Reverse Communication Interface in ELSI

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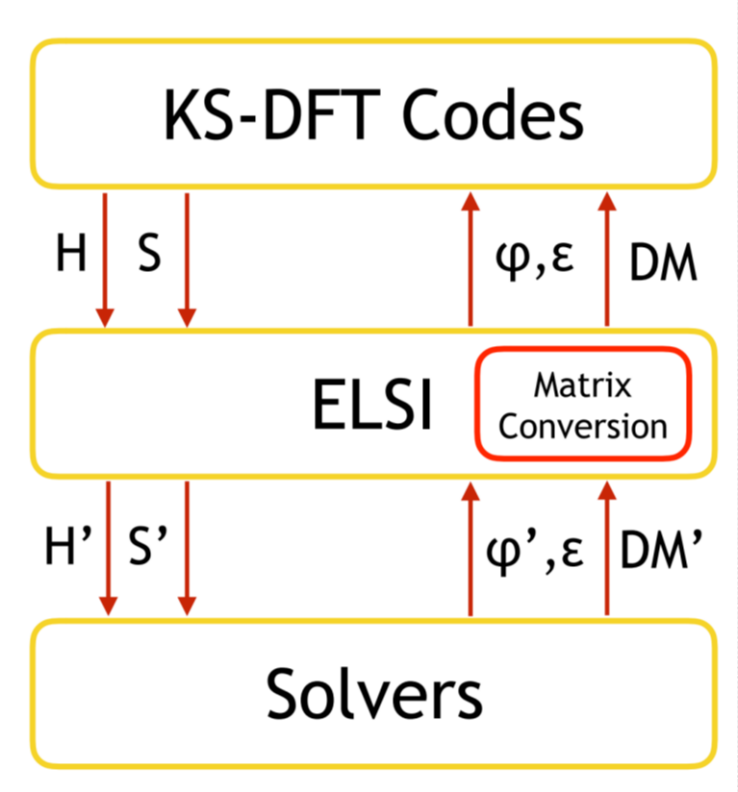
Eigenvalue Problem in KS DFT

$$H\psi = \lambda S\psi$$

- Here H is the Hamiltonian matrix, S is the overlapping matrix, λ is a eigenvalue and ψ is the corresponding eigenvector.
- In Kohn-Sham DFT, smallest k eigenpairs are needed.
- In practice, the size of the Hamiltonian matrix is large and k is proportional to the Hamiltonian size.
- Solving the eigenvalue problem is required in each self-consistency iteration.

ELectronic Structure Infrastructure: ELSI

- ELSI provides an stable interface layer between KS-DFT codes and various solvers (ELPA, libOMM, PEXSI, SIPs…)
- Matrix format conversion is performed automatically by ELSI
- ELSI and redistributed solvers supports five major compilers (Intel, GNU, IBM, PGI, Cray)
- Reverse Communication Interface for Iterative Eigensolvers.
  - Currently, we have Davidson, OMM and PPCG implemented.



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Davidson Method

- Ψ
- Solve Rayleigh Ritz problem $(\Psi^* \mathrm{H} \Psi, \Psi^* \Psi)$ for smallest eigenpairs Λ, Q
- $R = \mathrm{H}\Psi Q - \Psi \mathrm{Q} \Lambda$
- If $\|R\| < tol$, converged
- Approximately solve $(H - \Lambda_i I) V_i = R_i$ for all V_i
- $\Psi = [\Psi \, V]$

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Orbital Minimization Method

[Corsetti 2014]

- Solve an unconstrained minimization problem

$$\min_{\Psi} \mathrm{tr}\left((2I - \Psi^*\Psi)\Psi^*\mathrm{H}\Psi\right)$$

- with conjugate gradient method and exact line search.

- Ψ_m
- $G_m = \mathcal{P}\nabla f_{obj}(\Psi_m)$
- $D_m = G_m + \beta_m G_{m-1}$
- $\Psi_{m+1} = \Psi_m + \gamma_m D_m$

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Projected Preconditioned CG

[Vecharynski, et al 2015]

- Solve a constrained minimization problem

$$\min_{\Psi^*\Psi=I} \mathrm{tr}(\Psi^* \mathrm{H} \Psi)$$

- in the subspace of wavefunctions, gradient and conjugate gradient direction.

- Ψ_m
- $G_m = \mathcal{P}2(I - \Psi_m \Psi_m^*) H \Psi_m$
- Minimize the objective with $\Psi_{m+1} = \Psi_m C_\Psi + G_m C_G + D_m C_D$ and $C_?$ is diagonal
- $D_{m+1} = G_m C_G + D_m C_D$
- Solve Rayleigh Ritz problem for Ψ_{m+1} every few iterations

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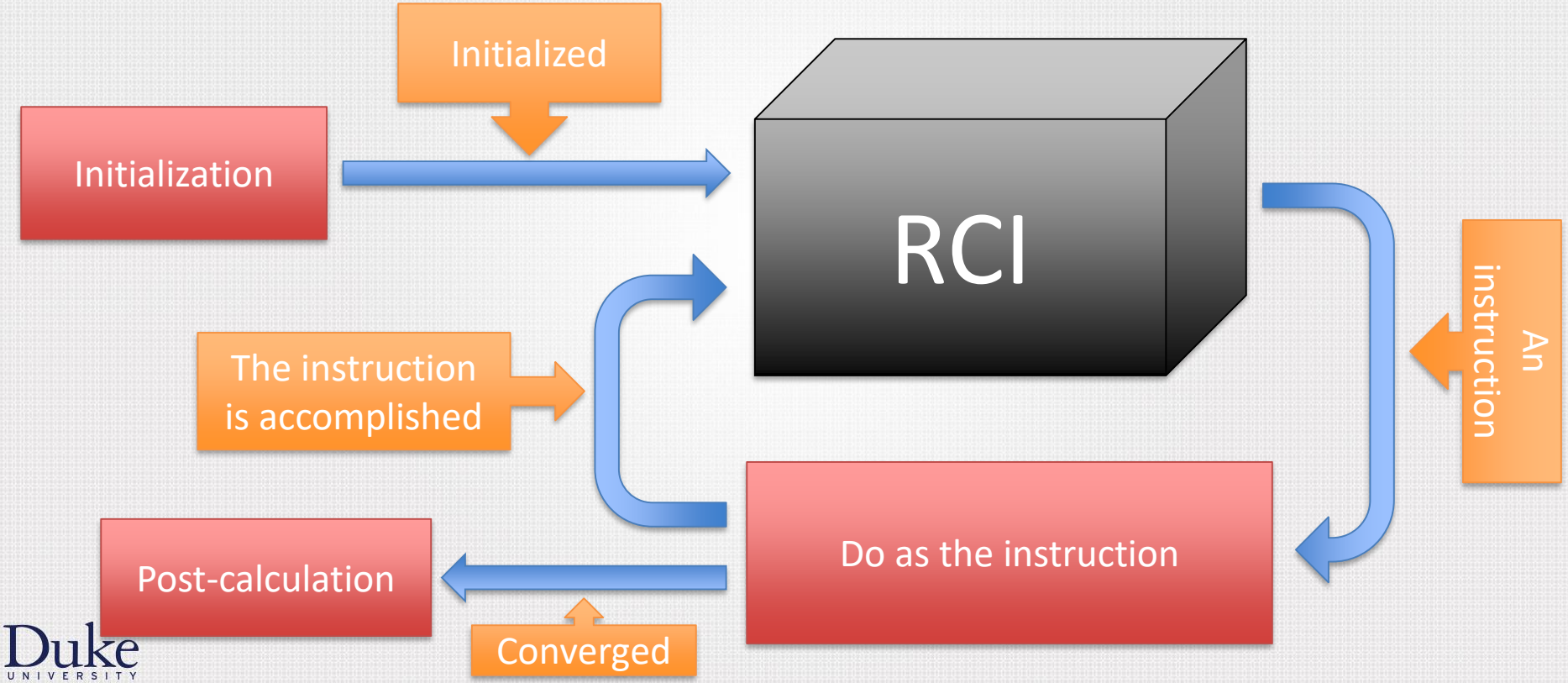
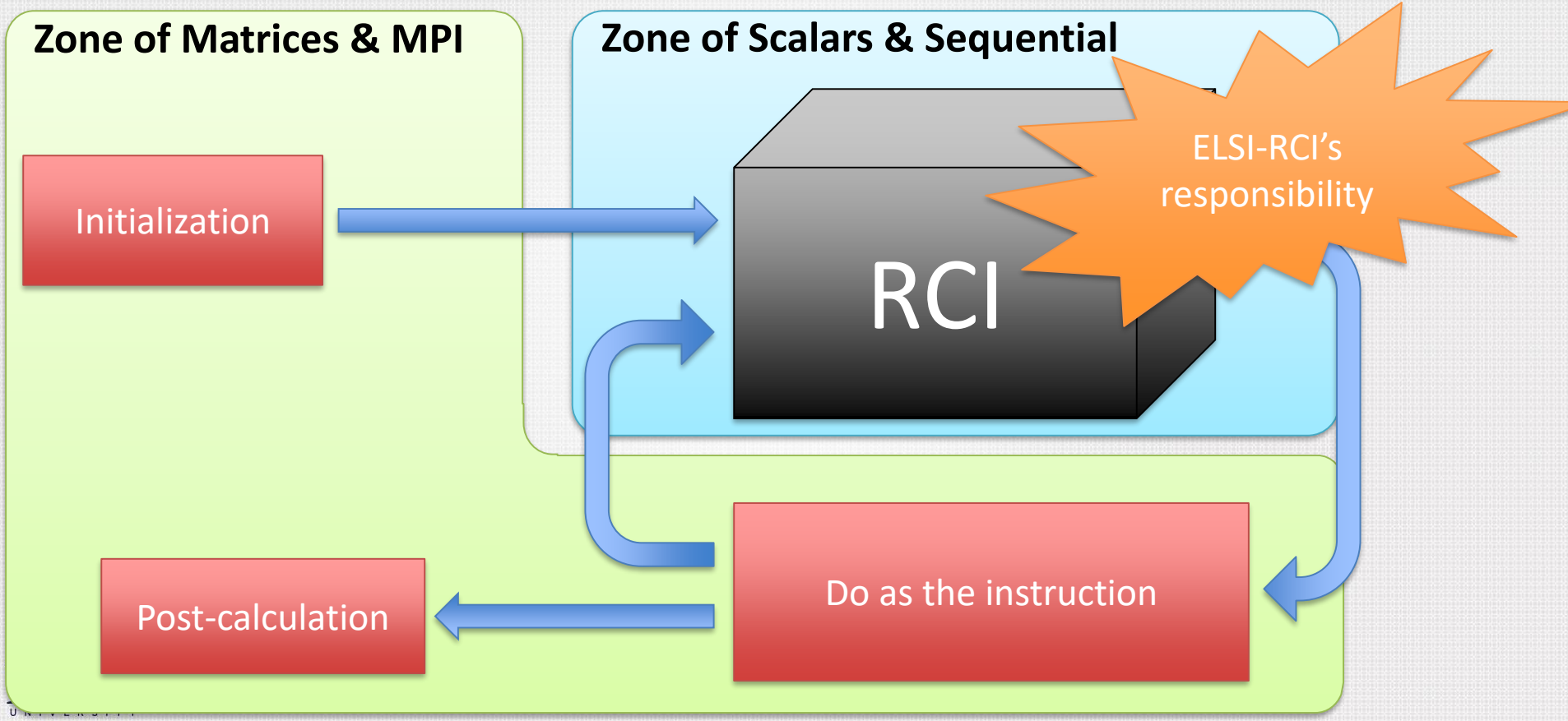
Reverse Communication Interface

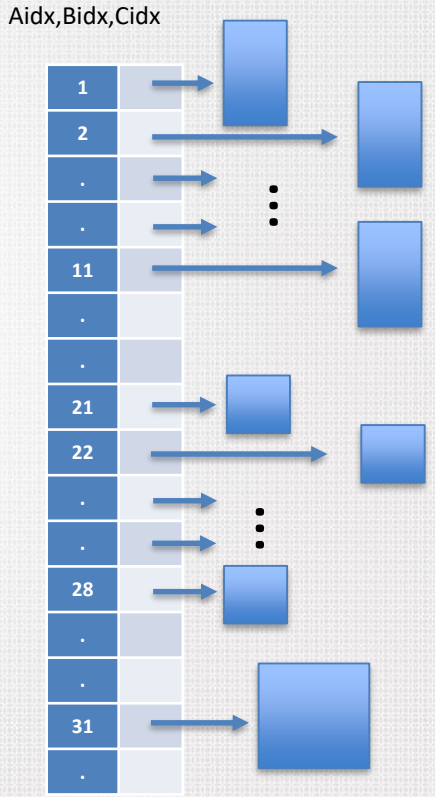


Reverse Communication Interface



Instruction Data Structure

```
type, public :: rci_instr

    character :: jobz, uplo, side ! job char; upper or lower; left or right
    character :: trH, trS, trP, trA, trB ! Operation for H, S, P, A, B

    integer   :: m, n ! size of the output matrix
    integer   :: k ! size of the intermedia multiplication
    integer   :: lda, ldb, ldc ! leading size for matrix A, B and C

    integer   :: rAoff,cAoff ! row and column offset of A
    integer   :: rBoff,cBoff ! row and column offset of B

    integer   :: Aidx, Bidx, Cidx ! indices for matrix A, B and C

    real(r8)  :: alpha, beta ! coefficients

  end type
```



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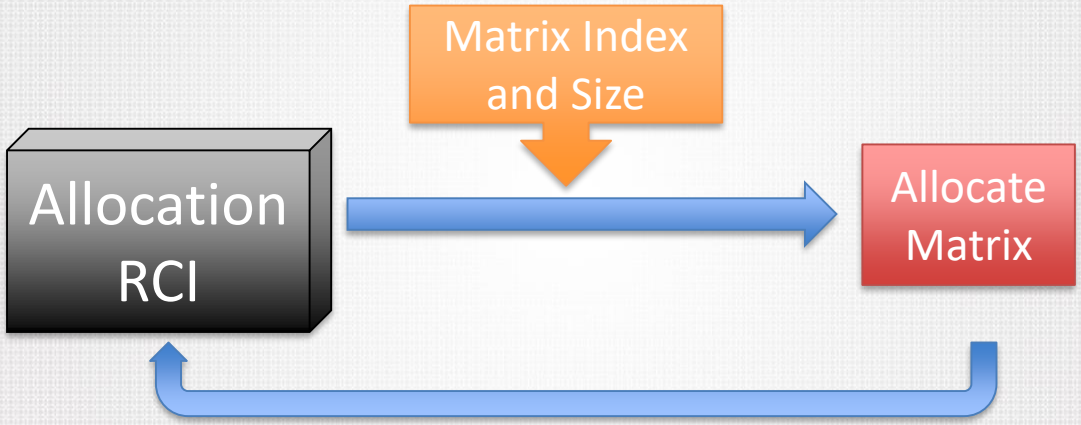
Initialization

- Allocate memory (RCI)



- Initialize the initial wave functions
  - All tests of iterative methods currently use random initial guess

Initialization

Common Instructions

- RCI_NULL
  - Null
- RCI_CONVERGE
  - Converged Flag
- RCI_STOP
  - Stop Flag
- RCI_ALLOCATE
  - Allocate a matrix
- RCI_DEALLOCATE
  - Deallocate a matrix
- RCI_H_MULTI
  - $B = op(H) * A$
- RCI_S_MULTI
  - $B = op(S) * A$
- RCI_P_MULTI
  - $B = op(P) * A$

Common Instructions

- RCI_COPY
  - $B = op(A)$
- RCI_SUBCOPY
  - $B\left(r_B + (1{:}m), c_B + (1{:}n)\right) = A(r_A + (1{:}m), c_A + (1{:}n))$
- RCI_SUBCOL
  - $B = A(:, res)$
- RCI_SUBROW
  - $B = A(res, :)$

Locking Technique Requires These Ops

- RCI_SCALE
  - $A = \alpha * A$
- RCI_COLSCALE
  - $A = A * \mathrm{diag}(res)$
- RCI_COL_NORM
  - $res = \sqrt{\mathrm{diag}(A' \cdot A)}$
- RCI_TRACE
  - $res = \mathrm{tr}(A)$
- RCI_DOT
  - $res = \mathrm{tr}(A * B) = A(:)' * B(:)$

Common Instructions

- RCI_GEMM
  - $C = \alpha * op(A) * op(B) + \beta * C$
- RCI_AXPY
  - $B = \alpha * A + B$
- RCI_HEGV
  - $A * C = B * C * \mathrm{diag}(res)$
- RCI_POTRF
  - $A = U' * U$ or $A = L * L'$
- RCI_TRSM
  - Solve $op(A) * X = \alpha * B$ or $X * op(A) = \alpha * B$ for X

Do As Instructions

```
ijob = RCI_INIT_IJOB
do
  call rci_solve(r_h, ijob, iS, task, resvec)
  select case (task)
  case (RCI_NULL)
  case (RCI_STOP)
     exit
  case (RCI_CONVERGE)
     exit
  case (RCI_H_MULTI)
     call dgemm(iS%TrH, 'N', n, n_state, n, 1.0, H, n, Work(iS%Aidx)%Mat, lda, 0.0, Work(iS%Bidx)%Mat, ldb)
  case (RCI_S_MULTI)
     call dgemm(iS%TrS, 'N', n, n_state, n, 1.0, S, n, Work(iS%Aidx)%Mat, lda, 0.0, Work(iS%Bidx)%Mat, ldb)
  case (RCI_P_MULTI) ! No preconditioner
     Work(iS%Bidx)%Mat = Work(iS%Aidx)%Mat
  case (RCI_GEMM)
     call dgemm(iS%trA, iS%trB, iS%m, iS%n, iS%k, iS%alpha, Work(iS%Aidx)%Mat, iS%lda, Work(iS%Bidx)%Mat, iS%ldb, iS%beta, Work(iS%Cidx)%Mat, iS%ldc)
  case (RCI_AXPY)
     call daxpy(iS%m*iS%n, iS%alpha, Work(iS%Aidx)%Mat, 1, Work(iS%Bidx)%Mat, 1)
  case (RCI_COPY)
     Work(iS%Bidx)%Mat = Work(iS%Aidx)%
  case (…)
      …….
  end select
end do
```

call rci_omm(r_h, ijob, iS, task, resvec)

call rci_davidson(r_h, ijob, iS, task, resvec)

call rci_ppcg(r_h, ijob, iS, task, resvec)

Do as the instruction

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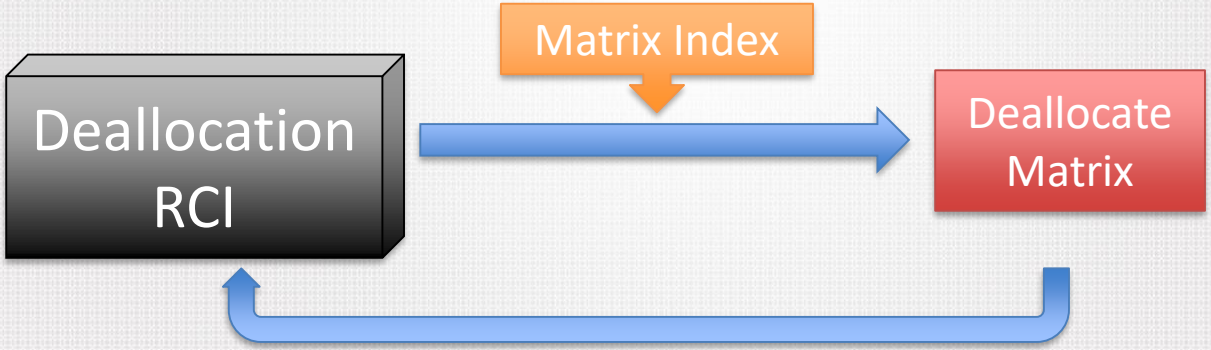
Post-calculation

- Obtain the converged wave functions and the energy
- Obtain eigenvalues or the density matrix if requested
- Deallocate matrices for the iterative method



Post-calculation

ELSI-RCI

Target Users

- Discretization methods such that the Hamiltonian matrix can only be applied as an operator.
- Discretization methods such that n_{basis}/n_{state} is relatively large.
- Eigenvalue problem beyond DFT, e.g., BSE eigenvalue problems.

Benefits

- Knowledge of (P)BLAS and (SCA)LAPACK is sufficient to use many different iterative eigensolvers in ELSI_RCI.
- Coding the driver for ELSI_RCI from an existing iterative eigensolver is relatively easy.
- One driver runs many iterative eigensolvers.

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Numerical Results

- Silicon $2 * 2 * 2$ and $4 * 4 * 4$
- Planewave discretization with Ecut = 20 Hatree
- ONCV pseudo potential
- Hamiltonian operator from a converged SCF calculation
- Random initial wave functions
- Kerker preconditioner is used
- Convergence criteria 10^{-7}

	Si8	Si64
N_{basis}	74088	571787
N_{basis}^{pw}	4553	37073
N_{state}	16	128

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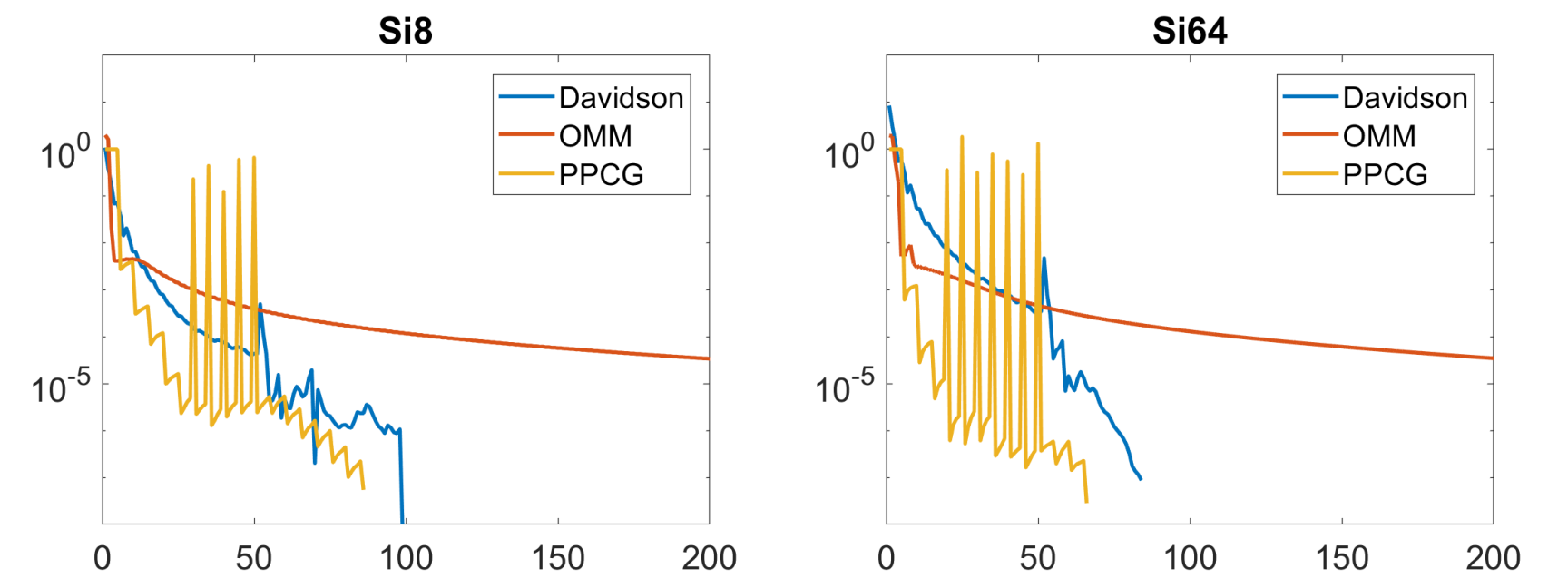
Numerical Results



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Conclusion & Future Work

- ELSI-RCI is a stand alone code without any dependency on other packages except I/O
- When any of H, S and P is not explicitly available, ELSI-RCI would be the choice in ELSI
- One time implementation of RCI driver benefits Davidson method, OMM, PPCG and more eigensolvers in the future

- Implement other iterative eigensolvers
- Reduce the memory usage in the absence of overlapping matrix

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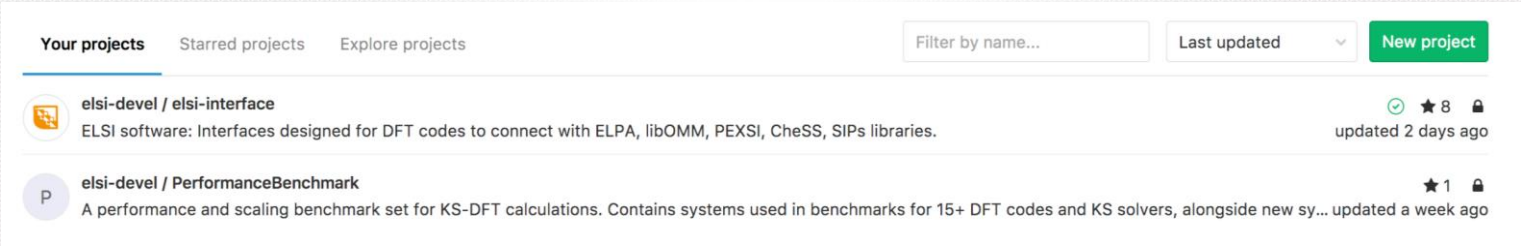
ELSI

- ELSI and ELSI-RCI are available on the ELSI Gitlab as a project at

www.elsi-interchange.org



Electronic Structure Library
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Thank
you