SAND2019-5616C

Matrix Powers Kernels for Thick-restart Lanczos with Explicit External Deflation

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IEEE International Parallel and Distributed Processing Symposium (IPDPS),
Rio de Janeiro, Brazil, May 15, 2019

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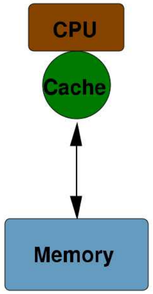
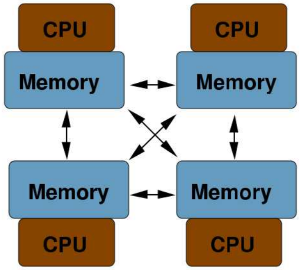
Lanczos for large-scale Hermitian Eigenvalue problems

- Lanczos is a powerful method for solving large SYEV, Av = λv
  - used is many applications
    - effective for computing a few exterior eigenvalues (and eigenvectors)
      - several approaches to improve convergence e.g., thick-restart
    - applicable for interior eigenvalues with spectrum transformation (e.g., shift-invert)
  - use two main kernels (based on Krylov subspace projection)
    - Matrix Vector multiply (SpMV)
      for generating Krylov subspace = span(q, Aq, A^2q, ...)
      - often, black box, provided by users
    - Orthgonalization
      for generating orthonormal basis vectors
      - our current focus

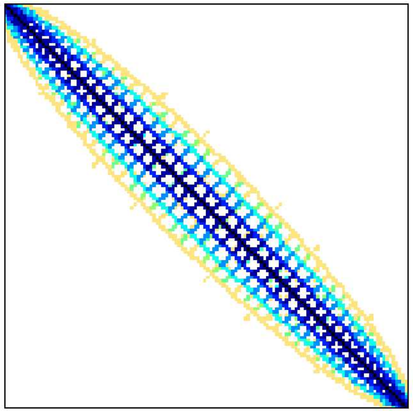




  - Communication can be expensive (time, and maybe power)
    - P2P + irregular data access for SpMV
    - all-reduce + BLAS-1 or 2 for Orthogonalization
    - becoming more expensive on a newer architecture

Challenges in computing many eigenvalues

- Some applications require many eigenvalues (e.g., >1% of n)
  - electronic structure calculation, normal-mode analysis in structure analysis, etc.



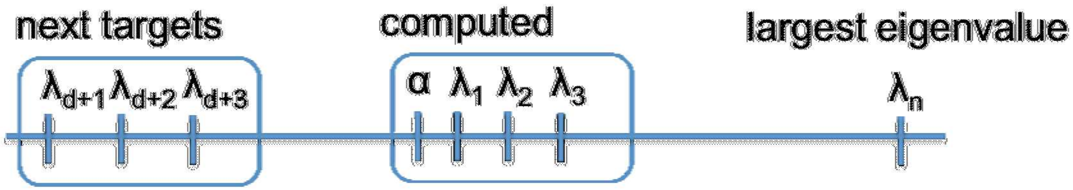
- Other approaches exist
  - Full eigenvalue decomposition
    - ScaLAPACK, ELPA, EigenExa, etc.
    - Stable, but expensive $O(n^3)$
  - Spectral Slicing
    - SLEPc, EVSL, z-Parse, FEAST, etc.
    - Scalable, but several parameters (e.g., windows) and duplicate/missing eigenvalues on the interface
- Lanczos: it is a challenge both numerically & computationally
  - often needs large subspace (e.g., $m=2n_d$)
  - require *locking* (i.e., multiple orthogonalization) to avoid computing the same eigenvalues (nm^2 flops)
  - This talk: combine s-step with EED+TRLan

Explicit external deflation

- Shift the computed eigenvalues away from the exterior:

$$A_d := A + \alpha U_d U_d^T$$

  where U_d contain computed eigenvectors



- Two issues
  - Numerical stability / accuracy (e.g., effects of the errors in the computed eigenvalues on the accuracy of the next eigenvalues to be computed)

    ➔ on-going studies

  - Performance of matrix powers kernel with sparse-plus-low-rank matrix

$$(A + \alpha U_d U_d^T)^k p_0 \qquad \text{for } k = 1, 2, \ldots, s$$

    - deflation of U_d becomes expensive as more eigenvectors are computed

      ➔ focus of this talk (SpMV as a black-box)

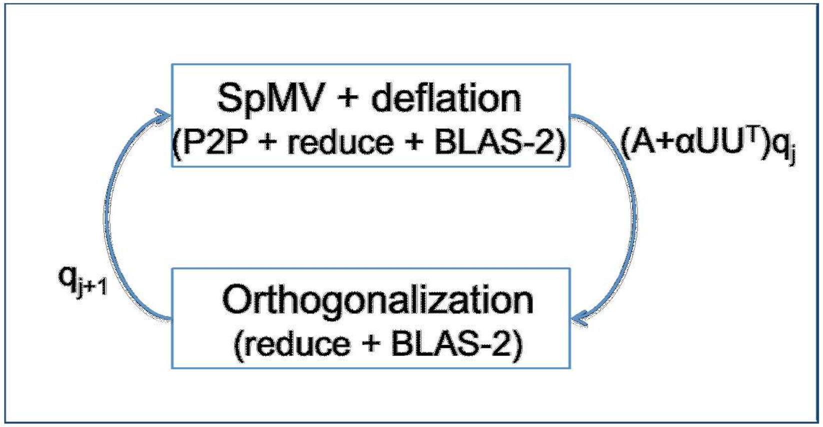
Matrix powers kernel for sparse plus low-rank matrix

- standard kernel

  for j=1, 2, …, s

  - $p_j := A\, p_{j-1} + \alpha U_d\, (U_d^T\, p_{j-1})$

  end



- Each step needs communication
  - p2p for SpMV, and global-reduce for deflation
  - BLAS-2 kernels (SpMV or GEMV)
- "Communication-avoiding" (CA) kernel
  - One global-reduce per every s steps
  - Potential to reduce the communication latency by a factor of s

Matrix powers kernel for sparse plus low-rank matrix

- specialized CA kernel
  - if the computed eigenpairs satisfy (exact and orthogonal)

    $AU_d = U_d \Lambda_d$ and $U_d^T U_d = I$

  - then recurrence for deflation can be un-rolled

$$
\begin{aligned}
p_j &:= (A+\alpha U_d U_d^T)^j p_0 \\
&:= A\,(A+\alpha U_d U_d^T)^{j-1} p_0 + \alpha U_d U_d^T\,(A+\alpha U_d U_d^T)^{j-1} p_0 \\
&:= A\,(A+\alpha U_d U_d^T)^{j-1} p_0 + \alpha U_d(\Lambda_d + \alpha\, I)\, U_d^T (A+\alpha U_d U_d^T)^{j-2} p_0 \\
&:= A p_{j-1} + \alpha U_d(\Lambda_d + \alpha I)^{j-1} U_d^T p_0
\end{aligned}
$$

    - SpMV with the previous vector p_{j-1}
    - GEMV with the starting vector p_0, followed by small local computation

      ➔ One all-reduce per s steps

Matrix powers kernel for sparse plus low-rank matrix

1. dot-products
   $\mathbf{b}_0 := \alpha U_d^H \mathbf{p}_0$

2. local computation
   for $j = 1, 2, \ldots, s-1$ do
   $\quad \mathbf{b}_j := W_{j-1}\mathbf{b}_0$
   end for

3. local matrix-matrix multiplication
   $[\mathbf{c}_0, \mathbf{c}_1, \ldots, \mathbf{c}_{s-1}] := U_d[\mathbf{b}_0, \mathbf{b}_1, \ldots, \mathbf{b}_{s-1}]$

4. MPK with a sparse matrix A
   for $j = 1, 2, \ldots, s$ do
   $\quad \mathbf{p}_j := A\mathbf{p}_{j-1} + \mathbf{c}_{j-1}$
   end for

- Specialized kernel
  1. only one dot-product through GEMV
     - not GEMM
  2. small local computation with small $W_j=(\Lambda+\alpha I)^j$ for deflation
  3. GEMM with local vectors
  4. followed by matrix-powers kernel with sparse matrix A

less communication (sx) and computation (2x) for deflation

	computation flop count	communication, intra volume	inter latency
standard	$s \cdot \text{nnz}(A) + 2nds$	$s \cdot \text{nnz}(A) + 2nds$	$s + s$
comm-avoid	$s \cdot \text{nnz}(A) + nd \cdot (s+1)$	$s \cdot \text{nnz}(A) + 2nd$	$1 + 1$

Accuracy of computed eigenvalues

- Computed eigenpairs are not exact
  - $U_d^T U_d = I + F$
    where F is the orthogonalization error
  - $A\, U_d = U_d\, \Lambda_d + E$
    where E is determined by the stopping criteria

- If the orthogonality is maintained (e.g., two classical Gram Schmidt), then norm of F is small

- It can be shown that if the computed eigenvalues satisfy

$$\frac{\|E\|_2}{\|A\|_2} \le \tau \le \frac{\epsilon\, n(\|A\|_2 + \alpha)^2}{\alpha\|A\|_2}, \quad \text{or} \quad \|E\|_2 \le \tau\|A\|_2 \le \frac{\epsilon\, n\|A\|_2}{\alpha}\|A\|_2,$$

then the effects of the errors in the computed eigepairs is small in the evaluation of MPK (i.e., the same order as the round-off errors)

General CA MPK: blocking cover, N. Knight, E. Carson, J. Demmel 2014

1. MPK with a sparse matrix A

```
for j = 1, 2, ..., s-1 do
    p_j := A p_{j-1}
end for
```

2. Block dot-product

$B := U_d^H \cdot [\mathbf{p}_0, \mathbf{p}_1, \ldots, \mathbf{p}_{s-1}]$

3. local computation, $O(ds^2)$ flops

```
for j = 1, 2, ..., s do
    c_j := b_j
    for i = 1, 2, ..., j-1 do
        c_j := c_j + X_i c_{j-i}
    end for
    c_j := α c_j
end for
```

4. generate low-rank correction

$Y := U_d \cdot [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_s]$

5. MPK with A to integrate low-rank correction

```
for j = 1, 2, ..., s do
    p_j := A p_{j-1} + y_j
end for
```

- Matrix-powers kernel for a general sparse-plus-low-rank matrix, $A+\alpha U_d U_d^T$
- No assumption on properties of A or U
- Require additional costs, s-1 additional SpMV and then block dot-product with GEMM
  - specialized CA MPK does not require additional SpMV, and perform GEMV instead of GEMM
- Can be applied for TRLan+EED
  (first performance studies of blocking cover for practical application)

	computation flop count	communication, intra volume	inter latency
ST	$s \cdot \text{nnz}(A) + 2nds$	$s \cdot \text{nnz}(A) + 2nds$	$s+s$
BC	$(2s-1) \cdot \text{nnz}(A) + 2nds$	$(2s-1) \cdot \text{nnz}(A) + 2nd$	$2+1$
CA	$s \cdot \text{nnz}(A) + nd \cdot (s+1)$	$s \cdot \text{nnz}(A) + 2nd$	$1+1$

Putting all together: s-step TRLan+EED

Krylov subspace generation

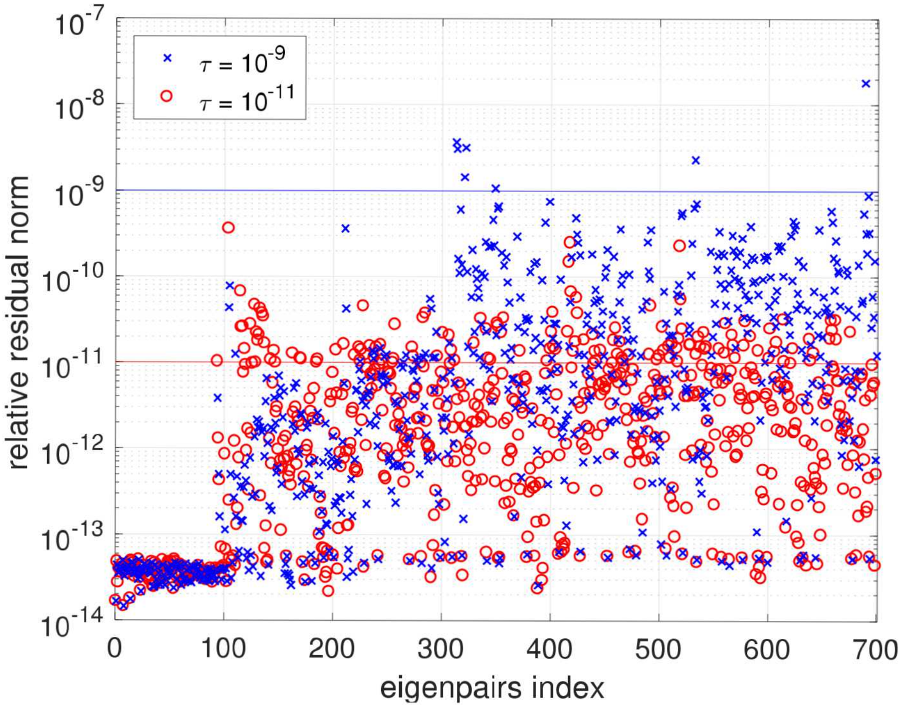
- Matrix powers kernel with sparse-plus-low-rank matrix
  - Standard kernel
  - Specialized/blocking cover CA kernel
- Block orthogonalization
  - block Gram Schmidt: orthogonalize s vectors against previous vectors at once (single all-reduce)
  - Cholesky QR: orthogonalize s vectors among themselves (single all-reduce)

set $\mathbf{q}_1 = \mathbf{q}/\|\mathbf{q}\|_2$, $k = 0$.
for $j = 1, 2, 3, \ldots$
  1. Initialization.
    a. $\mathbf{p} := (A + \alpha U_d U_d^H)\mathbf{q}_{k+1}$
    b. $\alpha_{k+1} := \mathbf{q}_{k+1}^H \mathbf{p}$
    c. $\mathbf{p} := \mathbf{p} - \alpha_{k+1}\mathbf{q}_{k+1} - \sum_{i=1}^{k} \beta_i \mathbf{q}_i$
    d. $\beta_{k+1} := \|\mathbf{p}\|_2$
    e. $\mathbf{q}_{k+2} := \mathbf{p}/\beta_{k+1}$
  2. The j-th restart-loop.
    for $i = k+2 : s : m$
    a. Starting vector $\mathbf{p}_i = \mathbf{q}_i$.
    b. Matrix Powers Kernel:
      for $\ell = i, i+1, \ldots, i+s-1$
        $\mathbf{p}_{\ell+1} := (A + \alpha U_d U_d^H)\mathbf{p}_\ell$
      end for
    c. Block three-term orthogonalization:
      $R_{i-s:i,\, i+1:i+s} := Q_{i-s:i}^H P_{i+1:i+s}$
      $P_{i+1:i+s} := P_{i+1:i+s} - Q_{i-s:i} R_{i-s:i,\, i+1:i+s}$
    d. Tall-skinny Cholesky QR factorization:
      $B := P_{i+1:i+s}^H P_{i+1:i+s}$
      $R_{i+1:i+s,\, i+1:i+s} := \mathrm{chol}(B)$
      $Q_{i+1:i+s} := P_{i+1:i+s} R_{i+1:i+s,i+1:i+s}^{-1}$
    e. Reorthogonalize $Q_{i+1:i+s}$ if necessary:
      Classical Gram Schmidt followed by Cholesky QR.
    f. Update the projected matrix T_m:
      see, e.g., [4, Sec. 4.2.2].
    end for
  3. The j-th restart.
    a. compute all eigenpairs of T_m and the corresponding residual norms for Ritz pairs by (2).
    b. if stopping criteria is satisfied then
    c.   compute desired Ritz vectors and exit.
    d. else restart:
    e.   update k (see [14], [13]).
    f.   select k Ritz values $\lambda_1, \ldots, \lambda_k$ of interest, and compute their Ritz vectors $\{\mathbf{q}_1, \ldots, \mathbf{q}_k\}$.
    g.   set $\alpha_i = \lambda_i$ and $\beta_i = \|A\mathbf{q}_i - \lambda_i \mathbf{q}_i\|_2$ by (2), for $i = 1, \ldots, k$,
    h.   set $\mathbf{q}_{k+1} = \mathbf{q}_{m+1}$.
    i. end if
end for

Experimental setups

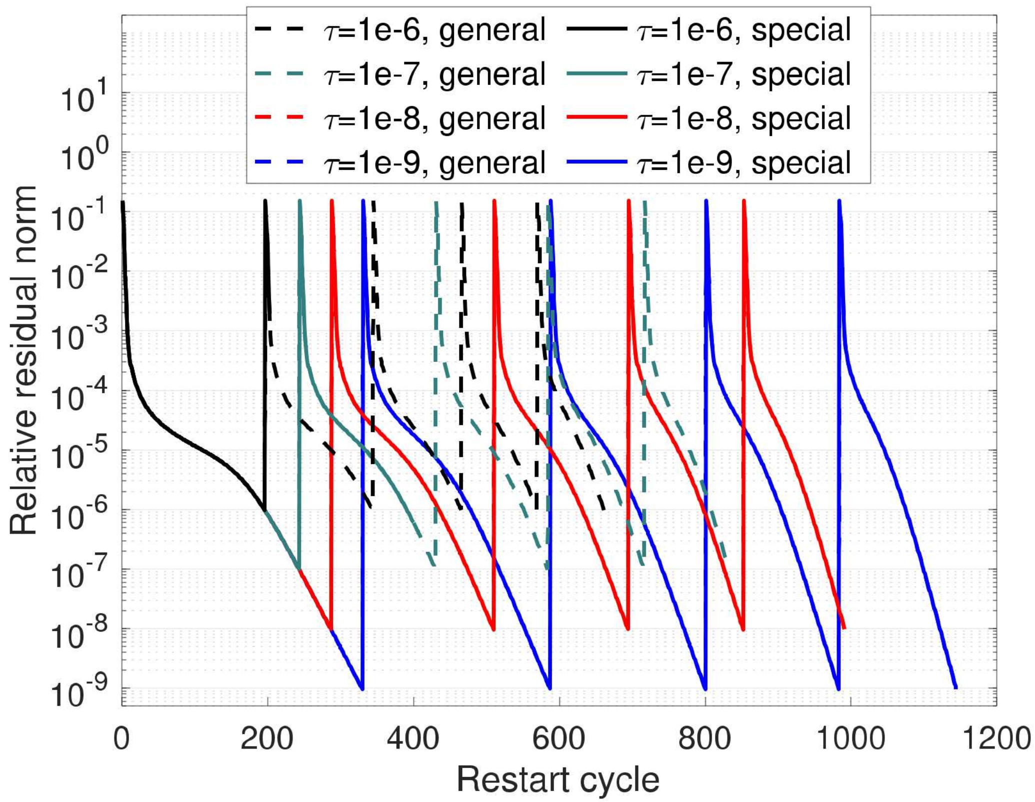
- NERSC Cori Haswell nodes
  - Each node with Intel Xion E5 at 2.3GHz with 128GB of main memory
  - Nodes are connected through Cray Aries (Dragonfly)
- Compiled using the Cray compiler wrapper
  - Linked to Intel's MKL
- Solver parameters
  - Shift is chosen based on the next target and the largest computed eigenvalue, $\alpha=\lambda_d+(\lambda_n-\lambda_d)/2$
  - Eigenpairs are considered to be converged with $\tau=10^{-11}$
  - One MPI process per core

Accuracy of computed eigenpairs with standard TRLan+EED



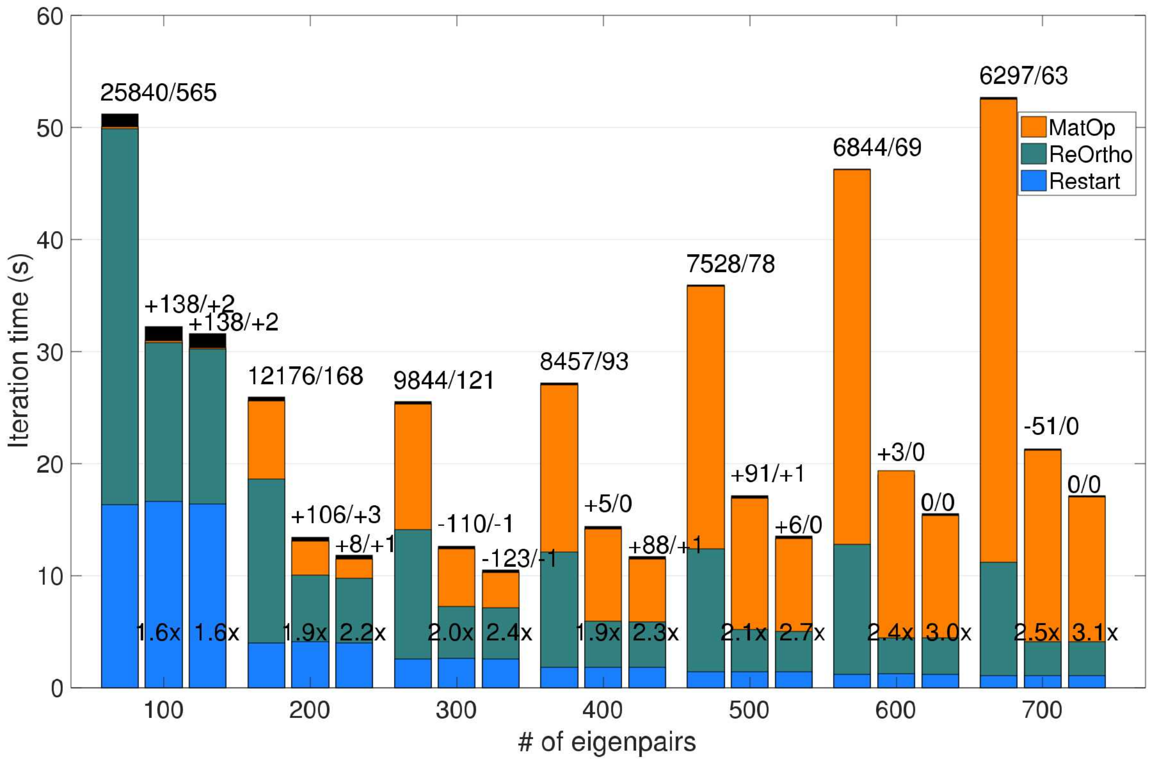
- Relative residual norms with TRLan+EED
  - Compute 100 eigenpairs at a time
  - SiH_4 for DFT electronic structure calculation from Suite Sparse matrix collection
  - TRLan+EED obtain desired accuracy

Accuracy of computed eigenvalues



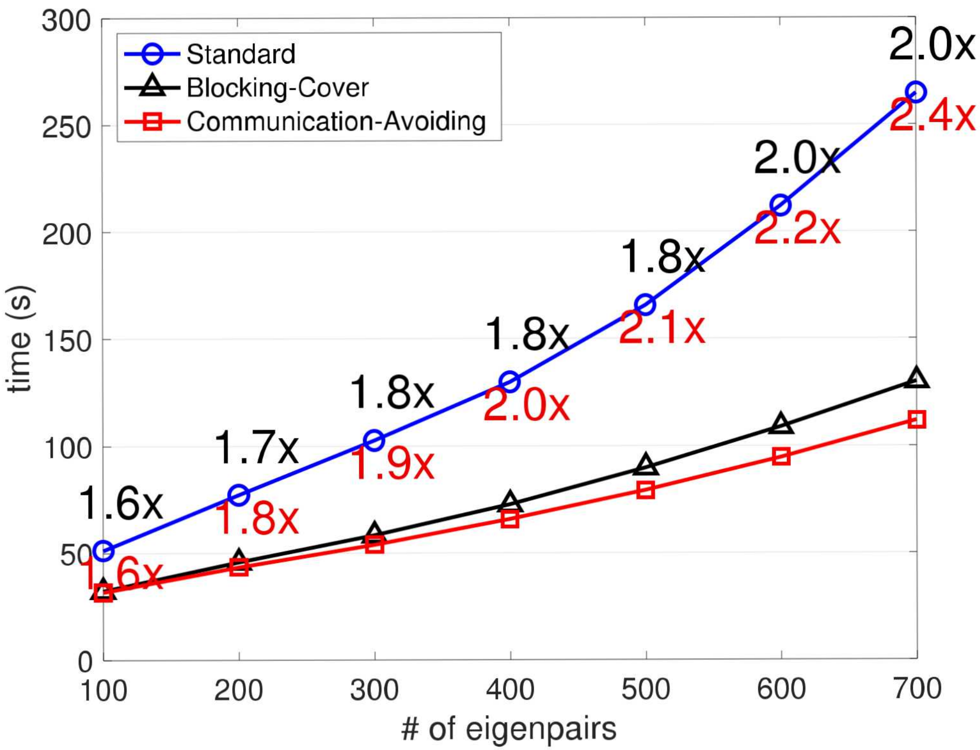
- Specialized MPK is as accurate as standard MPK when tolerance is selected carefully

Performance results using a diag($1^2,2^2,\ldots,n^2$) with n=10K



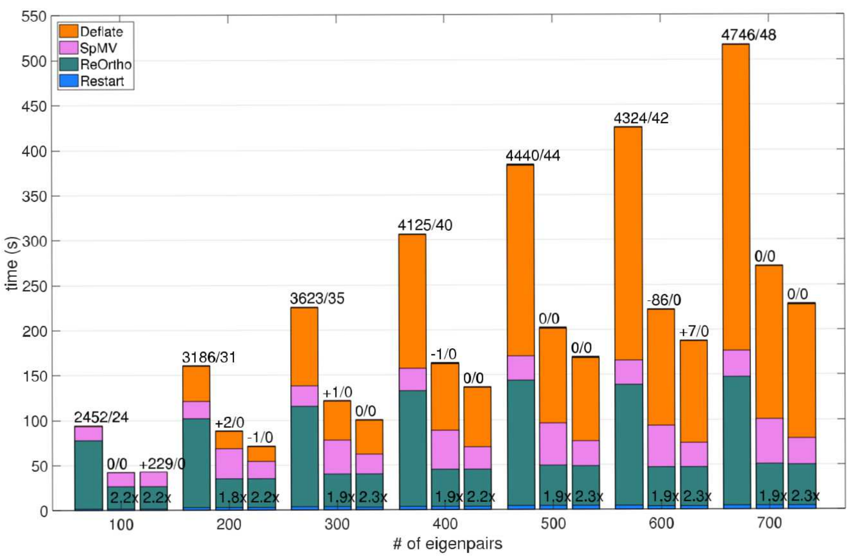
- ReOrtho time reduced through block orthogonalization
  - For computing first 100 eigenpairs, TRLan vs Ca-TRLan
- MatOp time reduced through MPK

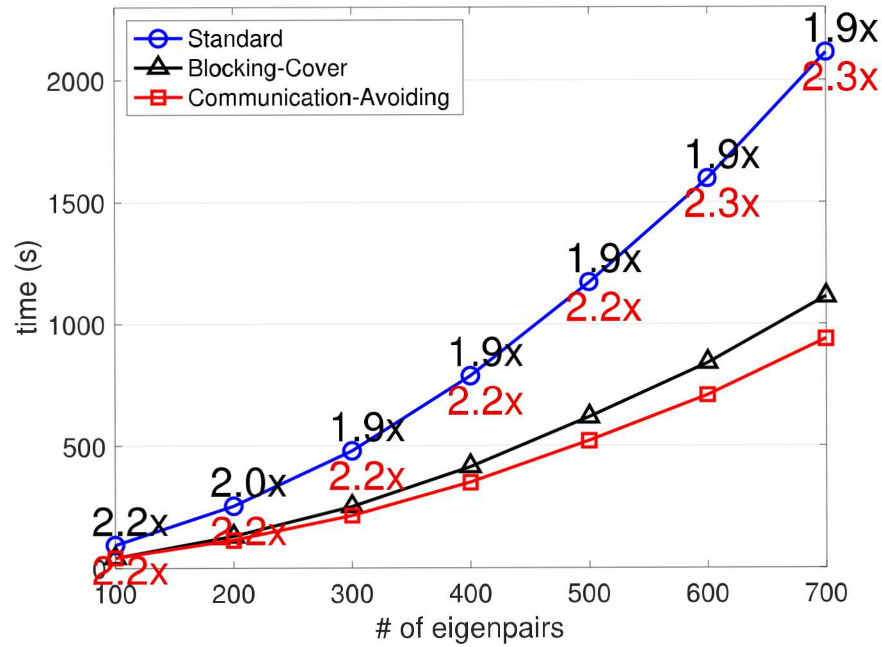
Performance results using a diag($1^2, 2^2, \ldots, n^2$) with n=10K



- Increasing benefits as more eigenvalues are needed

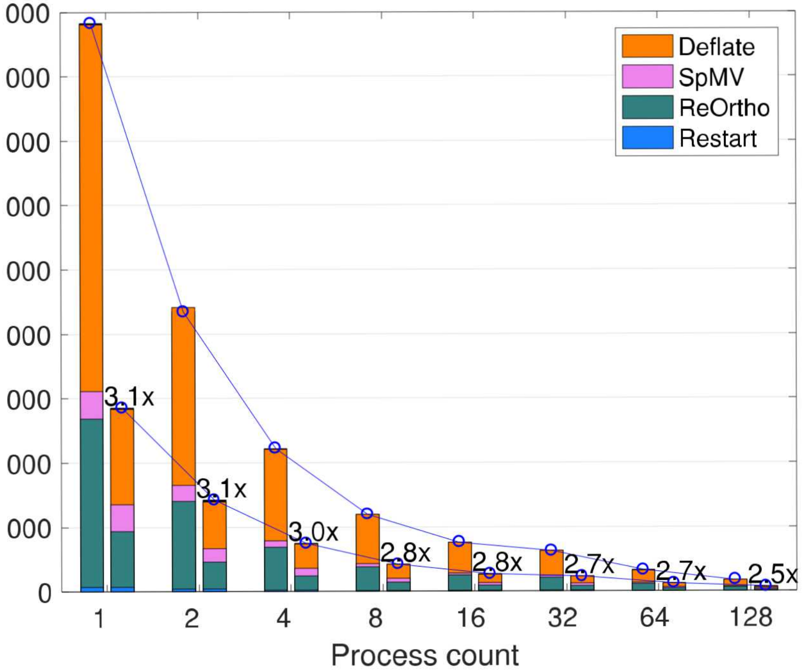
Performance results using a DFC matrix (n=97K)

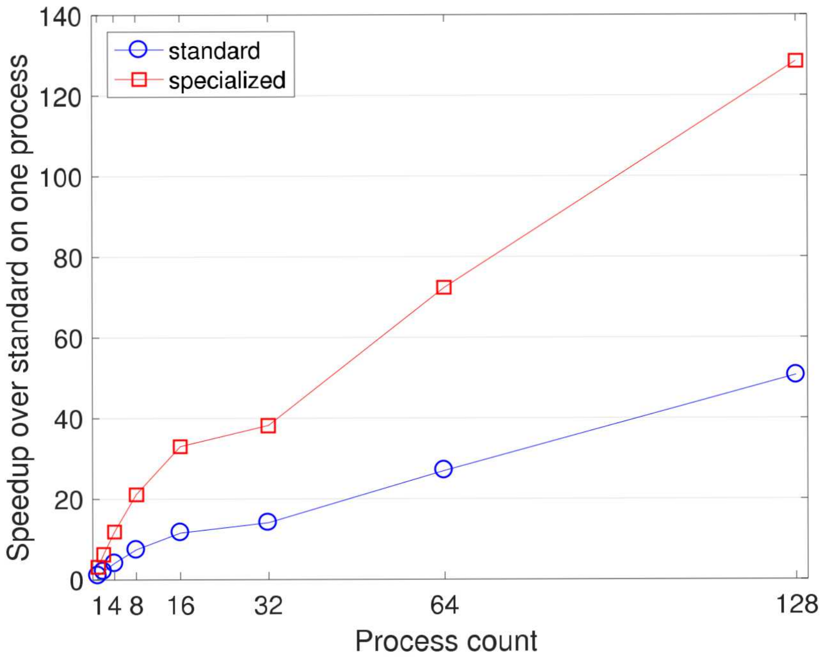




- Avoiding communication/computation can reduce the run time
  - Speedups of up to 2.3x

Performance results using a DFC matrix (n=240K)





- CA variants can maintain the performance benefits over multiple processes
  - Needs to address sequential part (e.g., restart)

Conclusion

- TRLan+EED for computing many eigenvalues
- s-step method for improving performance by avoiding communication
- Possible to avoid some computation when the tolerance is carefully selected

- More theoretical, numerical, and performance studies are underway
  - Low-synchronous orthogonalization kernels
  - Effects of inaccurate eigenpairs on EED

Thank you!!

- ECP PEEKS, for funding

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering and early testbed platforms, in support of the nations exascale computing imperative.