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Implementing a New Dense Symmetric Eigensolver using Mixed Precision Techniques on Multicore Systems with Hardware Accelerators

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Motivations

The importance of finding eigenvalues/eigenvectors arises from different scientific applications like quantum chemistry, quantum physics, the analysis of electrical networks, quantum mechanics, and statistics. Often their solutions comprise the most computationally expensive algorithmic components. It is essential that efficient solution techniques and high quality software are developed for the solution of eigenvalue problems on high performance computers. Several promising algorithms have been investigated in terms of accuracy and performance, such as the divide and conquer method (DSYEVD).

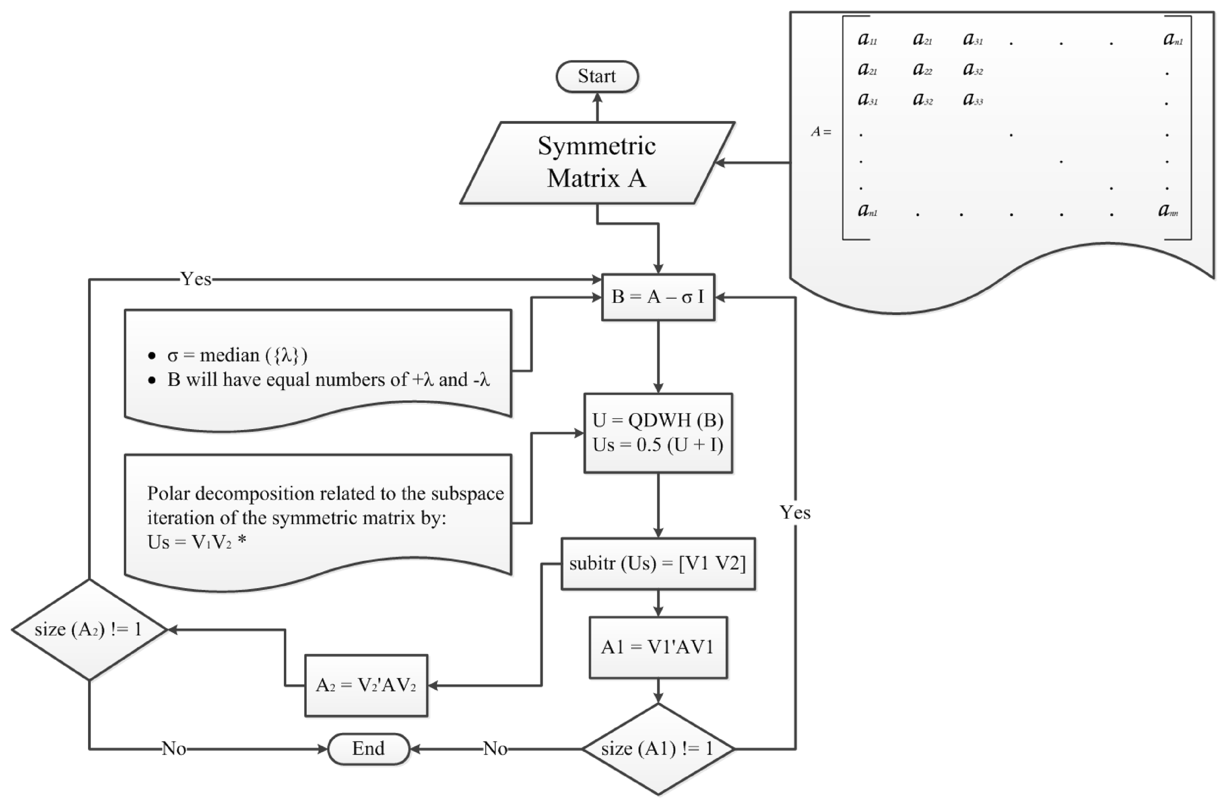
QDWHeig Eigensolver

Problem Definition: for a $n \times n$ real symmetric matrix A, the eigen decomposition is:

$$A = Q \Lambda Q^{\top},$$

where Λ is the matrix of all the eigenvalues, Q is the matrix of corresponding eigenvectors
QDWHeig Eigensolver:

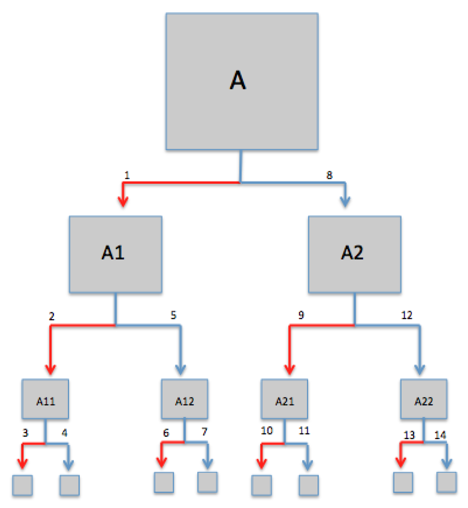
- QDWHeig is a spectral divide-and-conquer algorithm
- QDWHeig can easily be adjusted to find a portion of the spectrum
- Building blocks are matrix multiplication and QR, Cholesky factorization
- The main part of QDWHeig is the polar decomposition, which converges in at most 6 iterations



σ is estimated heuristically, as the median of diagonal elements.

Implementations

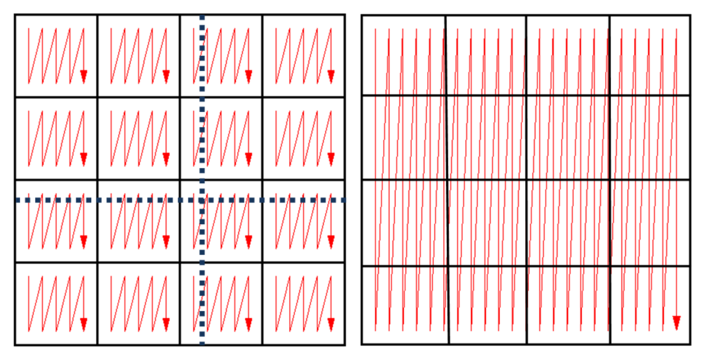
Recursive Formulation



QDWHeig is implemented using high performance kernels from:

- LAPACK library
- MAGMA: LAPACK for GPU's and multicore architectures
- PLASMA library with Naive, Tile and Tile_Async interfaces

	Algorithm	Storage
LAPACK	Block algorithm	CMDL
MAGMA	Block algorithm	CMDL
PLASMA	Tile algorithm	TDL



- We extend the existing PLASMA tile algorithms to run on top of column-major data layout
- We use mixed precision technique to find the polar decomposition

Environment Settings

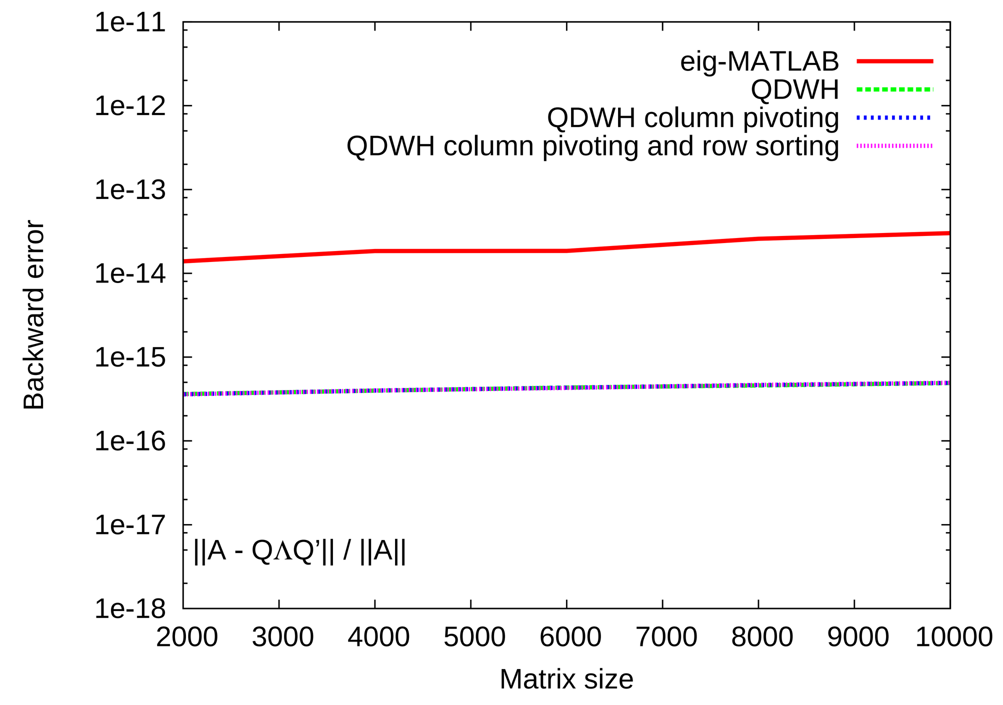
Software:

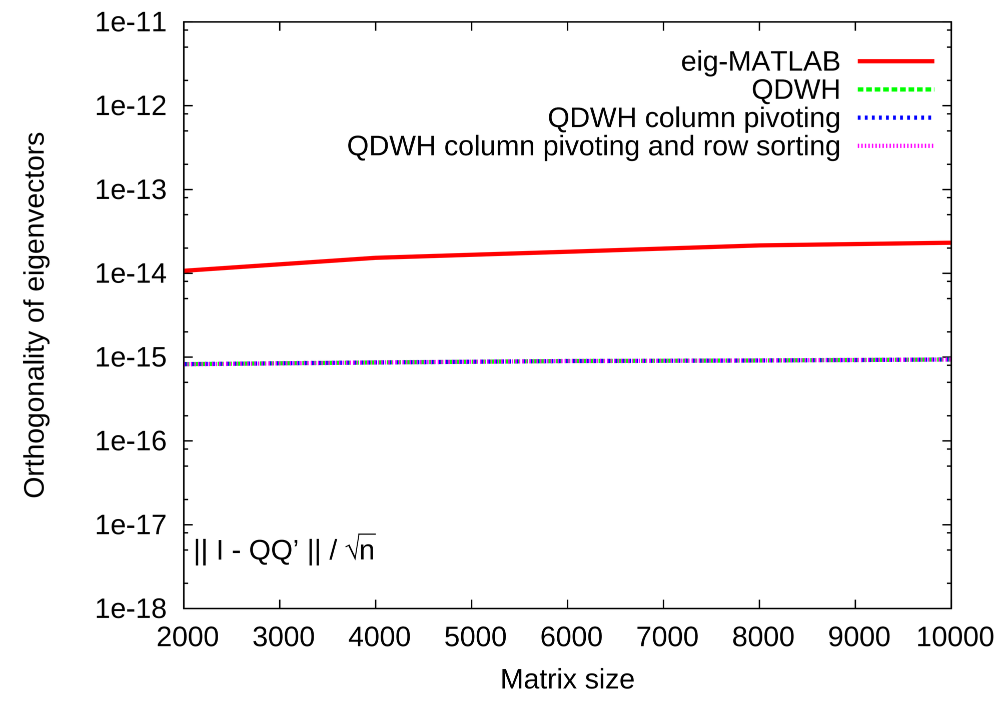
- Intel Compiler Suite 2013.1.117
- PLASMA 2.4.5, LAPACK 3.4.2, MAGMA 1.4.1(compiled w/-mkl=parallel)

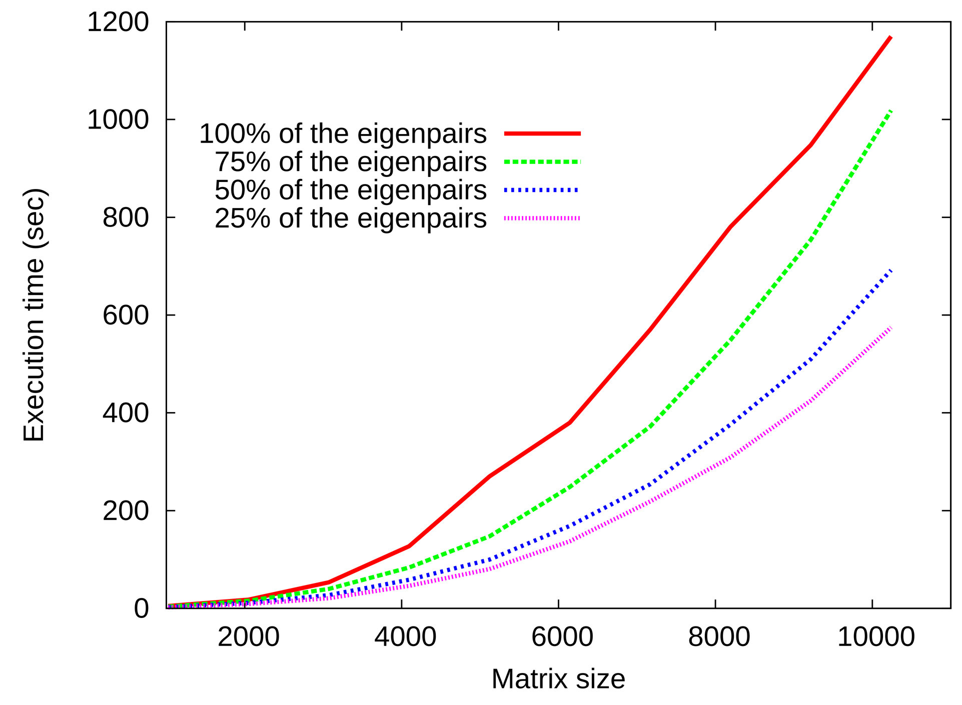
Hardware:

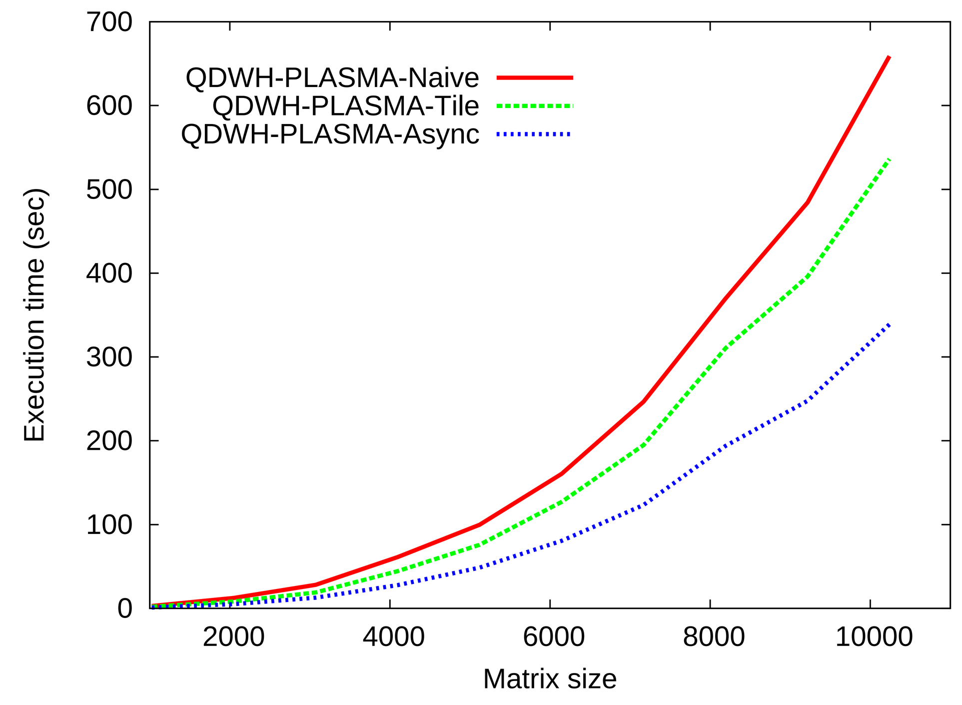
- Intel(R) Xeon(R) CPU E5-2650
- Dual-socket 8-core (16 cores total)
- 20M Cache, 2.00 GHz, 8.00 GT/s Intel(R) QPI
- Tesla K20c, 705.5 MHz clock, 6GB memory

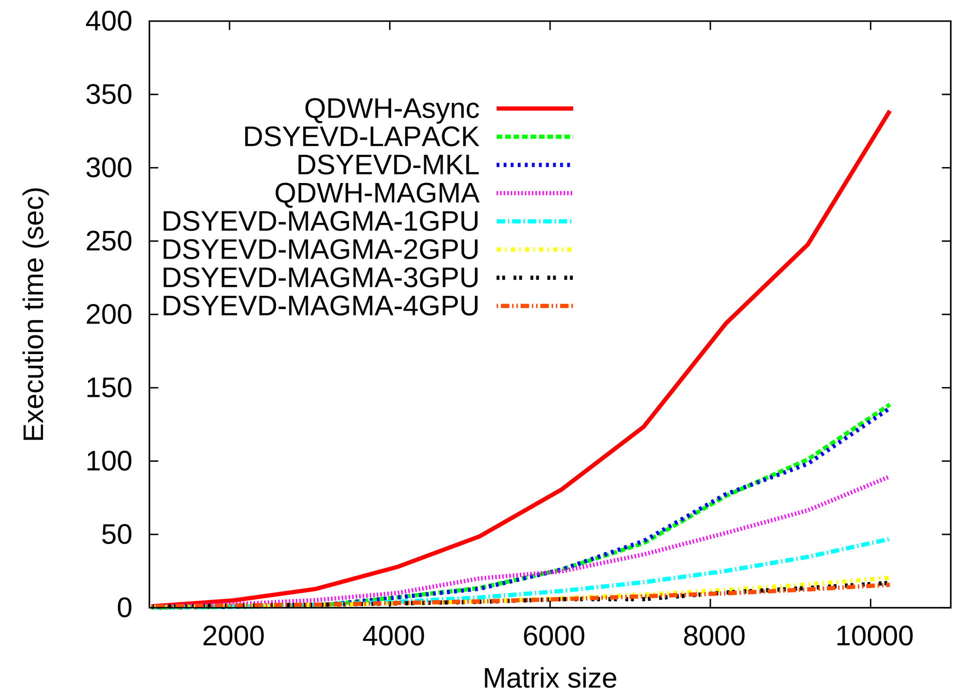
Numerical Accuracy and Performance Results

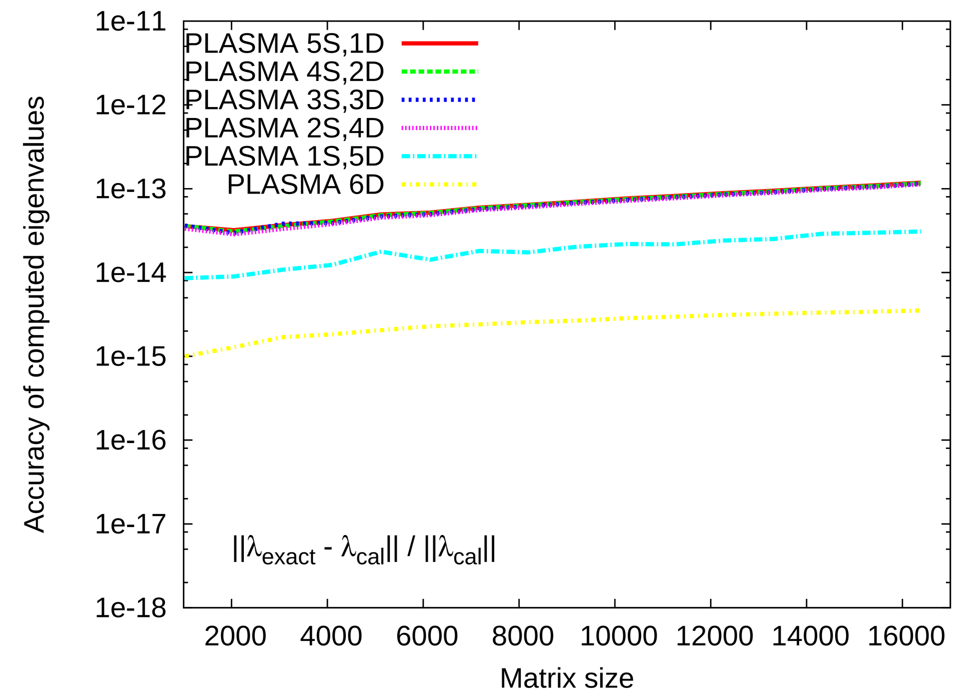












Future Research

- Implement QDWHeig using multi GPUs
- Implement QDWHeig using MORSE (Tile algorithm + GPU)
- Use the highly optimized Hierarchical QR (University of Colorado Denver) and 2.5D Matrix-Matrix multiplications (University of California Berkeley)
- Combine the depth-first version with a breadth-first of QDWHeig

References

[1] Y. Nakatsukasa and N. Higham. Stable and efficient spectral divide and conquer algorithms for the symmetric eigenvalue decomposition and the svd. *SIAM Journal on Scientific Computing*, 35(3):A1325–A1349, 2013.

[2] Emmanuel Agullo, Jim Demmel, Jack Dongarra, Bilel Hadri, Jakub Kurzak, Julien Langou, Hatem Ltaief, Piotr Luszczek, and Stanimire Tomov. Numerical linear algebra on emerging architectures: The plasma and magma projects. *Journal of Physics: Conference Series*, 180(1):012037, 2009.