A communication-avoiding parallel algorithm for the symmetric eigenvalue problem

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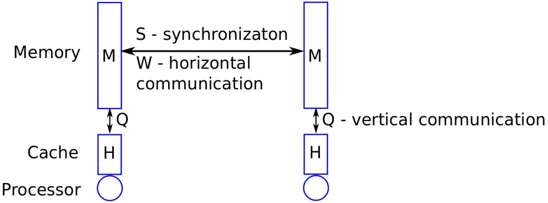
Beyond computational complexity

Algorithms should minimize communication, not just computation

- communication and synchronization cost more energy than flops
- two types of communication (data movement):



  - vertical (intranode memory–cache)
  - horizontal (internode network transfers)
- parallel algorithm design involves tradeoffs: computation vs communication vs synchronization
- parameterized algorithms provide optimality and flexibility

Cost model for parallel algorithms

We use the Bulk Synchronous Parallel (BSP) model (L.G. Valiant 1990)

- execution is subdivided into S supersteps, each associated with a global synchronization (cost α)
- at the start of each superstep, processors interchange messages, then they perform local computation
- if the maximum amount of data sent or received by any process is m_i (and work done is f_i) at superstep i then the BSP time is

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

We additionally consider vertical communication cost

- F – computation cost (local computation)
- Q – vertical communication cost (memory–cache traffic)
- W – horizontal communication cost (interprocessor communication)
- S – synchronization cost (number of supersteps)

Symmetric eigenvalue problem

Given a dense symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ find diagonal matrix $\boldsymbol{D}$ so

$$\boldsymbol{AX} = \boldsymbol{XD}$$

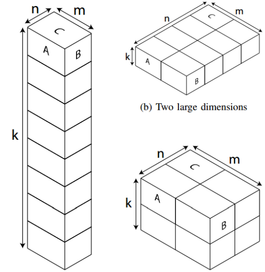
where $\boldsymbol{X}$ is an orthogonal matrix composed of eigenvectors of $\boldsymbol{A}$

- diagonalization – reduction of $\boldsymbol{A}$ to diagonal matrix $\boldsymbol{D}$
- computing the SVD has very similar computational structure
- we focus on tridiagonalization (bidiagonalization for SVD), from which standard approaches (e.g. MRRR, see Dhillon, Parlett, Vömel, 2006) can be used
- core building blocks:
  - matrix multiplication
  - QR factorization
- QR, SVD, diagonalization of lare matrices are needed for appications in scientific computing, data analysis and beyond

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 $W = O\Big(\big(\frac{mnk}{p}\big)^{2/3}\Big)$ provided sufficiently memory and sufficiently large p

- when $m = n = k$, 3D blocking gets $O(p^{1/6})$ improvement over 2D[1]
- when m, n, k are unequal, need appropriate processor grid[2]



(a) One large dimension

(b) Two large dimensions

(c) Three large dimensions

[1] J. Berntsen, Par. Comp., 1989; A. Aggarwal, A. Chandra, M. Snir, TCS, 1990; R.C. Agarwal, S.M. Balle, F.G. Gustavson, M. Joshi, P. Palkar, IBM, 1995; F.W. McColl, A. Tiskin, Algorithmica, 1999; ...

[2] J. Demmel, D. Eliahu, A. Fox, S. Kamil, B. Lipshitz, O. Schwartz, O. Spillinger 2013

Bandwidth-efficient QR and diagonalization

Goal: achieve the same communication complexity for QR and diagonalization as for matrix multiplication

- synchronization complexity expected to be higher

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

  product of communication and synchronization cost must be greater than the square of the number of columns[3]

- general strategy
  1. use communication-efficient matrix-multiplication for QR
  2. use communication-efficient QR for diagonalization

[3] E.S., E. Carson, N. Knight, J. Demmel, SPAA 2014 (TOPC 2016)

Communication complexity of dense matrix kernels

For $n \times n$ Cholesky with p processors, optimal parallel schedules attain

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

for any $\delta = [1/2, 2/3]$.
Achieving similar costs for LU, QR, and the symmetric eigenvalue problem requires some algorithmic tweaks.

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

✓ means costs attained (synchronization within polylogarithmic factors).

[4] B. Lipshitz, MS thesis 2013
[5] T. Wicky, E.S., T. Hoefler, IPDPS 2017
[6] A. Tiskin, FGCS 2007
[7] E.S., J. Demmel, EuroPar 2011
[8] E.S., G. Ballard, T. Hoefler, J. Demmel, SPAA 2017

QR factorization of tall-and-skinny matrices

Consider the reduced factorization $\boldsymbol{A} = \boldsymbol{QR}$ 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
- Householder-QR requires $S = \Theta(n)$ supersteps, $W = O(n^2)$
- Cholesky-QR2, TSQR, and HR-TSQR only $S = \Theta(\log(p))$ supersteps
- TSQR[9]: row-recursive divide-and-conquer, $W = O(n^2 \log(p))$

$$\begin{bmatrix} \boldsymbol{Q}_1\boldsymbol{R}_1 \\ \boldsymbol{Q}_2\boldsymbol{R}_2 \end{bmatrix} = \begin{bmatrix} \text{TSQR}(\boldsymbol{A}_1) \\ \text{TSQR}(\boldsymbol{A}_2) \end{bmatrix}, [\boldsymbol{Q}_{12}, \boldsymbol{R}] = \text{QR}\left(\begin{bmatrix} \boldsymbol{R}_1 \\ \boldsymbol{R}_2 \end{bmatrix} \right), \boldsymbol{Q} = \begin{bmatrix} \boldsymbol{Q}_1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q}_2 \end{bmatrix} \boldsymbol{Q}_{12}$$

- TSQR-HR[10]: TSQR + Householder-reconstruction, $W = O(n^2 \log(p))$
- Cholesky-QR2[11]: stable so long as $\kappa(\boldsymbol{A}) \leq 1/\sqrt{\epsilon}$, achieves $W = O(n^2)$

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[9] J. Demmel, L. Grigori, M. Hoemmen, J. Langou 2012

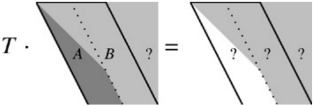
[10] G. Ballard, J. Demmel, L. Grigori, M. Jacquelin, H.-D. Nguyen, E.S. 2014

[11] Y. Yamamoto, Y. Nakatsukasa, Y. Yanagisawa, T. Fukaya 2015

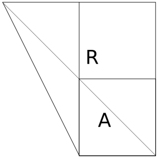
QR factorization of square matrices

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

- algorithms in ScaLAPACK, Elemental, DPLASMA use 2D layout, generally achieve $W = O(n^2/\sqrt{p})$ cost
- Tiskin's 3D QR algorithm[12] achieves $W = O(n^2/p^{2/3})$ communication



- however, requires slanted-panel matrix embedding



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

[12] A. Tiskin 2007, "Communication-efficient generic pairwise elimination"

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
  - 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 $\text{QR}\left(\begin{bmatrix}\boldsymbol{R_1}\\ \boldsymbol{R_2}\end{bmatrix}\right)$ 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

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

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

- can be done by successive column QR factorizations

$$\boldsymbol{T} = \underbrace{\boldsymbol{Q}_1^T \cdots \boldsymbol{Q}_n^T}_{\boldsymbol{Q}^T} \boldsymbol{A} \underbrace{\boldsymbol{Q}_1 \cdots \boldsymbol{Q}_n}_{\boldsymbol{Q}}$$

- two-sided updates harder to manage than one-sided
- can use n/b QRs on panels of b columns to go to band-width $b+1$
- $b = 1$ gives direct tridiagonalization

Multi-stage tridiagonalization

Writing the orthogonal transformation in Householder form, we get

$$\underbrace{(\boldsymbol{I} - \boldsymbol{U}\boldsymbol{T}\boldsymbol{U}^T)^T}_{\boldsymbol{Q}^T} \boldsymbol{A} \underbrace{(\boldsymbol{I} - \boldsymbol{U}\boldsymbol{T}\boldsymbol{U}^T)}_{\boldsymbol{Q}} = \boldsymbol{A} - \boldsymbol{U}\boldsymbol{V}^T - \boldsymbol{V}\boldsymbol{U}^T$$

where $\boldsymbol{U}$ are Householder vectors and $\boldsymbol{V}$ is

$$\boldsymbol{V}^T = \boldsymbol{T}\boldsymbol{U}^T + \frac{1}{2}\boldsymbol{T}^T\boldsymbol{U}^T \underbrace{\boldsymbol{A}\boldsymbol{U}}_{\text{challenge}} \boldsymbol{T}\boldsymbol{U}^T$$

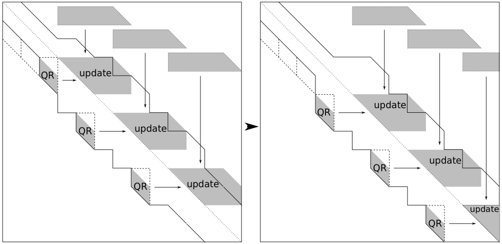
- when performing two-sided updates, computing $\boldsymbol{AU}$ dominates cost
- if $b = 1$, $\boldsymbol{U}$ is a column-vector, and $\boldsymbol{AU}$ is dominated by vertical communication cost (moving $\boldsymbol{A}$ between memory and cache)
- idea: reduce to banded matrix ($b \gg 1$) first[13]

[13] T. Auckenthaler, H.-J. Bungartz, T. Huckle, L. Krämer, B. Lang, P. Willems 2011

Successive band reduction (SBR)

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

- fewer nonzeros lead to lower computational cost, $F = O(n^2b/p)$
- however, transformations introduce fill/bulges
- bulges must be chased down the band[14]



- communication- and synchronization-efficient 1D SBR algorithm known for small band-width[15]

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[14] B. Lang 1993; C. Bischof, B. Lang, X. Sun 2000

[15] G. Ballard, J. Demmel, N. Knight 2012

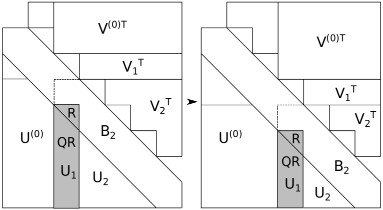
Communication-efficient eigenvalue computation

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

- implemented in ELPA, can outperform ScaLAPACK[16]
- with $n = n/\sqrt{p}$, 1D SBR gives $W = O(n^2/\sqrt{p})$, $S = O(\sqrt{p}\log^2(p))$[17]

We show the benefits of many-stage tridiagonalization

- use $\Theta(\log(p))$ intermediate band-widths to achieve $W = O(n^2/p^{2/3})$
- leverage communication-efficient rectangular QR with processor groups



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

[16] T. Auckenthaler, H.-J. Bungartz, T. Huckle, L. Krämer, B. Lang, P. Willems 2011

[17] G. Ballard, J. Demmel, N. Knight 2012

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 $W + F/\sqrt{H}$
- S – synchronization cost (number of supersteps)

Conclusion

Summary of contributions

- communication-efficient QR factorization algorithm
  - optimal communication cost for any matrix dimensions
  - variants that trade-off some accuracy guarantees for performance
- communication-efficient symmetric eigensolver algorithm
  - reduce matrix to successively smaller band-width
  - uses concurrent executions of 3D matrix multiplication and 3D QR

Practical implications

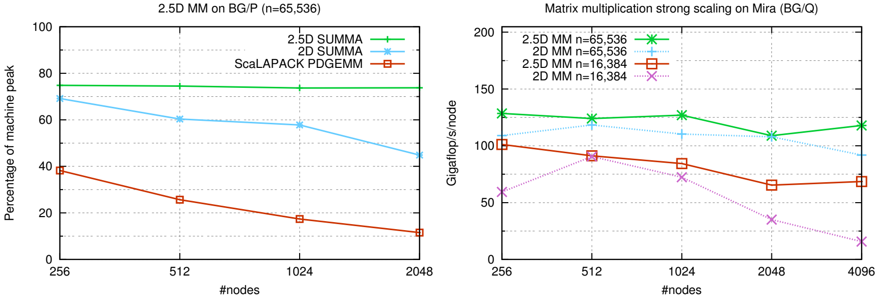
- ELPA demonstrated efficacy of two-stage approach, our work motivates 3+ stages
- partial parallel implementation is competitive but no speed-up

Future work

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

Backup slides

Communication-efficient matrix multiplication



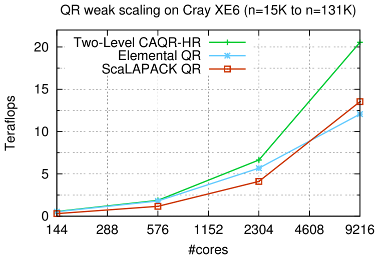
12X speed-up, 95% reduction in comm. for $n = 8\text{K}$ on 16K nodes of BG/P

Communication-efficient QR factorization

- Householder form can be reconstructed quickly from TSQR[18]

$$\boldsymbol{Q} = \boldsymbol{I} - \boldsymbol{Y}\boldsymbol{T}\boldsymbol{Y}^T \quad \Rightarrow \quad \text{LU}(\boldsymbol{I} - \boldsymbol{Q}) \to (\boldsymbol{Y}, \boldsymbol{T}\boldsymbol{Y}^T)$$

- Householder aggregation yields performance improvements

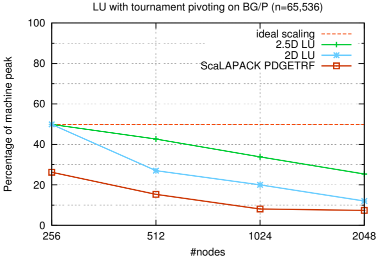


[18] Ballard, Demmel, Grigori, Jacquelin, Nguyen, S., IPDPS, 2014

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[19] extended to tournament pivoting[20]
- first implementation of a communication-optimal LU algorithm[11]

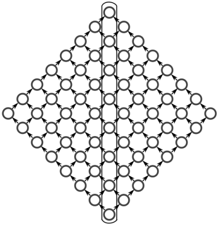
[19] Tiskin, FGCS, 2007

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

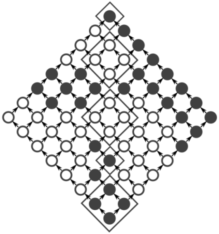
Tradeoffs in the diamond DAG

Computation vs synchronization tradeoff for the $n \times n$ diamond DAG,[21]

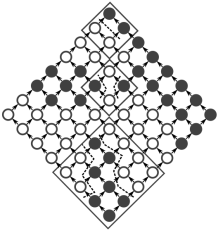
$$F \cdot S = \Omega(n^2)$$



Dependency chain P



Monochrome dependency intervals



Multicolored dependency intervals

We generalize this idea[22]

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

[21] Papadimitriou, Ullman, SIAM JC, 1987

[22] 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:[23]
For triangular solve with an $n \times n$ matrix,

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

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

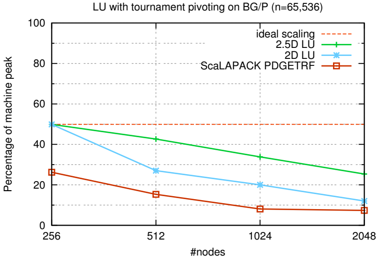
$$F_{\text{CHOL}} \cdot S_{\text{CHOL}}^2 = \Omega\left(n^3\right) \qquad W_{\text{CHOL}} \cdot S_{\text{CHOL}} = \Omega\left(n^2\right)$$

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

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[24] extended to tournament pivoting[25]
- first implementation of a communication-optimal LU algorithm[10]

[24] Tiskin, FGCS, 2007
[25] S., Demmel, Euro-Par, 2011