INVENTORS FOR THE DIGITAL WORLD

Large scale SVD using polar decomposition

M. Faverge

Outline

1. Classic solution to solve large SVD problems
2. Using the polar decomposition
   - The QDWH-based Polar Decomposition
   - The ZOLO-based Polar Decomposition
   - Preliminary results with Scalapack [D. Sukkari's PhD]
3. Task based algorithms
4. Alternative solutions to (partial-SVD)

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SVD - Singular Value Decomposition

$$A = U\Sigma V^T$$

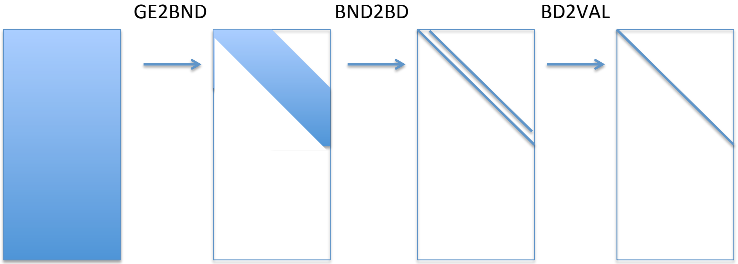
- A is general matrix
- Σ are the singular values of A
- U are the left singular vectors
- V are the right singular vectors

Singular Value Decomposition

$A = U\Sigma V^T$

- Focus on getting the singular values only (GEVAL)
- Use three steps algorithms:

GE2BND	Reduce the general matrix to general band
BND2BD	Reduce the general band to bidiagonal
BD2VAL	Compute the singular values from the bidiagonal



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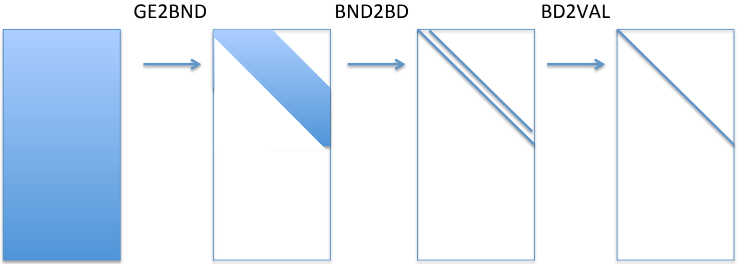
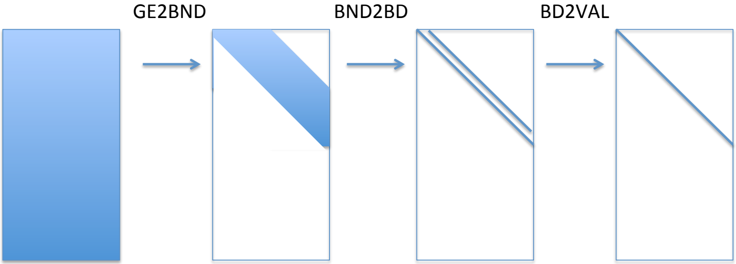


Singular Value Decomposition

$A = U\Sigma V^T$

- Focus on getting the singular values only (GEVAL)
- Use three steps algorithms:

GE2BND	**Reduce the general matrix to general band**
BND2BD	Reduce the general band to bidiagonal (PLASMA)
BD2VAL	Compute the singular values from the bidiagonal

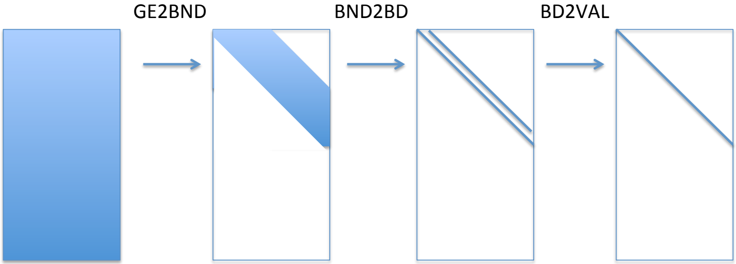


Singular Value Decomposition

$A = U\Sigma V^T$

- Focus on getting the singular values only (GEVAL)
- Use three steps algorithms:

GE2BND	**Reduce the general matrix to general band**
BND2BD	Reduce the general band to bidiagonal (PLASMA)
BD2VAL	Compute the singular values from the bidiagonal (MKL)



Two(-Three) stages algorithms

1. Reduction to tridiagonal form $A = U'BV'^T$
   - B is a bidiagonal matrix
   - U' and V' are unitary matrices
2. Find the singular values of the bidiagonal matrix B: $B = Q * \Sigma * P^t$
3. Eventually compute the eigenvectors: $U = U'Q$, and $V^t = (V'P)^t$

Problem: Reduction to tridiagonal is using BLAS 2

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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

A Major Building Block Toward Important DLA Algorithms

The polar decomposition can be used as a pre-processing step toward solving:

- *the symmetric eigenvalue problem*: $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top$, $V = [V_1 V_2]$
- *the singular value decomposition*: $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$

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

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QDWH Polar Decomposition Algorithm

$$A = U_p H$$

where, $U_p U_p^\top = I_n$, H is symmetric positive semidefinite

- Backward stable algorithm for computing the polar decomposition
- Based on conventional computational kernels, i.e., Cholesky/QR factorizations (≤ 6 iterations for double precision) and GEMM
- The total flop count for QDWH depends on the condition number of the matrix κ:

κ	1	10^{16}
flops	$(10 + \frac{2}{3})n^3$	$43n^3$

QDWH Polar Decomposition Algorithm (cont'd)

The QDWH iteration is:

$$X_0 = A/\alpha, \begin{bmatrix} \sqrt{c_k} X_k \\ I \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R, \; X_{k+1} \quad = \frac{b_k}{c_k} X_k + \frac{1}{\sqrt{c_k}} \left(a_k - \frac{b_k}{c_k} \right) Q_1 Q_2^\top, \; k \geq 0 \tag{1}$$

When, X_k becomes well-conditioned, it is possible to replace Equation 1 with a Cholesky-based implementation as follows:

$$X_{k+1} = \frac{b_k}{c_k} X_k + \left(a_k - \frac{b_k}{c_k} \right) (X_k W_k^{-1}) W_k^{-\top}, W_k \quad = \text{chol}(Z_k), \; Z_k = I + c_k X_k^\top X_k \tag{2}$$

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QDWH/ZOLO 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:

$$\begin{bmatrix} X_k \\ \sqrt{c_{2j-1}} I \end{bmatrix} = \begin{bmatrix} Q_{j1} \\ Q_{j2} \end{bmatrix} R_j, \; X_{k+1} = X_k + \Sigma_{j=1}^{r} \frac{a_j}{\sqrt{c_{2j-1}}} Q_{j1} Q_{j2}^*.$$

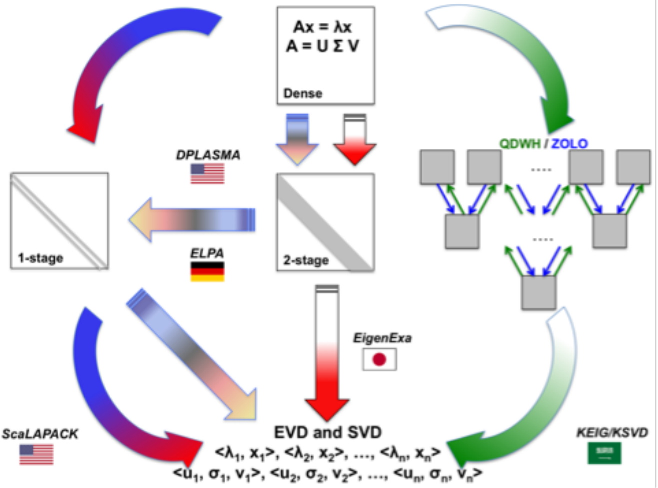
- For Ill-conditioned matrices, in double precision, QDWH converges after 6 **successive** iterations, while ZOLO converges after 2 **successive** iterations, each execute 8 **independent** embarrassingly parallel factorizations

ZOLO Arithmetic Complexity VS QDWH

Table 1: Algorithmic complexity and memory footprint for various PD algorithms with $\kappa_2(A) = 10^{12}$.

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

The Big Picture (Similar w/ SVD)



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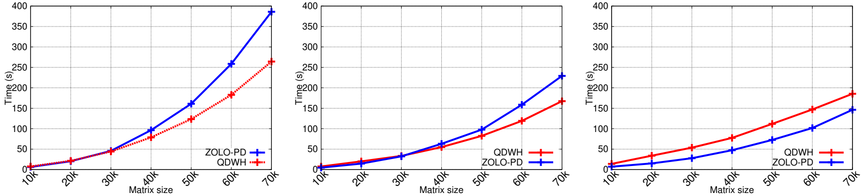
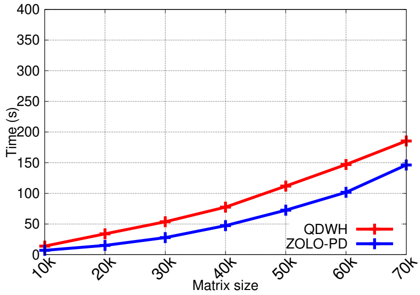
Performance Comparison on *Shaheen-2* (Polar-Decomposition)



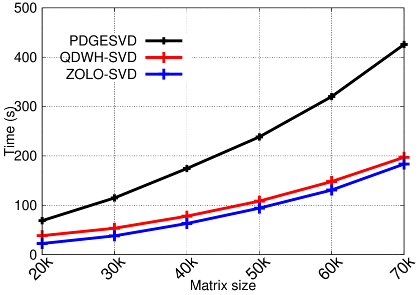
(a) 200 nodes. (b) 400 nodes. (c) 800 nodes.

Figure 1: QDWH versus ZOLO-PD.

Performance Results: From PD To SVD on 800 nodes of *Shaheen-2*



(a) Polar Decomposition



(b) SVD solvers

Outline

Summary of what is done

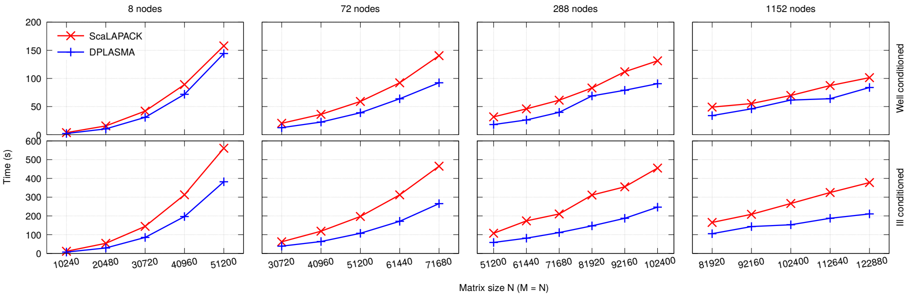
QDWH

- DPLASMA [Cluster 2019]
  Distributed memory / No GPUs
- Chameleon [TPDS 2017]
  Shared Memory / GPUs
- Distributed+GPUs ???

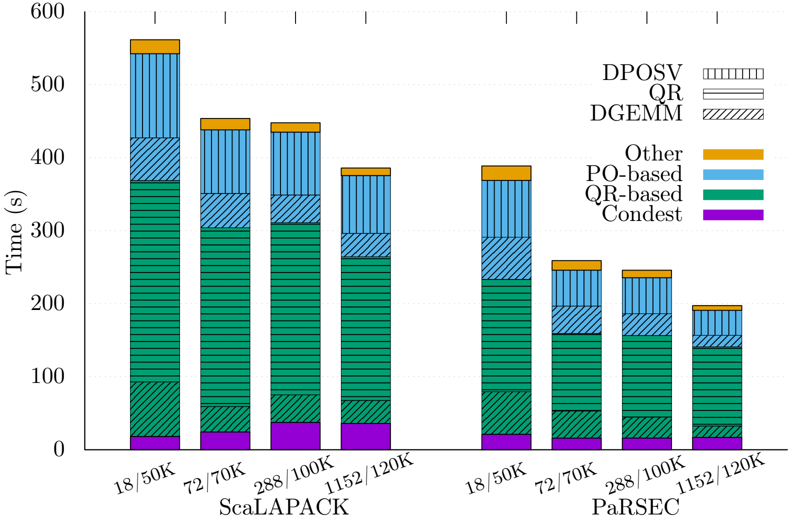
ZOLO

- Chameleon: on-going

Performance Comparisons Using Well and Ill-Conditioned Matrices



Performance Breakdown on # Nodes / Matrix Size N



What is missing for an efficient ZOLO algorithm

- Is it possible to save some memory thanks to the task-based algorithm ? (Avoid the 48 factor)
- Exploit the dynamic task-based computations to better balanced the replicated problems
- Efficient reduction step to merge the partial solutions together
- Will there be scheduling issues with the very large amount of tasks and the pipelining of the stages?

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4. **Alternative solutions to (partial-SVD)**

Other solutions that can be used for (partial-)SVD

- Randomized SVD (cf Diodon project)
- Partial QR with column pivoting
  Pb with the norm computations and the pivoting
- Randomized QR with column pivoting
  Similar issue as before but can localize the pivoting in a smaller matrix than can be replicated to avoid communications.
- Truncated QR factorization algorithms
  Issue with the storage of the updates
- In previous solutions, the pivoting strategy can be replace by a rotation solution, that replaces the column pivoting by a matrix-matrix product.

Thank you ☺

Sequential Task Graph: StarPU pseudo-code with Cholesky factorization

```
for (k = 0; k < NT; k+)
  potrf( RW, A[k][k] );
  for (n = k+1; n < NT; n++)
    trsm( READ, A[k][k], RW, A[k][n] );
  for (m = k+1; m < NT; m++)
    syrk( READ, A[k][m], RW, A[m][m] );
    for (n = m+1; n < NT; n++) {
      gemm( READ, A[k][m], READ, A[k][n],
                 RW, A[m][n] );
```

Leveraging QDWH-TB from Shmem to Distmem

1877 Zolotarev, best rational approximant for the scalar sign function.

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.

Parametrized Task Graph: PaRSEC pseudo-code with Cholesky factorization (POTRF and TRSM)

```
potrf(k)

  // Execution space
  k = 0 .. NT-1

  // Parallel partitioning
  :A(k, k)

  RW T   <- (k == 0) ? A(k, k)
              [U]
         <- (k != 0) ? T syrk(k
    -1, k) [U]

         -> T trsm(k, k+1..NT
    -1)        [U]
         -> A(k, k)
              [U]
```

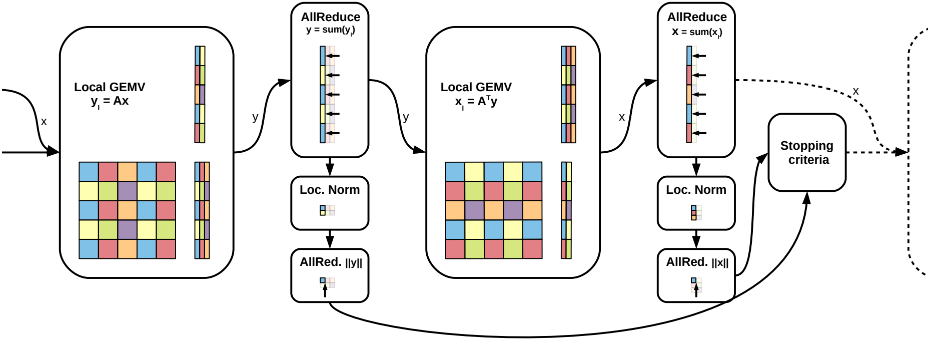
```
trsm(k, n)
  // Execution space
  k = 0   .. NT-2
  n = k+1 .. NT-1
  // Parallel partitioning
  : A(k, n)

  READ T <- T potrf(k)
              [U]
  RW   C <- (k == 0) ? A(k, n)
         <- (k != 0) ? C gemm(k
    -1, n, k)
         -> A syrk(k, n)
         -> A gemm(k, n, n+1..
    NT-1)
         -> B gemm(k, k+1..n-1,
     n)
         -> A(k, n)
```

Parametrized Task Graph: PaRSEC pseudo-code with Cholesky factorization (SYRK and GEMM)

```
syrk(k, m)
  // Execution space
  k = 0   .. NT-2
  m = k+1 .. NT-1
  // Parallel partitioning
  : A(m, m)

  READ A <- C trsm(k, m)

  RW   T <- (k == 0) ? A(m, m)
           [U]
         <- (k != 0) ? T syrk(k
    -1, m)    [U]

         -> (m == k+1) ? T
    potrf(m)       [U]
         -> (m != k+1) ? T
    syrk(k+1, m)  [U]
```

```
gemm(k, m, n)
  // Execution space
  k = 0   .. NT-3
  m = k+1 .. NT-1
  n = m+1 .. NT-1
  // Parallel partitioning
  : A(m, n)

  READ A <- C trsm(k, m)
  READ B <- C trsm(k, n)
  RW   C <- (k == 0) ? A(m, n)
         <- (k != 0) ? C gemm(k
    -1, m, n)
         -> (m == k+1) ? C
    trsm(m, n)
         -> (m != k+1) ? C
    gemm(k+1, m, n)
```

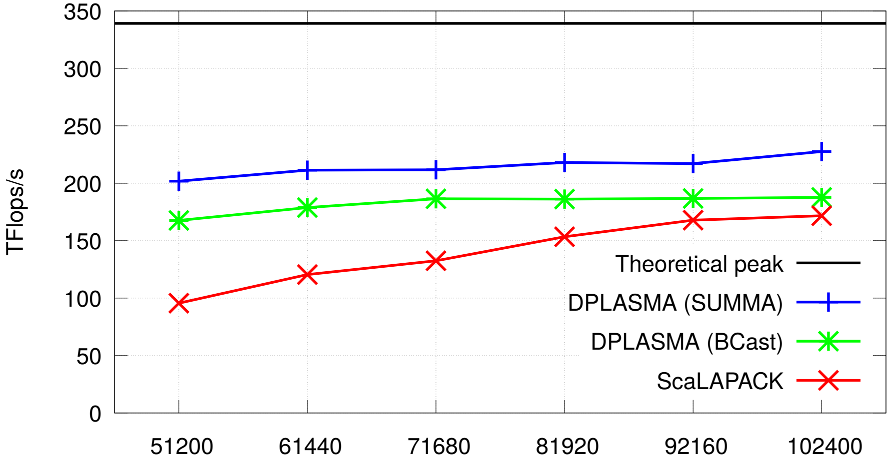
(1) Task-based Design of the Matrix Two-Norm Estimation



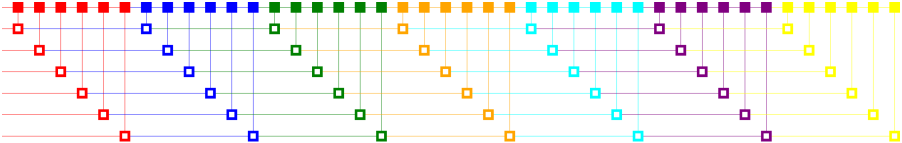
(2) Scalable Universal Matrix Multiplication Algorithm (SUMMA)

- SUMMA replaces standard broadcasts with pipelined rings of communication
- Already implemented in ScaLAPACK for distributed-memory GEMM operations
- Fine-grained computations expose a low-level control of communications, which provide more flexibility for scheduling of computational tasks and communications.
- For instance: overlapping, network congestion, communication load balancing, etc.

Performance Impact in TFlop/s on 288 nodes w/ SUMMA for Matrix-Matrix Multiplication

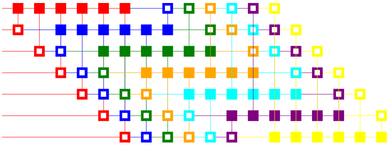


(3) Hierarchical QR Factorization Using Tree Reduction: Flat Tree $Flat(0)$ (or Domino)



Long critical path ☹
High communication volume ☹

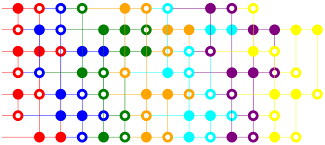
(3) Hierarchical QR Factorization Using Tree Reduction: $Flat(k)$



Short critical path ☺

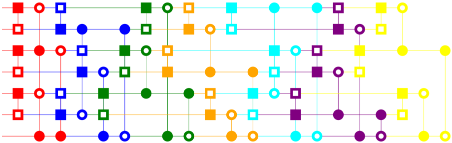
High communication volume ☹

(3) Hierarchical QR Factorization Using Tree Reduction: Greedy



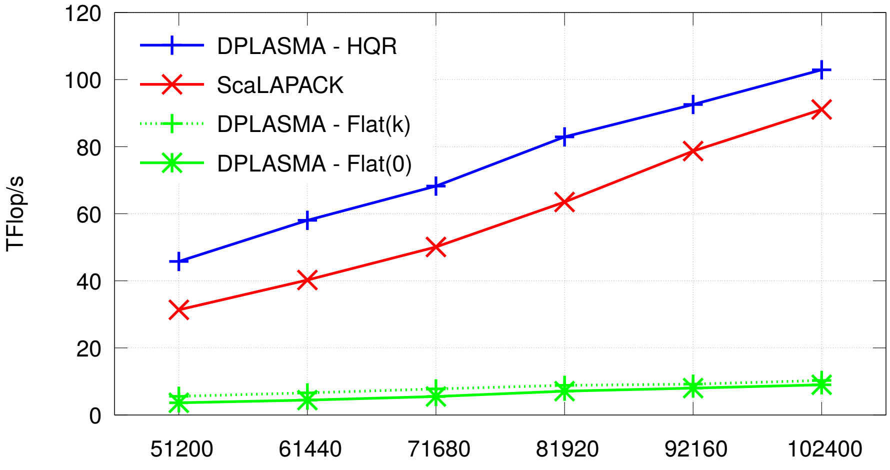
Short critical path ☺
Low communication volume ☺
Low kernels' arithmetic intensity ☹

(3) Hierarchical QR Factorization Using Tree Reduction: Mixing Greedy + flat

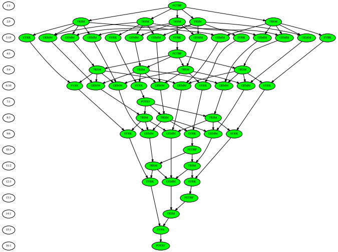


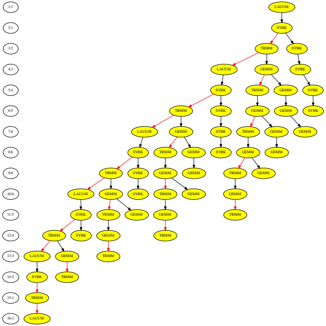
Short critical path ☺
Low communication volume ☺
High kernels' arithmetic intensity ☺

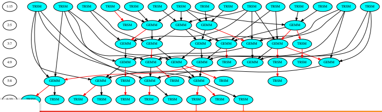
Performance Impact in TFlop/s on 288 nodes w/ HQR for the QR Factorization

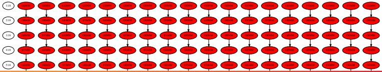


(4) Composing Directed Acyclic Graphs









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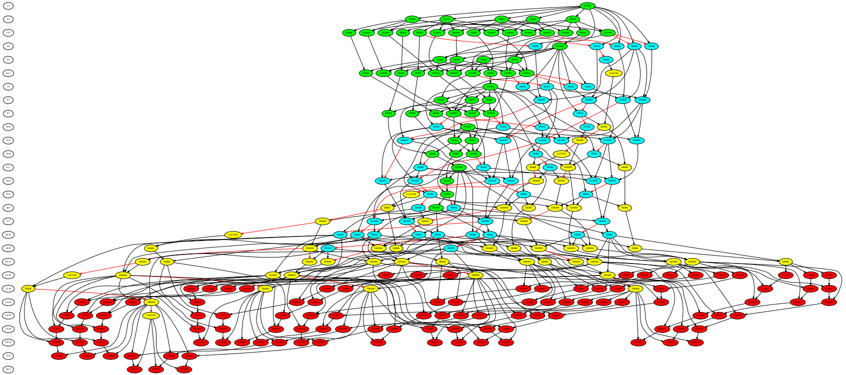

Performance Impact in TFlop/s on 288 nodes w/ DAG Composition for Cholesky-based Linear Solvers