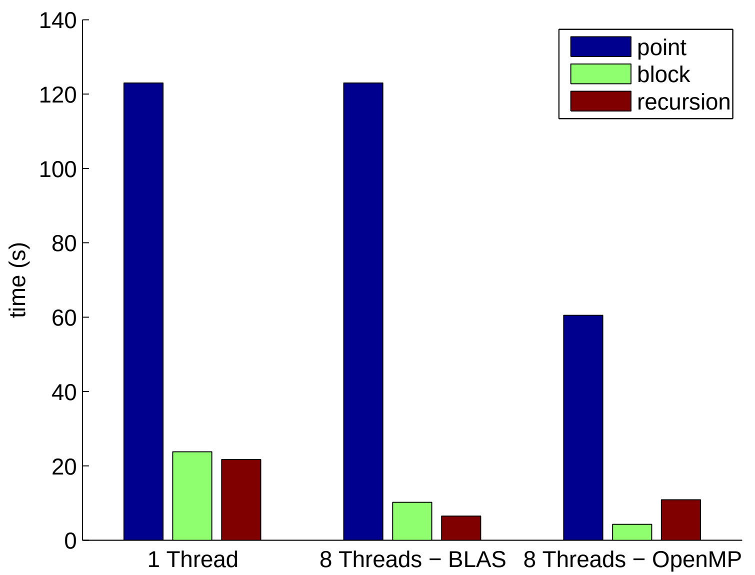
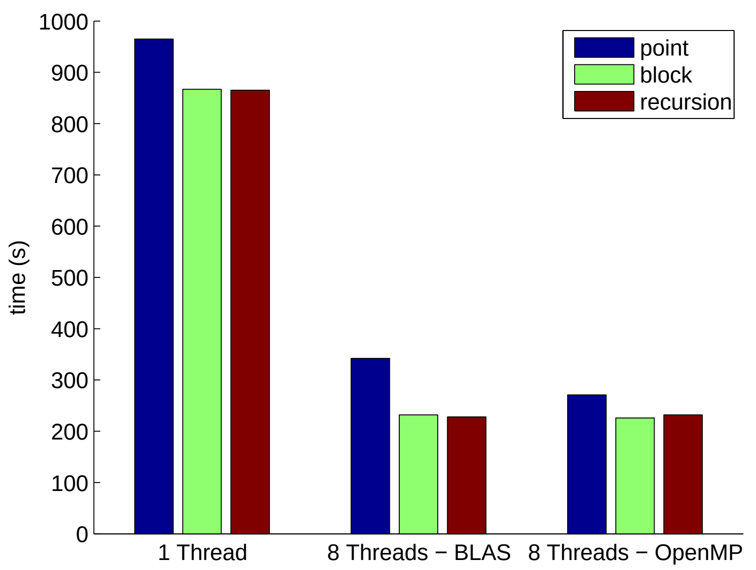


# Parallel Results for 4000 $\times$ 4000 Triangular Matrices



# Parallel Results for 4000 × 4000 Full Matrices



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- Condition estimation:
  - Condition number estimates and residual bounds are available for the matrix square root.
  - Condition number is expensive to compute.

# Implementation for the NAG Library

- Real and complex routines, with or without condition estimation, and extra routines specifically for triangular matrices.
- Test programs:
  - Check the residual $(\sqrt{A})^2 - A$ against the theoretical residual bound.
  - Test against computation in VPA using condition estimate.
  - Tricky test cases e.g. almost singular matrices, nearly negative eigenvalues.
  - Error exits and illegal inputs.

# Summary

- Recursive blocking can be fast, when the algorithm allows.
- NAG implementation uses OpenMP, so will use standard blocking.
- Matrix square root is a key computational kernel - BLAS?
- The fastest method in serial is not necessarily the fastest method in parallel.

# References

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