Communication-avoiding factorization algorithms

Edgar Solomonik

Department of Computer Science, University of Illinois at Urbana-Champaign

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L P N A @CS@Illinois

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Algorithms should minimize communication, not just computation

- communication and synchronization cost more energy than flops

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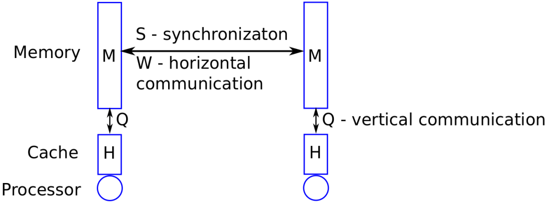

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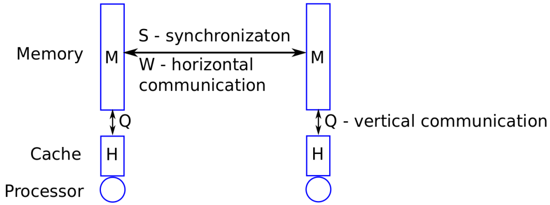

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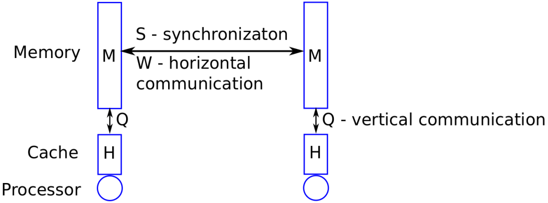

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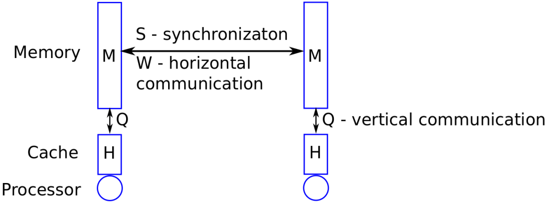

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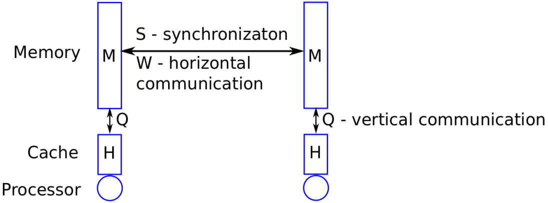

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- parallel algorithm design involves tradeoffs: computation vs communication vs synchronization
- parameterized algorithms provide optimality and flexibility

Cost model for parallel algorithms

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$$T = \sum_{i=1}^{S} \alpha + w_i \cdot \beta + q_i \cdot \nu + f_i \cdot \gamma = O(S \cdot \alpha + W \cdot \beta + Q \cdot \nu + F \cdot \gamma)$$

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  where typically $\alpha \gg \beta \gg \nu \gg \gamma$
- we mention vertical communication cost only when it exceeds $Q = O(F/\sqrt{H} + W)$ where H is cache size

Communication complexity of matrix multiplication

Multiplication of $\boldsymbol{A} \in \mathbb{R}^{m \times k}$ and $\boldsymbol{B} \in \mathbb{R}^{k \times n}$ can be done in $O(1)$ supersteps with communication cost $W = O\left(\left(\frac{mnk}{p}\right)^{2/3}\right)$ provided sufficient memory and sufficiently large p

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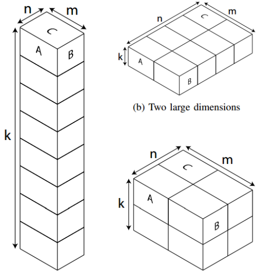
- when m, n, k are unequal, need appropriate processor grid[2]



(a) One large dimension (b) Two large dimensions (c) Three large dimensions

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Communication complexity of dense matrix kernels

For $n \times n$ Cholesky with p processors

$$F = O(n^3/p), \quad W = O(n^2/p^\delta), \quad S = O(p^\delta)$$

given memory to store $p^{2\delta-1}$ copies of the matrix for any $\delta = [1/2, 2/3]$.

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Can achieve similar costs for LU, QR, and the symmetric eigenvalue problem (modulo logarithmic factors on synchronization), but algorithmic changes (as opposed to parallel schedules) are necessary.

triangular solve	square TRSM ✓[3]	rectangular TRSM ✓[4]
LU with pivoting	pairwise pivoting ✓[5]	tournament pivoting ✓[6]
QR factorization	Givens on square ✓[3]	Householder on rect. ✓[7]
SVD (sym. eig.)	singular values only ✓[8]	singular vectors X

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Tradeoffs between costs based on dependency graphs

Definition ((ϵ, σ)-path-expander)

Graph $G = (V, E)$ is a (ϵ, σ)-**path-expander** if there exists a path $(u_1, \ldots u_n) \subset V$, such that the dependency interval $[u_i, u_{i+b}]_G$ for each i, b has size $\Theta(\sigma(b))$ and a minimum cut of size $\Omega(\epsilon(b))$.

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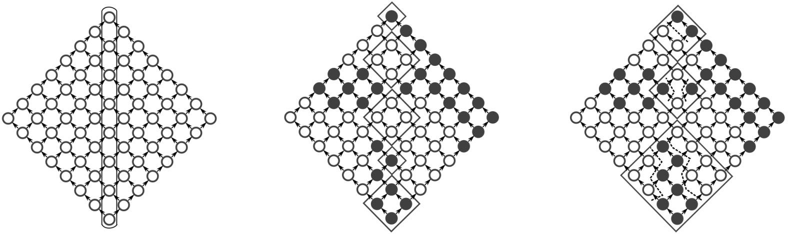

Dependency chain P   Monochrome dependency intervals   Multicolored dependency intervals

- computation-synchronizaton tradeoff in diamond DAG[8]: $F\cdot S=\Omega(n^2)$
- extends to triangular solve, matrix factorization, and iterative methods[9]

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Theorem (Path-expander communication lower bound)

*Any parallel schedule of an algorithm with a (ϵ, σ)-**path-expander** dependency graph about a path of length n and some $b \in [1, n]$ incurs computation (F), communication (W), and synchronization (S) costs:*

$$F = \Omega\left(\sigma(b) \cdot n/b\right), \quad W = \Omega\left(\epsilon(b) \cdot n/b\right), \quad S = \Omega\left(n/b\right).$$

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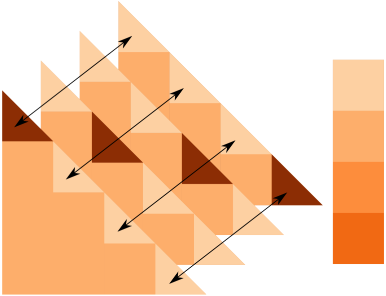
Corollary (Computation-sync. and bandwidth-sync. tradeoffs)

If $\sigma(b) = b^d$ and $\epsilon(b) = b^{d-1}$, the above theorem yields,

$$F \cdot S^{d-1} = \Omega(n^d), \;\; W \cdot S^{d-2} = \Omega(n^{d-1}).$$

New algorithms can circumvent lower bounds

For TRSM, we can achieve a lower synchronization/communication cost by performing triangular inversion on diagonal blocks



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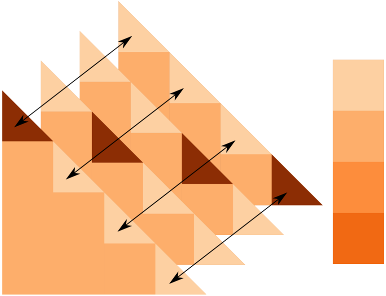

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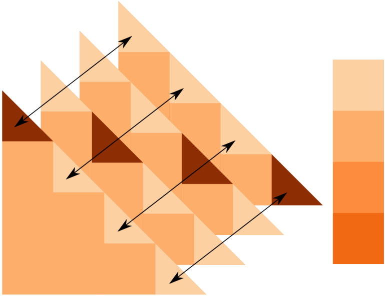

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- optimal communication for any number of right-hand sides

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QR factorization of tall-and-skinny matrices

Consider the reduced factorization $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}$ with $\boldsymbol{A}, \boldsymbol{Q} \in \mathbb{R}^{m\times n}$ and $\boldsymbol{R} \in \mathbb{R}^{n\times n}$ when $m \gg n$ (in particular $m \geq np$)

- $\boldsymbol{A}$ is tall-and-skinny, each processor owns a block of rows

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- Cholesky-QR2[13] stable so long as $\kappa(\boldsymbol{A}) \leq 1/\sqrt{\epsilon}$, achieves $W{=}O(n^2)$, $S{=}O(1)$, Cholesky-QR3[14] gets same and is unconditionally stable

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Square matrix QR algorithms generally use 1D QR for panel factorization

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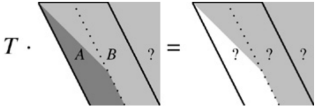
- Tiskin's 3D QR algorithm[15] achieves $W = O(n^2/p^{2/3})$ communication



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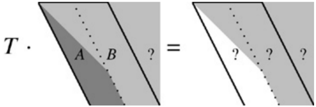
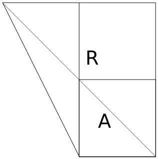


- however, requires slanted-panel matrix embedding



which is highly inefficient for rectangular (tall-and-skinny) matrices

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Communication-avoiding rectangular QR

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- note: interleaving rows of $\boldsymbol{R_1}$ and $\boldsymbol{R_2}$ gives a slanted panel

[16] E.S., G. Ballard, J. Demmel, and T. Hoefler, SPAA 2017

Communication-avoiding rectangular QR

For $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ existing algorithms are optimal when $m = n$ and $m \gg n$

- cases with $n < m < np$ underdetermined equations are important
- new algorithm[16]
  - subdivide p processors into m/n groups of pn/m processors
  - perform row-recursive QR (TSQR) with tree of height $\log_2(m/n)$
  - compute each tree-node elimination $\boldsymbol{Q_{12}R} = \begin{bmatrix}\boldsymbol{R_1}\\ \boldsymbol{R_2}\end{bmatrix}$ using Tiskin's QR with pn/m or more processors
- note: interleaving rows of $\boldsymbol{R_1}$ and $\boldsymbol{R_2}$ gives a slanted panel
- obtains ideal communication cost for any m, n, generally

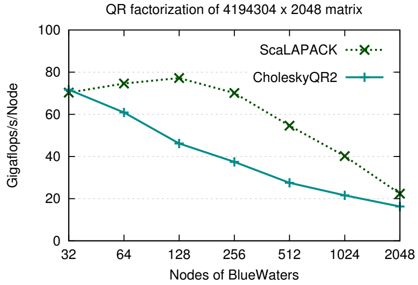
$$W = O\left(\left(\frac{mn^2}{p}\right)^{2/3}\right)$$

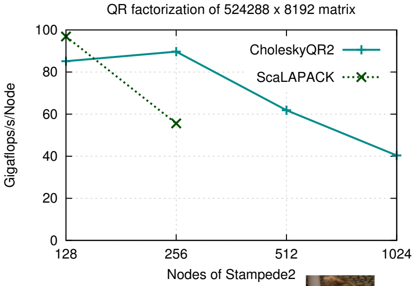
[16] E.S., G. Ballard, J. Demmel, and T. Hoefler, SPAA 2017

Cholesky-QR2 for rectangular matrices

Cholesky-QR2[17] with 3D Cholesky gives a practical 3D QR algorithm[18]

- Compute $\boldsymbol{A} = \hat{\boldsymbol{Q}}\hat{\boldsymbol{R}}$ using Cholesky-QR $\boldsymbol{A}^T\boldsymbol{A} = \hat{\boldsymbol{R}}^T\hat{\boldsymbol{R}}, \quad \hat{\boldsymbol{Q}} = \boldsymbol{A}\hat{\boldsymbol{R}}^{-1}$
- Correct approximate factorization by Cholesky-QR $\boldsymbol{Q}\bar{\boldsymbol{R}} = \hat{\boldsymbol{Q}}$, $\boldsymbol{R} = \bar{\boldsymbol{R}}\hat{\boldsymbol{R}}$
- Simple algorithm to achieve minimize comm. and sync. for any m, n, p





Analysis and implementation by PhD student Edward Hutter

[17] T. Fukaya, Y. Nakatsukasa, Y. Yanagisawa, Y. Yamamoto 2014

[18] E. Hutter, E.S. 2018

Tridiagonalization

Reducing the symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ to a tridiagonal matrix

$$\boldsymbol{T} = \boldsymbol{Q}^T \boldsymbol{A} \boldsymbol{Q}$$

via a two-sided orthogonal transformation is most costly in diagonalization (eigenvalue computation, SVD similar)

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- $b = 1$ gives direct tridiagonalization

Successive band reduction (SBR)

After reducing to a banded matrix, we need to transform the banded matrix to a tridiagonal one

[19] Lang 1993; Bischof, Lang, Sun 2000

[20] Ballard, Demmel, Knight 2012

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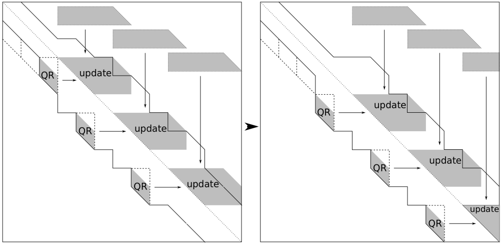

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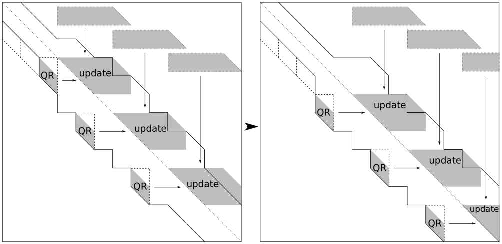

- communication- and synchronization-efficient 1D SBR algorithm known for small band-width[20]

[19] Lang 1993; Bischof, Lang, Sun 2000

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Communication-efficient eigenvalue computation

Previous work (start-of-the-art): two-stage tridiagonalization

- implemented in ELPA, can outperform ScaLAPACK[21]

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[23] E.S., G. Ballard, J. Demmel, T. Hoefler, SPAA 2017

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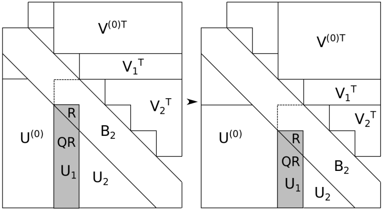

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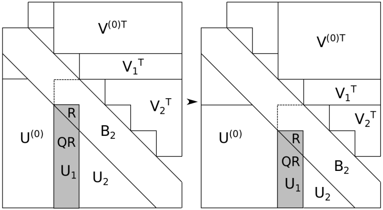

- 3D SBR (each QR and matrix multiplication update parallelized)

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[21] Auckenthaler, Bungartz, Huckle, Krämer, Lang, Willems 2011

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[23] E.S., G. Ballard, J. Demmel, T. Hoefler, SPAA 2017

Symmetric eigensolver results summary

Algorithm	W	Q	S
ScaLAPACK	$n^2/\sqrt{p}$	n^3/p	$n\log(p)$
ELPA	$n^2/\sqrt{p}$	-	$n\log(p)$
two-stage + 1D-SBR	$n^2/\sqrt{p}$	$n^2\log(n)/\sqrt{p}$	$\sqrt{p}(\log^2(p)+\log(n))$
many-stage	$n^2/p^{2/3}$	$n^2\log(p)/p^{2/3}$	$p^{2/3}\log^2 p$

- costs are asymptotic (same computational cost F for eigenvalues)
- W – horizontal (interprocessor) communication
- Q – vertical (memory–cache) communication excluding $W + F/\sqrt{H}$ where H is cache size
- S – synchronization cost (number of supersteps)

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Summary of new communication avoiding algorithms

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Future work

- back-transformations to compute eigenvectors in less computational complexity than $F = O(n^3 \log(p)/p)$

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- back-transformations to compute eigenvectors in less computational complexity than $F = O(n^3 \log(p)/p)$
- QR with column pivoting / low-rank SVD / sparse factorization

Acknowledgements

Collaborators on this work

- Edward Hutter (Department of Computer Science, University of Illinois at Urbana-Champaign)
- Grey Ballard (Department of Computer Science, Wake Forest University)
- James Demmel (Department of Computer Science and Department of Mathematics, University of California, Berkeley)
- Tobias Wicky (Department of Computer Science, ETH Zurich)
- Torsten Hoefler (Department of Computer Science, ETH Zurich)
- Erin Carson (Courant Institute of Mathematical Sciences, NYU)
- Nicholas Knight (Courant Institute of Mathematical Sciences, NYU)

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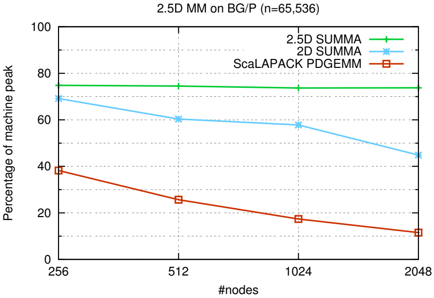
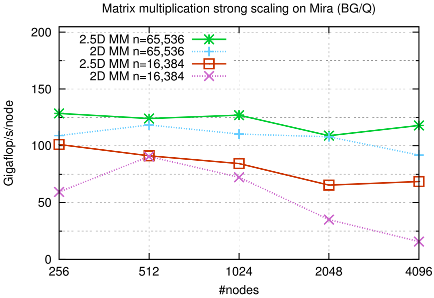
- DOE Computational Science Graduate Fellowship
- ETH Zurich Postdoctoral Fellowship
- XSEDE/TACC (Stampede2) and NCSA (BlueWaters)

Backup slides

Communication-efficient matrix multiplication





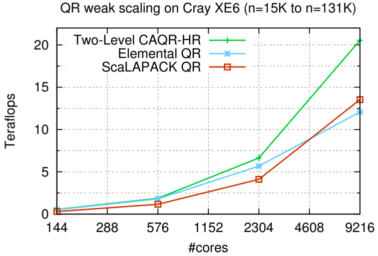
12X speed-up, 95% reduction in comm. for $n = 8$K on 16K nodes of BG/P

Communication-efficient QR factorization

- Householder form can be reconstructed quickly from TSQR[24]

$$\boldsymbol{Q} = \boldsymbol{I} - \boldsymbol{Y}\boldsymbol{T}\boldsymbol{Y}^T \qquad \Rightarrow \qquad \mathrm{LU}(\boldsymbol{I} - \boldsymbol{Q}) \rightarrow (\boldsymbol{Y}, \boldsymbol{T}\boldsymbol{Y}^T)$$

- Householder aggregation yields performance improvements

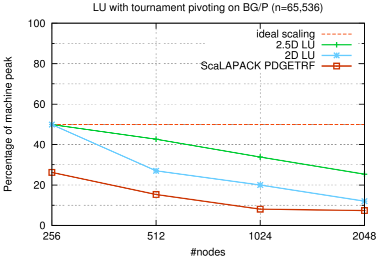


[24] Ballard, Demmel, Grigori, Jacquelin, Nguyen, S., IPDPS, 2014

Communication-efficient LU factorization

For any $c \in [1, p^{1/3}]$, use cn^2/p memory per processor and obtain

$$W_{\text{LU}} = O(n^2/\sqrt{cp}), \qquad S_{\text{LU}} = O(\sqrt{cp})$$



- LU with pairwise pivoting[25] extended to tournament pivoting[26]
- first implementation of a communication-optimal LU algorithm[11]

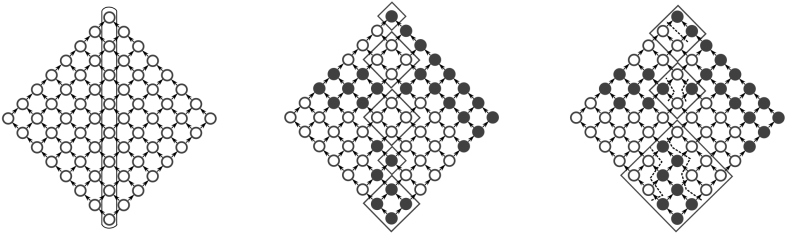
[25] Tiskin, FGCS, 2007

[26] S., Demmel, Euro-Par, 2011

Tradeoffs in the diamond DAG

Computation vs synchronization tradeoff for the $n \times n$ diamond DAG,[27]

$$F \cdot S = \Omega(n^2)$$



Dependency chain P   Monochrome dependency intervals   Multicolored dependency intervals

We generalize this idea[28]

- additionally consider horizontal communication
- allow arbitrary (polynomial or exponential) interval expansion

[27] Papadimitriou, Ullman, SIAM JC, 1987

[28] S., Carson, Knight, Demmel, SPAA 2014 (extended version, JPDC 2016)

Tradeoffs involving synchronization

We apply tradeoff lower bounds to dense linear algebra algorithms, represented via dependency hypergraphs:[29]
For triangular solve with an $n \times n$ matrix,

$$F_{\mathsf{TRSV}} \cdot S_{\mathsf{TRSV}} = \Omega\left(n^2\right)$$

For Cholesky of an $n \times n$ matrix,

$$F_{\mathsf{CHOL}} \cdot S_{\mathsf{CHOL}}^2 = \Omega\left(n^3\right) \qquad W_{\mathsf{CHOL}} \cdot S_{\mathsf{CHOL}} = \Omega\left(n^2\right)$$

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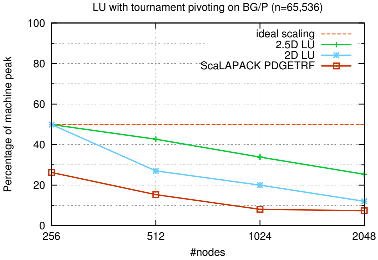

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