

Overview

Eigenvalue problems arise in a number of SciDAC applications. We highlight some recent progress on 1) computing a large number eigenpairs of a Hermitian matrix in the context of density functional theory based electronic structure calculation 2) computing a few selected eigenpairs of a non-Hermitian matrix in the context of equation-of-motion coupled cluster (EOM-CC) calculation and complex scaling configuration interaction 3) computing the full spectrum of Bethe–Salpeter Hamiltonian matrix which has a special structure.

Computing a large invariant subspace of a Hermitian matrix

Motivation:

- Large-scale density functional theory based electronic structure calculations require computing a large number of lowest eigenpairs (10^3 pairs or more).
- Density functional perturbation theory requires many more lowest eigenpairs (10^3 - 10^5).

The challenge:

- Existing eigensolvers contain repeated calls of the Rayleigh–Ritz procedure that becomes a bottleneck when many eigenpairs are computed on a massively distributed-memory parallel machines.
- Standard computational kernels for solving dense eigenvalue problems (ScaLAPACK) do not scale beyond a certain number of cores.

Our goal:

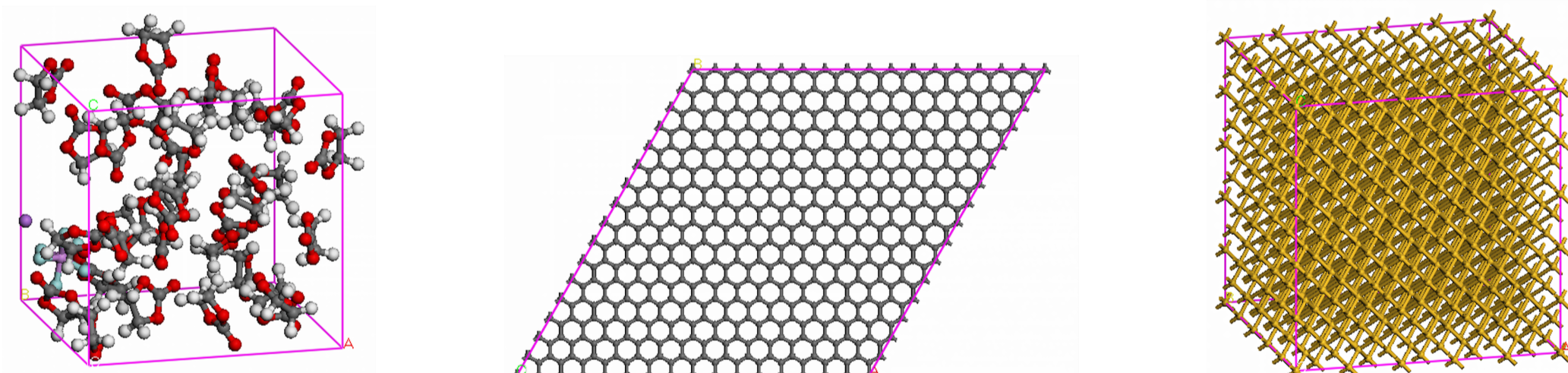
- Compute many lowest eigenpairs on massively parallel high performance computers.
- Avoid or reduce the amount of the RR computations.

The Projected Preconditioned Conjugate Gradient (PPCG) algorithm

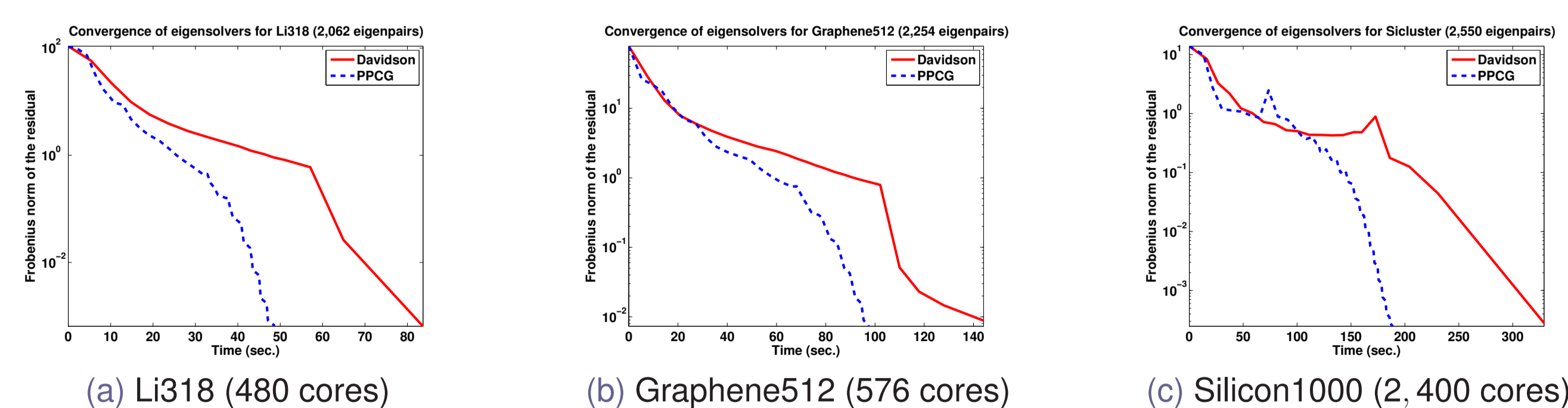
- The new eigensolver for computing large invariant subspaces of Hermitian matrices.
- The standard Rayleigh–Ritz procedure is replaced by a sequence of small dense eigenvalue problems plus the QR factorization of the approximate eigenspace.
- The Rayleigh–Ritz computation is performed only once every 5-10 iterations.
- Takes advantage of the available preconditioning techniques.
- Relatively easy to implement.
- The solver has been tested in within the Quantum Espresso and QBox electronic structure packages.

E. Vecharynski and C. Yang: *A Projected Preconditioned Conjugate Gradient Algorithm for Computing a Large Invariant Subspace of a Hermitian Matrix*, in preparation

Performance of the PPCG algorithm in Quantum Espresso

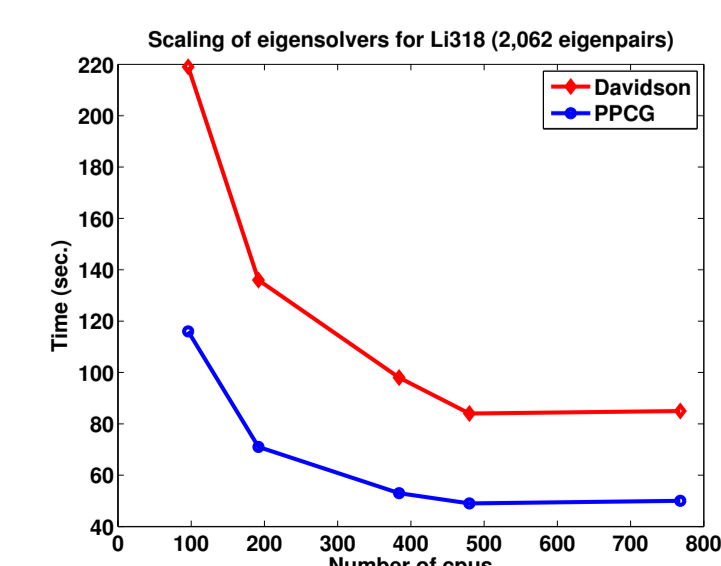


Benchmark systems: the solvation of LiPF₆ in ethylene carbonate and propylene carbonate liquids containing 318 atoms (left), the 16 by 16 supercell of graphene containing 512 carbon atoms (center), and 5 by 5 supercell of bulk silicon containing 1000 silicon atoms (right).



Performance profile

component	PPCG	Davidson
HX	10	6.4
RR	10	55
GEMM	15	10
Cholesky QR	6	0
Total	41	71.4



Non-Hermitian eigenvalue problems: applications and computational challenges

Computing a subset of eigenpairs closest to the given shift σ

- Electronic resonant states (method of complex coordinate rotation).
- Equation-of-motion coupled-cluster (EOM-CC) method.

Difficulties with the existing solution approaches

- Require inverting $A - \sigma I$ (“shift-and-invert”).
- Performance issues
 - Limited degree of parallelism (“one-by-one” eigenpair computation).
 - Failure to fully take advantage of BLAS3.
- Robustness issues.

Our goal:

- Develop a novel eigensolver that overcomes the known difficulties.

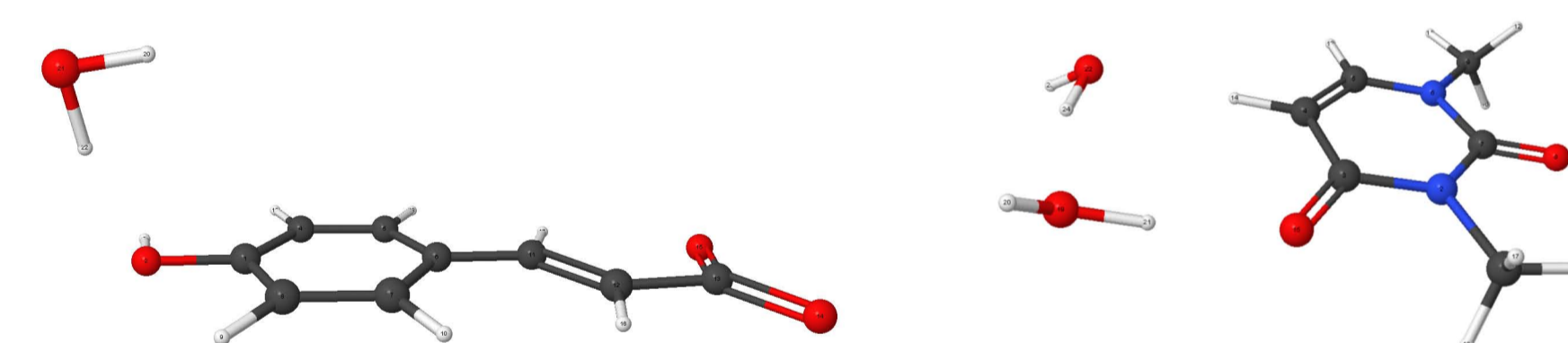
The Generalized Preconditioned Locally Harmonic Residual (GPLHR) method

- Uses the harmonic Rayleigh–Ritz procedure to extract approximate eigenpairs from low-dimensional search subspaces.
- Performs block iterations, effectively leverages BLAS3 kernels, provides multiple levels of concurrency.
- Takes advantage of the available preconditioning techniques.
- Robust, better convergence if memory is limited/tight.
- Provides an option of switching between the approximate eigenvector and Schur vectors iterations.

E. Vecharynski, F. Xue, and C. Yang: *Computing interior eigenpairs of non-Hermitian matrices*, in preparation

D. Zuev, E. Vecharynski, C. Yang, N. Orms, and A. I. Krylov: *New algorithms for iterative matrix-free eigensolvers in quantum chemistry*, J. Comp. Chem., submitted (2014)

GPLHR in Q-Chem: EOM-CC benchmark

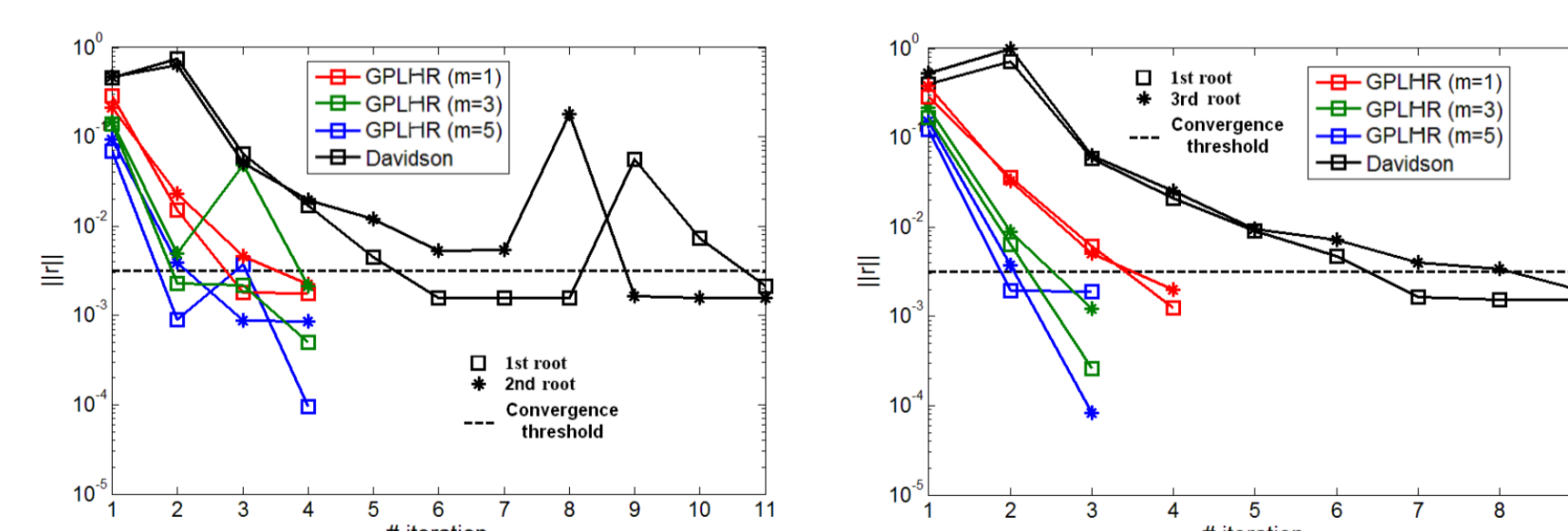


Benchmark systems: hydrated photoactive yellow protein chromophore PYPa-W_p (left) and dihydrated 1,3-dimethyluracil (mU)₂-(H₂O)₂ (right).

PYPa-W_p/6-31+G(d,p) GPLHR ($\sigma = 11$ a.u.)

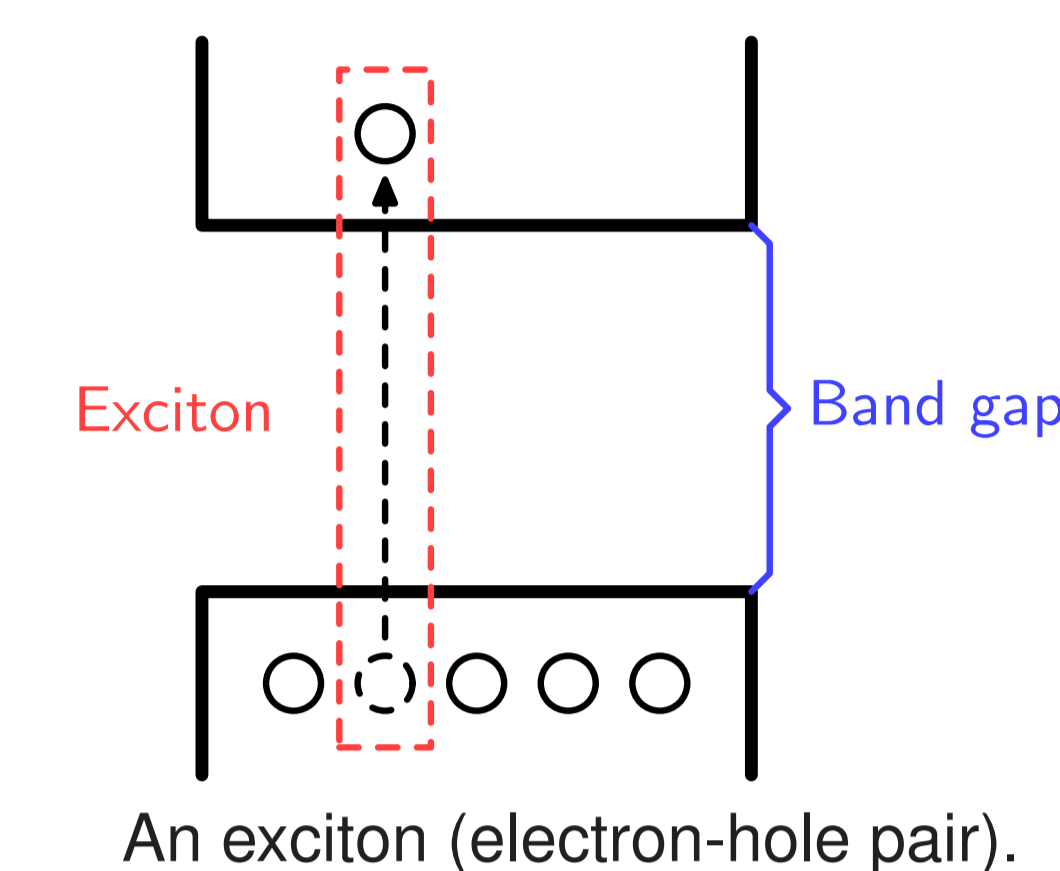
nroots ^a	niters ^b	m	Max. # of stored vectors	# matvec ^c
1	4	1	8	9
2	4	1	16	18
3	4	1	24	27
5	8	1	40	63

^a The number of requested eigenpairs. ^b The number of iterations to converge all eigenpairs. ^c The total number of matrix-vector multiplications. Davidson failed to deliver the solution.



Left: PYPa-W_p/6-31+G(d,p) for the pairs with converged energies of 4.11 and 4.20 eV;
Right: (mU)₂-(H₂O)₂/6-31+G(d,p) for the pairs with converged energies of 8.89 and 10.04 eV.

Computing all eigenpairs of the Bethe–Salpeter eigenvalue problem



Bethe–Salpeter eigenvalue (BSE) problem

- Exciton energies can be obtained by solving the Bethe–Salpeter eigenvalue problem $Hx = \lambda x$.
- We compute all eigenpairs of the complex Hamiltonian matrix

$$H = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix},$$

- where $A = A^* \in \mathbb{C}^{2n \times 2n}$ is Hermitian,
- $B = B^T \in \mathbb{C}^{2n \times 2n}$ is complex symmetric.
- The spectrum of H is symmetric w.r.t. real and imaginary axes.

Several existing candidates

- Hamiltonian QR algorithm
- Hamiltonian SR algorithm
- Hamiltonian Jacobi algorithm
- Embedding into a $4n \times 4n$ real Hamiltonian matrix

Difficulties

- None of above preserves the structure of the spectrum of H in floating-point arithmetic.
- Some are difficult to parallelize.

Our goal:

- Develop a fully structure-preserving parallel algorithm for BSE.

Ongoing work on a Cholesky-QR/Hamiltonian-URV method

Observations

- H is unitarily similar to

$$\hat{H} = \sqrt{-1} \begin{bmatrix} \text{Im}(A) + \text{Im}(B) & -\text{Re}(A) + \text{Re}(B) \\ \text{Re}(A) + \text{Re}(B) & \text{Im}(A) - \text{Im}(B) \end{bmatrix} = -\sqrt{-1} J_n (\tilde{A} + \tilde{B}),$$

where

$$J_n = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad \tilde{A} = \begin{bmatrix} \text{Re}(A) & \text{Im}(A) \\ -\text{Im}(A) & \text{Re}(A) \end{bmatrix}, \quad \tilde{B} = \begin{bmatrix} \text{Re}(B) & -\text{Im}(B) \\ -\text{Im}(B) & -\text{Re}(B) \end{bmatrix}.$$

Both \tilde{A} and \tilde{B} are real symmetric.

- $J_n(\tilde{A} + \tilde{B})$ is a $2n \times 2n$ real Hamiltonian matrix.
- In practice $\tilde{A} + \tilde{B}$ is often positive definite
- \leadsto all eigenvalues of H are real.

Key of the new method

- Transform to a skewsymmetric-s.p.d. pencil whenever possible.
- Use the symplectic URV decomposition to handle the most generic case.

Features

- Fully structure-preserving
- Avoid complex arithmetic
- Potentially high parallel efficiency