Task-Based Polar Decomposition Using SLATE on Massively Parallel Systems with Hardware Accelerators

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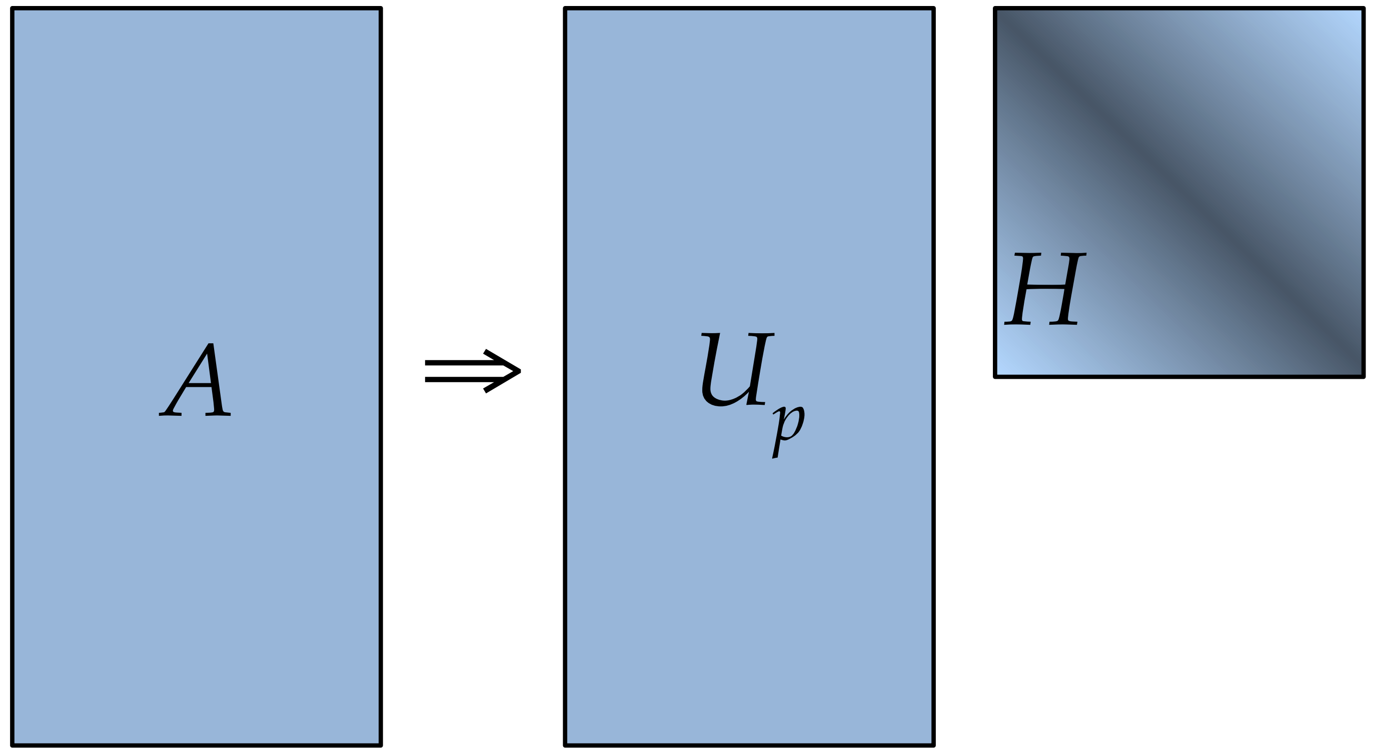
Polar Decomposition (PD)

- Factor matrix $A \in \mathbb{C}^{m \times n}$ $(m \geq n)$ into

$$A = U_p H$$



- Unitary matrix U_p
- Hermitian positive semi-definite matrix $H = \sqrt{A^H A}$,

$$HH = A^H A$$

- Useful in aerospace computations, factor analysis, computing SVD and pseudo-inverse

Motivation: Subaru telescope

- 8.2-meter telescope of the National Astronomical Observatory of Japan, located at Mauna Kea, Hawaii
- Adaptive Optics to measure and correct for atmospheric turbulence using pseudo-inverse in real time
- Used MAGMA-based Polar Decomposition (QDWH) SVD for pseudo-inverse, 2018

Polar Decomposition to SVD

- Compute $A = U_p H$
- Substitute Hermitian eigenvalues $H = V \Lambda V^H$
- Yields SVD: $A = U_p H = (U_p V) \Lambda V^H = U \Lambda V^H$
- See also High-Performance SVD Partial Spectrum Computation, Keyes et al., Thu 11 a.m.
- Or in reverse, compute PD from SVD:

$$A = U \Sigma V^H = U(V^H V) \Sigma V^H = (U V^H)(V \Sigma V^H) = U_p H$$

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Factorizations

- LU: $A = P^T LU,$ triangular L and U
- Cholesky: $A = LL^H,$ Hermitian positive definite A, triangular L
- QR: $A = QR,$ unitary Q, triangular R
- Eigenvalue: $A = V \Lambda V^{-1},$ diagonal Λ
- $A = V \Lambda V^H,$ Hermitian A, unitary V, real diagonal Λ
- SVD: $A = U \Sigma V^H,$ unitary U and V, real diagonal Σ
- Polar: $A = U_p H,$ unitary U_p, Hermitian semi-definite H

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History of Polar Decomposition

- 1902 — Autonne. Definition of polar decomposition.
- 1986 — Higham. Scaled Newton's Method.
- 1990 — Gander. Halley's Iteration.
- 1994 — Higham and Papadimitriou. Matrix inverse dynamically weight Halley (DWH).
- **2010 — Nakatsukasa et. al. Inverse-free QR-based DW Halley (QDWH).**
- 2013 — Nakatsukasa and Higham. QDWH Eig, SVD.
- 2016 — Sukkari, Ltaief, Keyes. Block algorithm, GPUs (**MAGMA**).
- 2016 — Sukkari, Ltaief, Keyes. ScaLAPACK, distributed memory (**POLAR**, Cray LibSci).
- 2017 — Sukkari, Ltaief, Faverge, Keyes. Task-based, shared memory (**Chameleon**).
- 2018 — Ltaief, Sukkari, Guyon, Keyes. QDWH SVD.
- 2019 — Sukkari, Ltaief, Keyes, Faverge. Task-based, distributed memory (**DPLASMA**).
- 2023 — Sukkari et al. Distributed, task-based, GPUs (**SLATE**).
- 2023 — Keyes, Ltaief, Nakatsukasa, Sukkari. QDWH Partial SVD. (Thu 11 a.m.)

Methods

- **Newton's Method**

$$X_0 = A,$$
$$X_{k+1} = \frac{1}{2}\left(X_k + X_k^{-H}\right) \qquad X_k \to U_p$$

  - Quadratic convergence, but initially slow
  - Explicit inverse, stability issues

- **Scaled Newton's Method**

$$X_{k+1} = \frac{1}{2}\left(z_k X_k + (z_k X_k)^{-H}\right)$$

  - Improves convergence

Higham. SIAM, 1986.

Methods

- **Halley Iteration**

$$X_0 = A,$$

$$X_{k+1} = X_k \left(3I + X_k^H X_k\right) \left(I + 3X_k^H X_k\right)^{-1}$$

  - Cubic convergence, but initially slow; explicit inverse

- **Dynamically Weighted Halley (DWH) Iteration**

$$X_0 = A / \left\| A \right\|_2,$$

$$X_{k+1} = X_k \left(a_k I + b_k X_k^H X_k\right) \left(I + c_k X_k^H X_k\right)^{-1}$$

  - Improves convergence: 6 iterations for cond(A) $= 10^{16}$

Gander. SIAM, 1990.

Yuji Nakatsukasa, Zhaojun Bai, and François Gygi. SIAM, 2010.

Methods

- Goal: implement DWH without inverse

$$X_{k+1} = X_k \left(a_k I + b_k X_k^H X_k\right) \left(I + c_k X_k^H X_k\right)^{-1}$$

- **QR-based Dynamically Weighted Halley (QDWH) Iteration**

$$\begin{bmatrix} \sqrt{c_k} X_k \\ I \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R$$ QR factorization

$$X_{k+1} = \alpha Q_1 Q_2^H + \beta X_k,$$ matrix multiply (gemm)

$$\alpha = \frac{1}{\sqrt{c_k}} \left(a_k - \frac{b_k}{c_k} \right),$$

$$\beta = \frac{b_k}{c_k}$$

Yuji Nakatsukasa, Zhaojun Bai, and François Gygi. SIAM, 2010.

Methods

- Goal: implement DWH as X_k becomes well-conditioned

$$X_{k+1} = X_k \left(a_k I + b_k X_k^H X_k\right) \left(I + c_k X_k^H X_k\right)^{-1}$$

- **Cholesky-based Dynamically Weighted Halley Iteration**

$$Z_k = I + c_k X_k^H X_k,$$ matrix multiply (herk)

$$L_k = \mathrm{chol}(Z_k),$$ Cholesky factorization

$$X_{k+1} = \left(a_k - \frac{b_k}{c_k}\right) X_k L_k^{-1} L_k^{-H} + \frac{b_k}{c_k} X_k$$ Cholesky solve, add

Yuji Nakatsukasa and Nicholas J. Higham. SIAM, 2013.

Algorithm

function polar_qdwh(input A; output U_p, H)

X_k = A / norm2est(A)

QR factor of X_k

$smin$ = norm1(R) / cond1est(R) / sqrt(n) // $smin$ is lower bound of $\sigma_{\min}$ of X_k

until convergence: $|smin - 1| < \text{tol}$

update weights $smin, a_k, b_k, c_k$

if ill-conditioned: $c_k > 100$

do QR-based iteration

else

do Cholesky-based iteration

$U_p = X_k$

$H = U_p^H A$ matrix multiply: gemm, herkx (cuBLAS, rocBLAS), or gemmt (MKL)

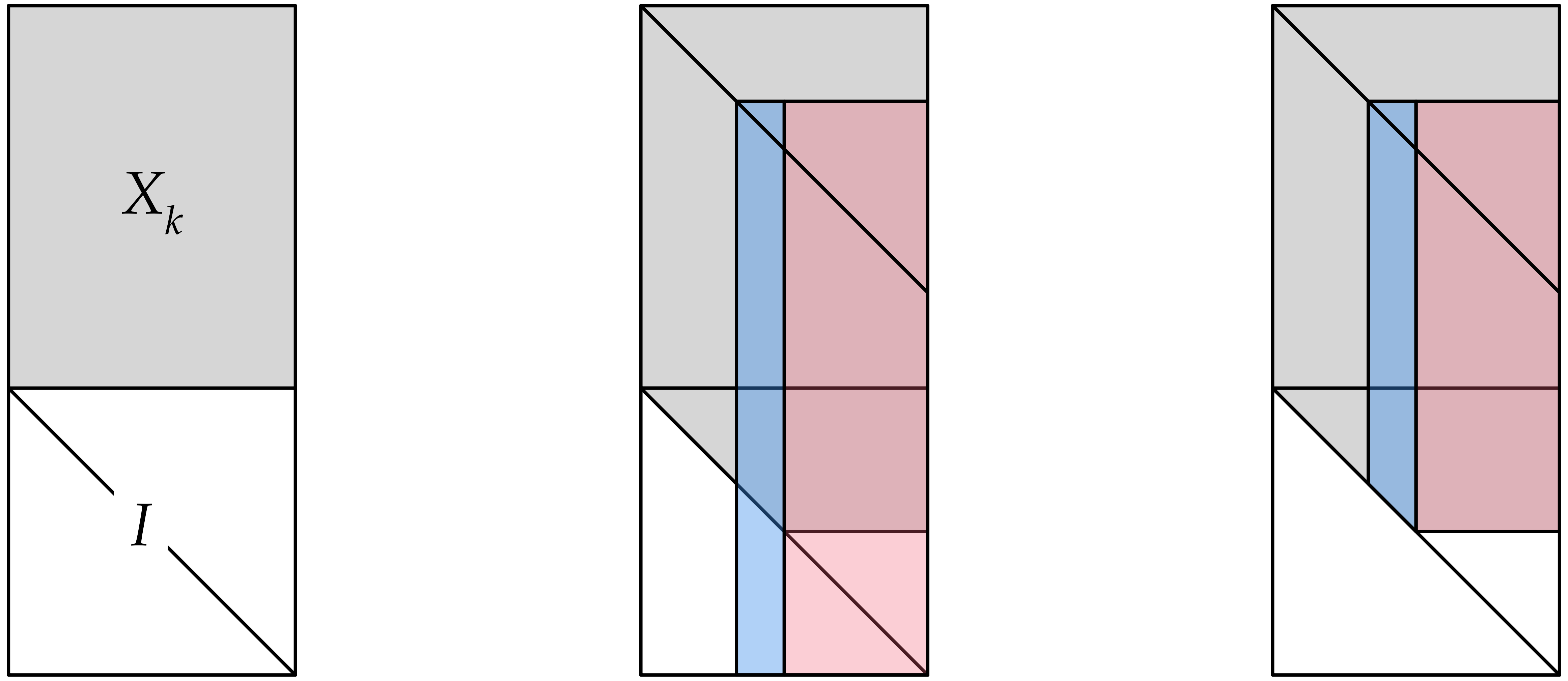
QR optimization

- QR of dense matrix on top of diagonal (identity)

$$\begin{bmatrix} \sqrt{c_k} X_k \\ I \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R$$

QR factorization

- Modify standard QR so panels go only to diagonal of lower block



SLATE: Software for Linear Algebra Targeting Exascale

- **Distributed, GPU-accelerated, dense linear algebra library**
  - BLAS
  - Linear systems
  - Least squares
  - Eigenvalues, SVD, Polar

- **Built on BLAS++ and LAPACK++ portability layer**
  - Wrappers around CPU and GPU BLAS & LAPACK
- **Modern replacement for ScaLAPACK**
  - C++ templates, MPI, OpenMP tasks

SLATE Coverage

Basic linear algebra $(C = AB, \ldots)$

	ScaLAPACK	SLATE
Level 1 PBLAS	✔	✘
Level 2 PBLAS	✔	✔ Level 2+ optimizations
Level 3 PBLAS	✔	✔
Auxiliary routines (add, set, scale, ...)	✔	✔
Matrix norms	✔	✔
Test matrix generation	✔	✔

Least squares $(Ax \cong b)$

	ScaLAPACK	SLATE
QR	✔	✔
Cholesky QR	✘	✔
LQ	✔	✔
Least squares solver	✔	✔
PAQR (pivoting avoiding)	✘	✔ dev branch

Linear systems $(Ax = b)$

	ScaLAPACK	SLATE
LU (partial pivoting, threshold)	✔	✔
CALU (tournament pivoting)	✘	✔
LU, band (pp)	✔	✔
LU (non-pivoting)	✘	✔
Cholesky	✔	✔
Cholesky, band	✔	✔
Symmetric Indefinite (block Aasen)	✘	✔ CPU only
Mixed precision (single-double)	✘	✔
Inverses (LU, Cholesky)	✔	✔
Condition estimate	✔	✔

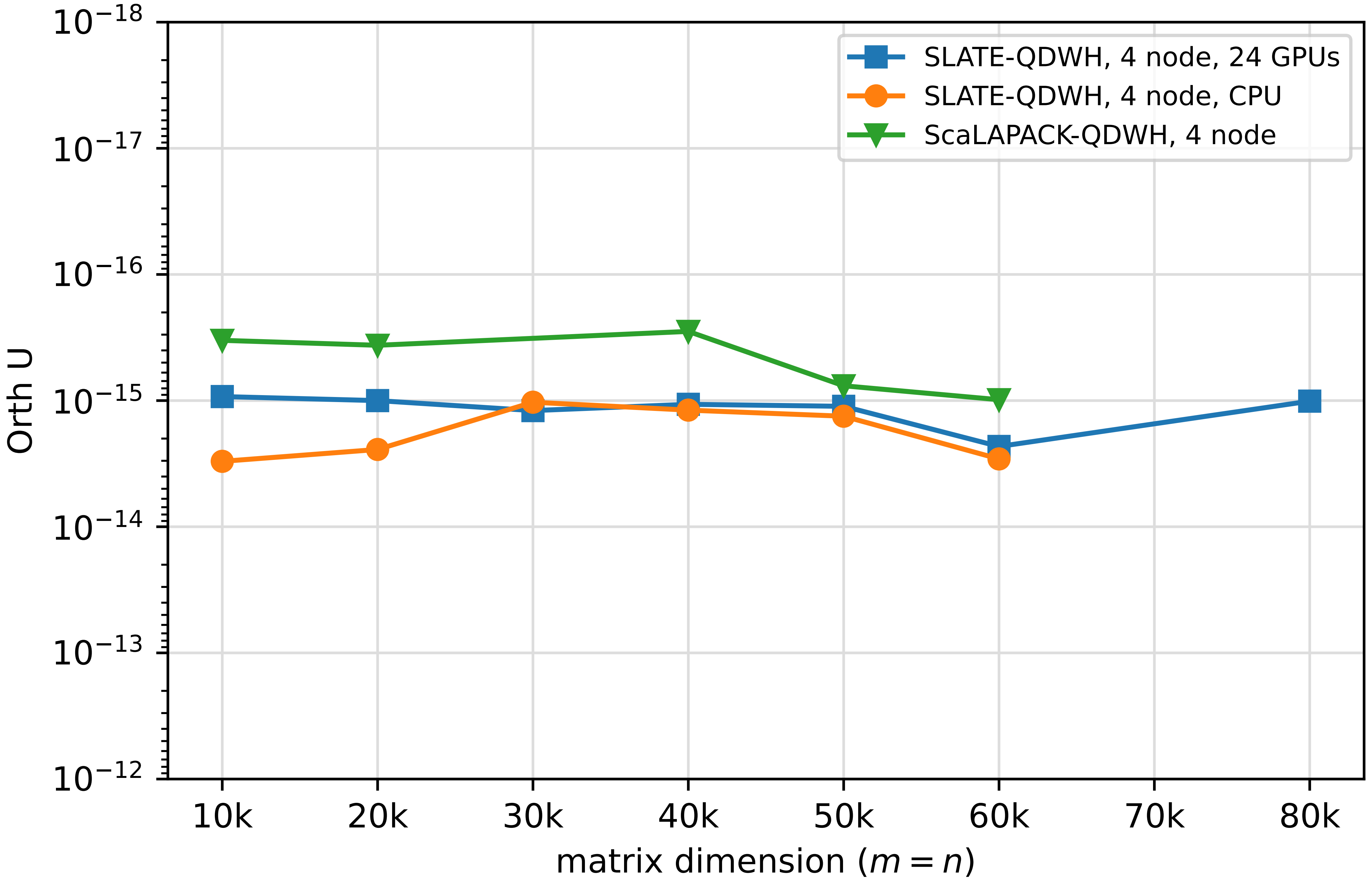
SVD, Eig, PD $(A = U\Sigma V^H, Ax = \lambda x, A = UH)$

	ScaLAPACK	SLATE
Singular value decomposition (SVD)	✔	✔ values & vectors
Hermitian eigenvalue	✔	✔ values & vectors
Generalized Hermitian eigenvalue	✔	✔ values & vectors
Polar decomposition (QDWH)	✘	✔ dev branch
LOBPCG	✘	✔ dev branch
Non-symmetric eigenvalue	pieces	✘ future
Complex–symmetric eigenvalue	✘	✘ future

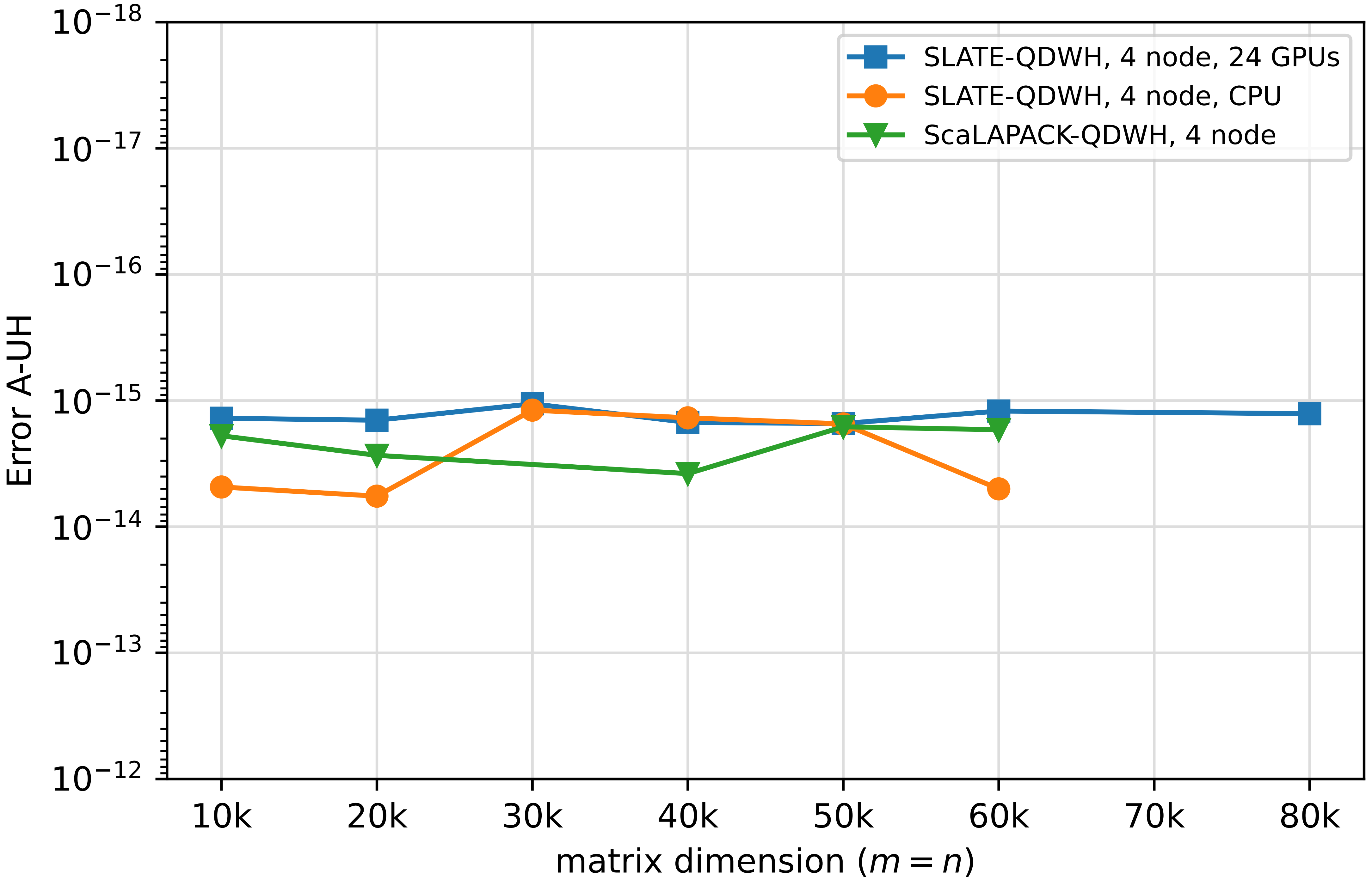
Unless noted, all routines are GPU-accelerated

Results

- Orthogonality of U_p

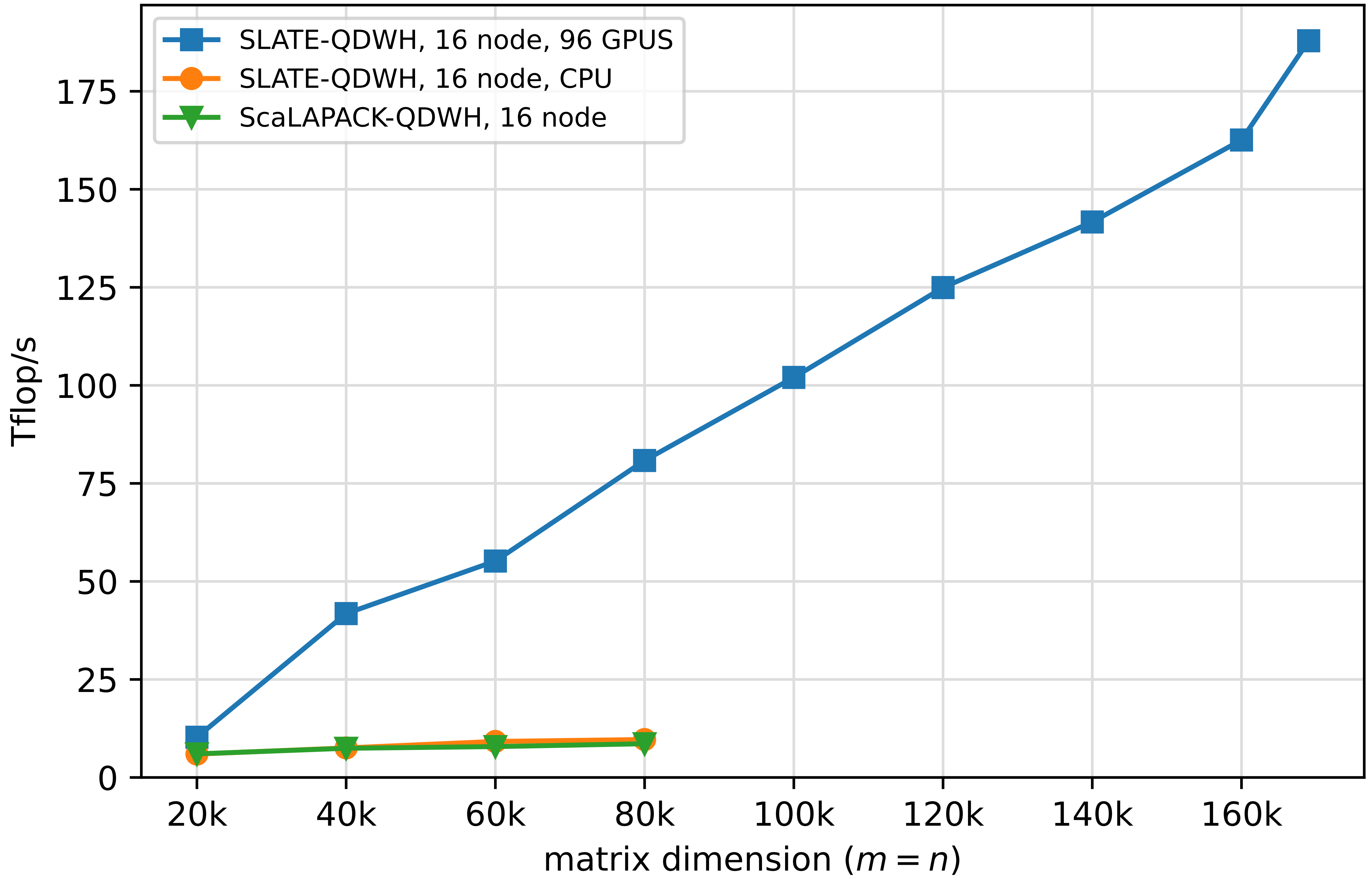


- Backward Error, $A - U_p\, H$



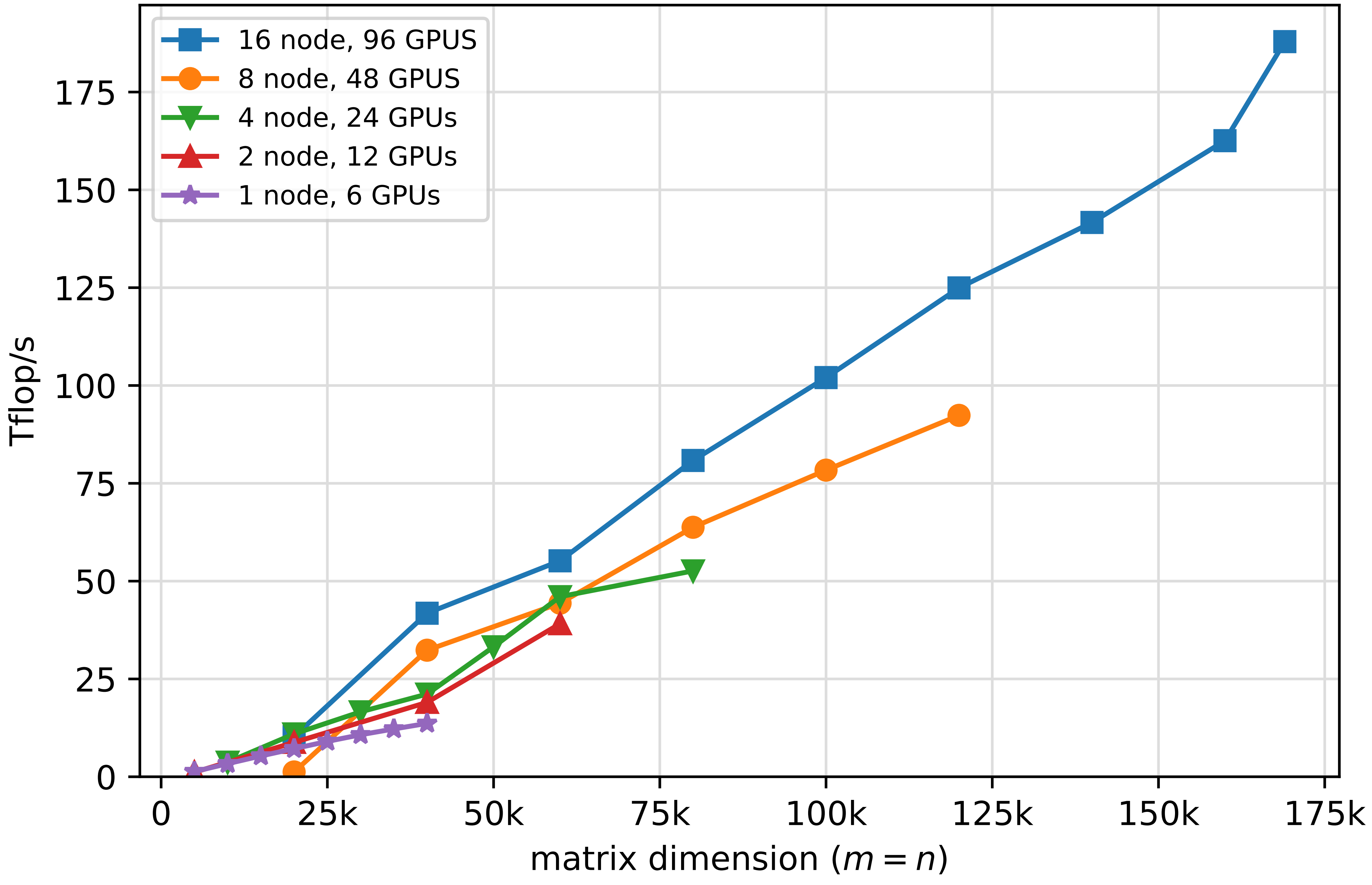
Results on Summit

- 16 node, SLATE GPU, SLATE CPU, ScaLAPACK CPU



Up to 18x speedup using GPUs

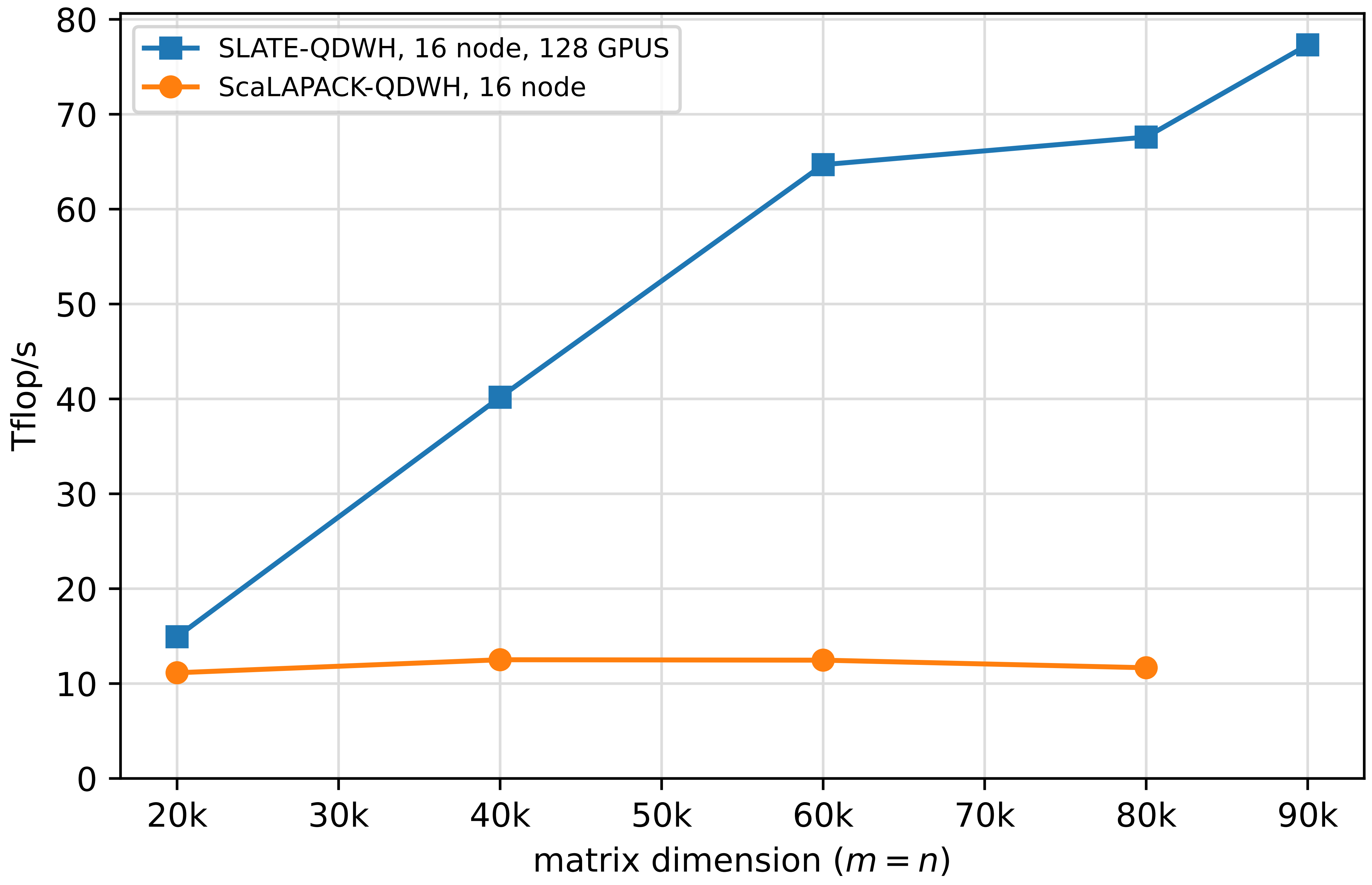
- 1 to 16 nodes, SLATE GPU



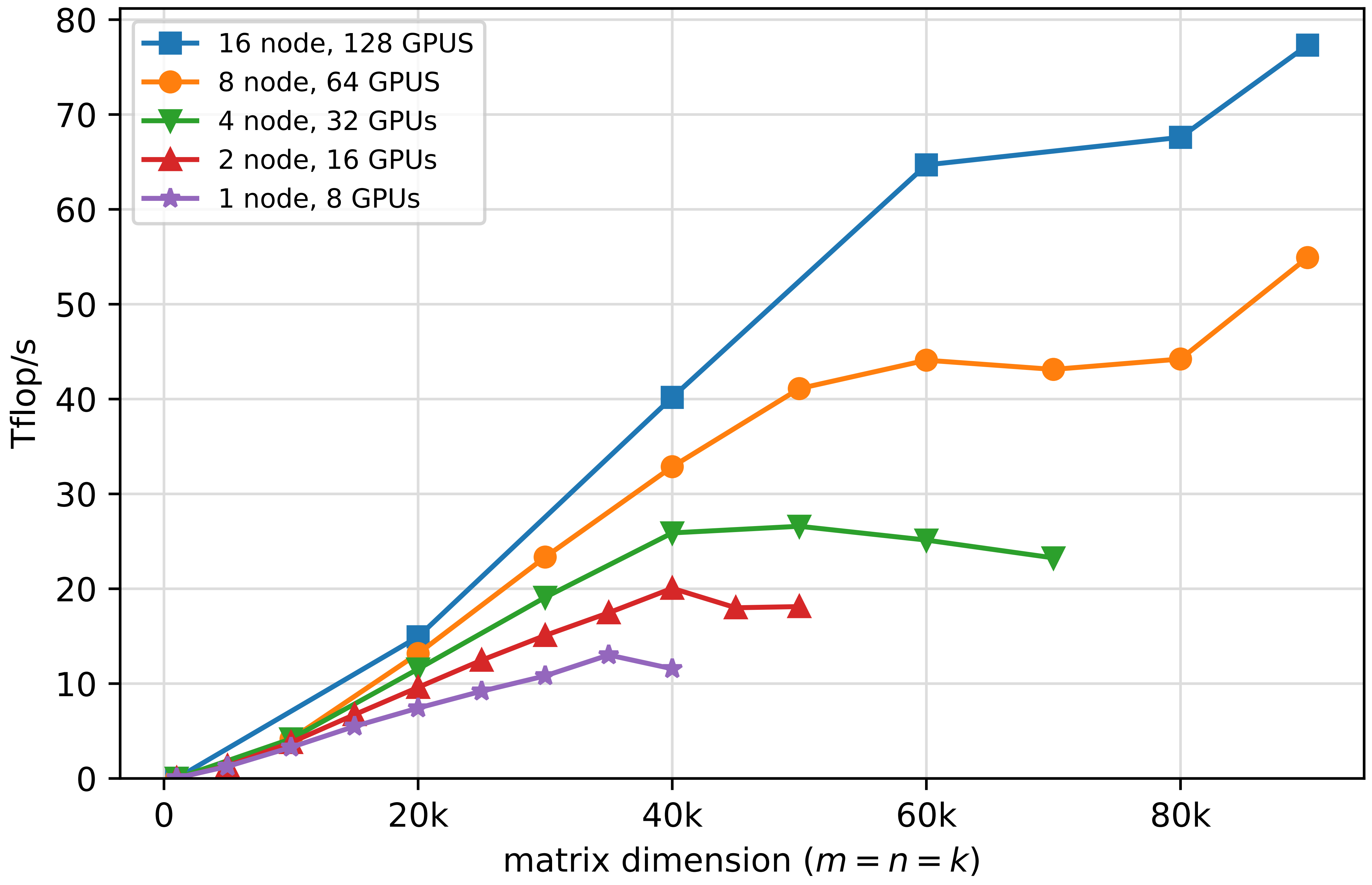
2x 22-core IBM POWER 9 CPU
+ 6 NVIDIA V100 GPUs per node

Results on Frontier

- 16 node, SLATE GPU, ScaLAPACK CPU



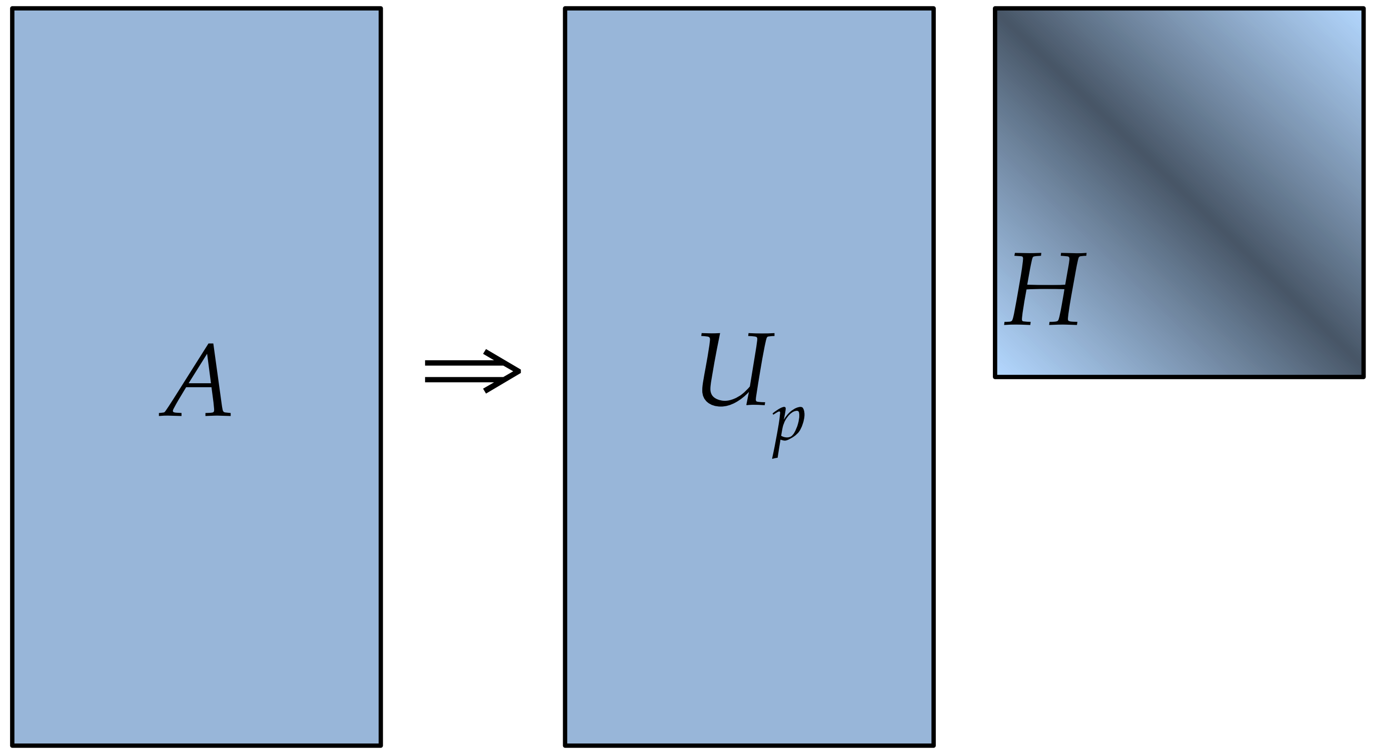
- 1 to 16 nodes, SLATE GPU



64-core AMD 3rd gen EPYC CPU
+ 8 AMD MI250X GPU GCDs per node

Summary

- Polar Decomposition using QR-based Dynamic Weighted Halley Iteration (QDWH)



- With SLATE, get CPU and GPU-accelerated, distributed implementation
- 18x speedup over ScaLAPACK CPU-based version in POLAR / Cray LibSci

Links and Acknowledgements

- SLATE, BLAS++, and LAPACK++ libraries
    - https://github.com/icl-utk-edu/slate/
    - https://github.com/icl-utk-edu/blaspp/
    - https://github.com/icl-utk-edu/lapackpp/

ECP
EXASCALE COMPUTING PROJECT

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