Massively Parallel Polar Decomposition on Distributed-Memory Systems

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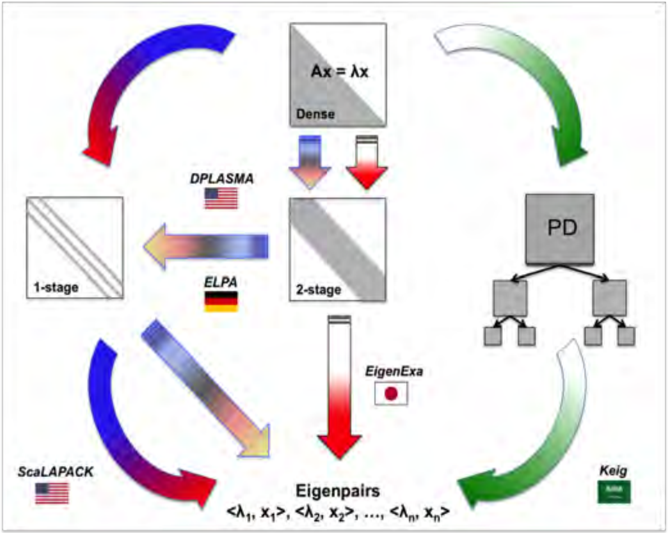
The Big Picture (Similar w/ SVD)



Cray LibSci 17.11.1

What is The Polar Decomposition ?

- The polar decomposition:

$$\mathbf{A} = \mathbf{U_p H}, \ A \in \mathbb{R}^{m \times n} (m \geq n),$$

where U_p is an orthogonal matrix and $H = \sqrt{A^\top A}$ is a symmetric positive semidefinite matrix

- The polar decomposition is a critical numerical algorithm for various applications, including aerospace computations, chemistry, factor analysis

Application to Symmetric Eigensolvers and SVD

The polar decomposition can be used as pre-processing step toward calculating the:

- The SVD $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^\top$:

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

- The EVD: $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^\top$, $V = [V_1 V_2]$

$$\begin{aligned} A &= U_p H \\ U_p + I &= \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} I_k & 0 \\ 0 & -I_{n-k} \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^* + I \\ &= \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^* \\ &= 2V_1 V_1^* \end{aligned}$$

$$A_1 = V_1^\top A V_1, A_2 = V_2^\top A V_2$$

Background

- **1877** — Zolotarev, best rational approximant for the scalar sign function.
- **1902** — Autonne, *SMF, definition of the polar decomposition.*
- **1994** — Higham and Papadimitriou, *SIAM, matrix inversion QDWH, shared-memory systems.*
- **2010** — Nakatsukasa et. al, *SIAM, inverse-free QDWH, theoretical accuracy study.*
- **2013** — Nakatsukasa and Higham, *SIAM, QDWH-EIG, QDWH-SVD, theoretical accuracy study.*
- **2014** — Nakatsukasa, *SIAM, ZOLO-PD, ZOLO-SVD, ZOLO-EIG, theoretical accuracy study.*
- **2016** — Sukkari, Ltaief and Keyes, *TOMS, QDWH-SVD, block algorithm, shared-memory system equipped with* multiple GPUs*.*
- **2016** — Sukkari, Ltaief and Keyes, *Euro-Par, QDWH, QDWH-SVD, block algorithm, distributed-memory system.*
- **2017** — Sukkari, Ltaief, Faverge and Keyes, *TPDS, QDWH, task-based, shared-memory system equipped with* multiple GPUs*.*
- **2018** — Sukkari, Ltaief, Esposito, Nakatsukasa and Keyes, *TOPC, ZOLO-PD, block algorithm, distributed-memory system.*

The Polar Decomposition Algorithms

- QDWH:

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

$$X_{k+1} = \frac{b_k}{c_k} X_k + \frac{1}{\sqrt{c_k}} \left(a_k - \frac{b_k}{c_k} \right) Q_1 Q_2^*.$$

- Zolo-PD:

$$\begin{bmatrix} X_k \\ \sqrt{c_{2j-1}} I \end{bmatrix} = \begin{bmatrix} Q_{j1} \\ Q_{j2} \end{bmatrix} R_j,$$

$$X_{k+1} = X_k + \Sigma_{j=1}^{r} \frac{a_j}{\sqrt{c_{2j-1}}} Q_{j1} Q_{j2}^*.$$

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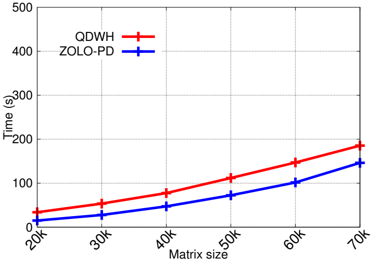
Under Consideration by Cray LibSci

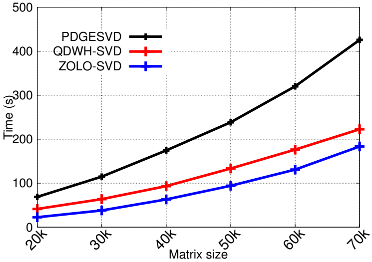
For Ill-conditioned matrices, in double precision, QDWH converges after 6 **successive** iterations, while ZOLO-PD converges after 2 **successive** iterations, each execute 8 **independent** embarrassingly parallel factorizations

Arithmetic Compexity and Performance

	QDWH	Successive ZOLOPD	Independent ZOLOPD
# QR-based iter	2	8	1
# Cholesky-based iter	4	8	1
Algorithmic complexity	$33n^3$	$100n^3$	15 n^3
Memory footprint	$6n^2$	$6n^2$	$48n^2$



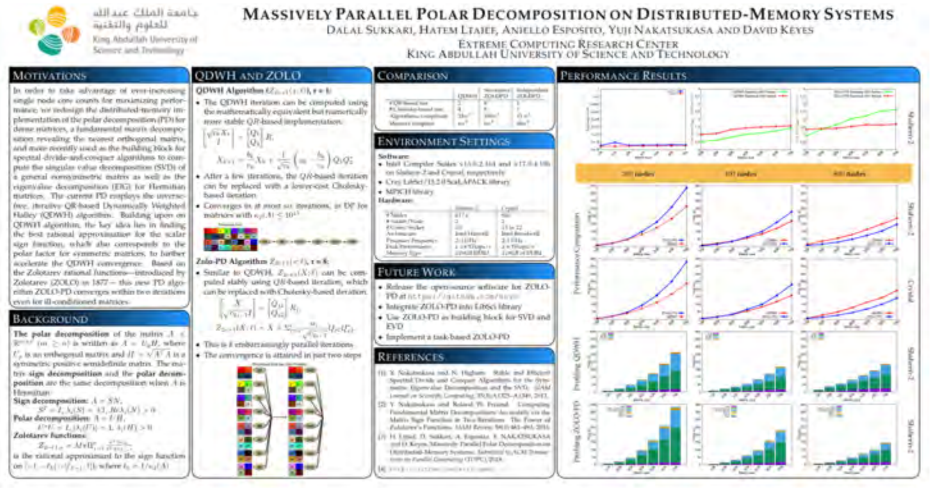
(a) Polar Decomposition



(b) SVD solvers

Cray XC40, 800 nodes, Intel Haswell 2.3GHz two-sockets 16 cores

Thank you


MASSIVELY PARALLEL POLAR DECOMPOSITION ON DISTRIBUTED-MEMORY SYSTEMS
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