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 all or a selected number of eigenpairs of the Bethe–Salpeter and Casida Hamiltonian matrices which have 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 or more).
- Density functional perturbation theory requires many lowest eigenpairs (10^-10^-3).

**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 a 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.


### 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).

- **LiPF6 (480 cores)**
- **Graphene512 (576 cores)**
- **Silicon1000 (2400 cores)**

**Performance profile**
- **LSTAB_NS, k=7**
- **Number of matrix-vector multiplications**
- **Residual norm**
- **Number of roots: 5, Total number of eigenvalues: 11799**

### 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.


### GPLHR in Q-Chem: EOM-CC benchmark

**Benchmark systems:** hydrated photosynthetic yellow protein chlorophyll PYPx-W_{16} (left) and dicyanovinyl 1,3 dimethylmalononitrile (mu_3)H_2O (right).

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<tr>
<th>PYPx-W_{16}/6-31+G(d,p)</th>
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- The number of requested eigenpairs.
- The number of iterations to converge all eigenpairs.
- The total number of matrix-vector multiplications. Davidson failed to deliver the solution.

### GPLHR in other applications

GPLHR exhibits a rapid and reliable convergence for a variety of standard and generalized eigenvalue problems across different applications (e.g., crystal growth simulation or stability analysis of fluid flows).

### Eigenvalue problems with a paired matrix structure

- The Bethe–Salpeter eigenvalue (BSE) problem
- The linear response (LR) eigenvalue problems in time-dependent density functional theory (TDFFT)

### Computing all/selected eigenpairs of the Casida Hamiltonian

**Problem setting**
- The Casida Hamiltonian matrix is of the form
  \[ H = \begin{bmatrix} A & B \\ \ast & \ast \end{bmatrix} \in \mathbb{C}^{2n\times2n} \]
- where \( A = A^T \) is Hermitian, \( B = B^T \) is complex symmetric, with \( [A B] \neq 0 \) (i.e., \( [A B] \) is Hermitian positive definite.)
- In BSE, often all eigenpairs of \( H \) are required.
- In TDFFT, \( H \) is real and sparse for molecules, and only several smallest eigenpairs are needed.

**Our goal:**
- Develop structure-preserving parallel eigensolver for BSE.
- Develop and apply block preconditioned eigensolver techniques tailored specifically to the LR problem.

**Methodology**
- BSE can be reduced to a real positive definite Hamiltonian eigenvalue problem and solved by a skew-symmetric eigensolver.
- When \( H \) is real it is equivalent to solving an \( n \times n \) product eigenvalue problem \( MKx = \lambda^2 Kx \), where \( M = A + B \geq 0, K = A - B \geq 0 \).
- Cholesky factorization and SVD are used to solve \( MKx = \lambda^2 Kx \) when all eigenpairs are needed.
- Several smallest eigenpairs of \( MK \) are computed by properly preconditioned iterative eigensolver applied to the symmetric generalized eigenvalue problem \( KMx = \lambda Kx \).

### Experimental results

**Parallel scalability of the dense BSE solver**
- The parallel solver is built on top of ScalAPACK.
- The scalability of the solver is comparable to that of GEMM.

**Efficiency of new LR eigensolvers**
- New eigensolvers (LOBPCG-LR and Davidson-LR) achieve 2x speedup compared to the traditional Davidson approach for the LR eigenproblem.
- The proposed approaches require 2x less matrix-vector products and offer a significant reduction in memory usage.