Part 1: Avoiding Communication in Eigenvalue and Singular Value Decompositions

Grey Ballard

CS 294/Math 270: Communication-Avoiding Algorithms
UC Berkeley

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U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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Plan

- Eigenvalue and singular value decompositions of dense matrices
  - want to compute most/all of the values and (possibly) the vectors
  - iterative solvers for large sparse matrices another CA topic

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  - EVD of symmetric matrix
  - EVD of nonsymmetric square matrix
  - SVD of general (rectangular) matrix
  - generalized versions
  - subsets of values/vectors desired

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  - EVD of symmetric matrix
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  - SVD of general (rectangular) matrix
  - generalized versions
  - subsets of values/vectors desired
- Overall approach is two-phase reduction to condensed form
  - based on orthogonal (similarity) transformations
  - alternative "divide-and-conquer" approaches another CA topic

Outline

1. EVD/SVD via Reduction to Condensed Form
2. Standard Algorithms
3. Two-Phase Approach
   - Full to Band(-Hessenberg)
   - Band Reduction
4. Open Problems

Canonical Forms for Real Matrices

- EVD of symmetric matrix

$$A = V \Lambda V^T$$

  - Λ is diagonal (eigenvalues) and V is orthogonal (eigenvectors)
- SVD of general rectangular matrix

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

  - Σ is diagonal (sing. values) and U, V are orthogonal (sing. vectors)
- EVD of nonsymmetric square matrix

$$A = U T U^T$$

  - Real Schur form: T is almost triangular and U is orthogonal

Computational and Numerical Considerations

- Canonical forms are based on orthogonal transformations
  - algorithms that apply orthogonal (similarity) transformations remain numerically stable
- Computing canonical forms requires iterative algorithms
  - unlike LU or QR decomposition, for example
  - computation depends on numerical values
- Reducing to condensed forms before applying iterative methods saves computation (and usually communication)
  - iterating on dense matrices is expensive
  - there are direct methods for reducing to simpler/sparser forms

Condensed Forms for Real Matrices

- EVD of symmetric matrix

$$A = QTQ^T \qquad \leftarrow \qquad A = V\Lambda V^T$$

  - T is tridiagonal and Q is orthogonal
- SVD of general rectangular matrix

$$A = Q_U B Q_V^T \qquad \leftarrow \qquad A = U\Sigma V^T$$

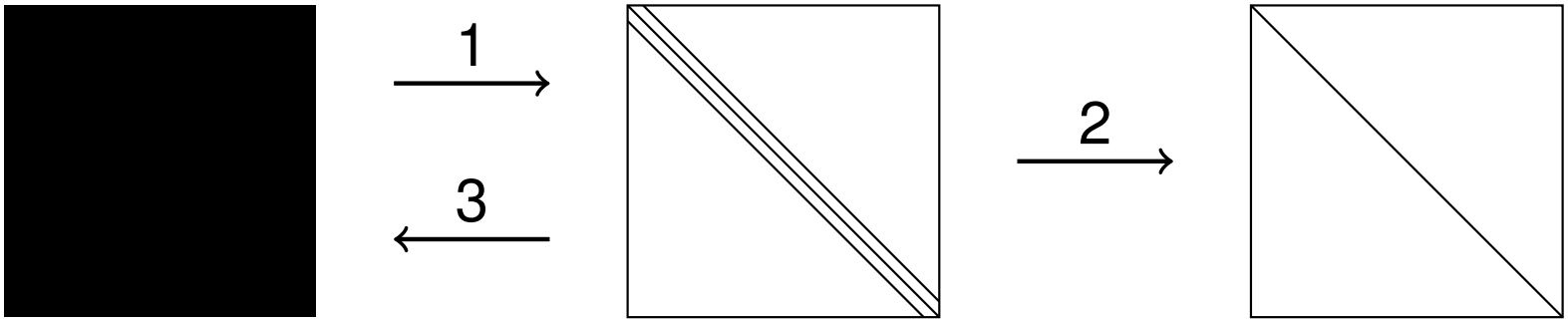
  - B is bidiagonal and Q_U, Q_V are orthogonal
- EVD of nonsymmetric square matrix

$$A = QHQ^T \qquad \leftarrow \qquad A = UTU^T$$

  - H is Hessenberg and Q is orthogonal

Symmetric EVD via Tridiagonalization

We typically compute the symmetric EVD with 3 steps:



1. Reduction-to-tridiagonal via orthogonal similarity transformations

$$A = QTQ^T$$

2. Solve the symmetric tridiagonal eigenvalue problem

$$T = V\Lambda V^T$$

3. Back-transformation of eigenvectors (if desired)

$$A = (QV)\Lambda(QV)^T$$

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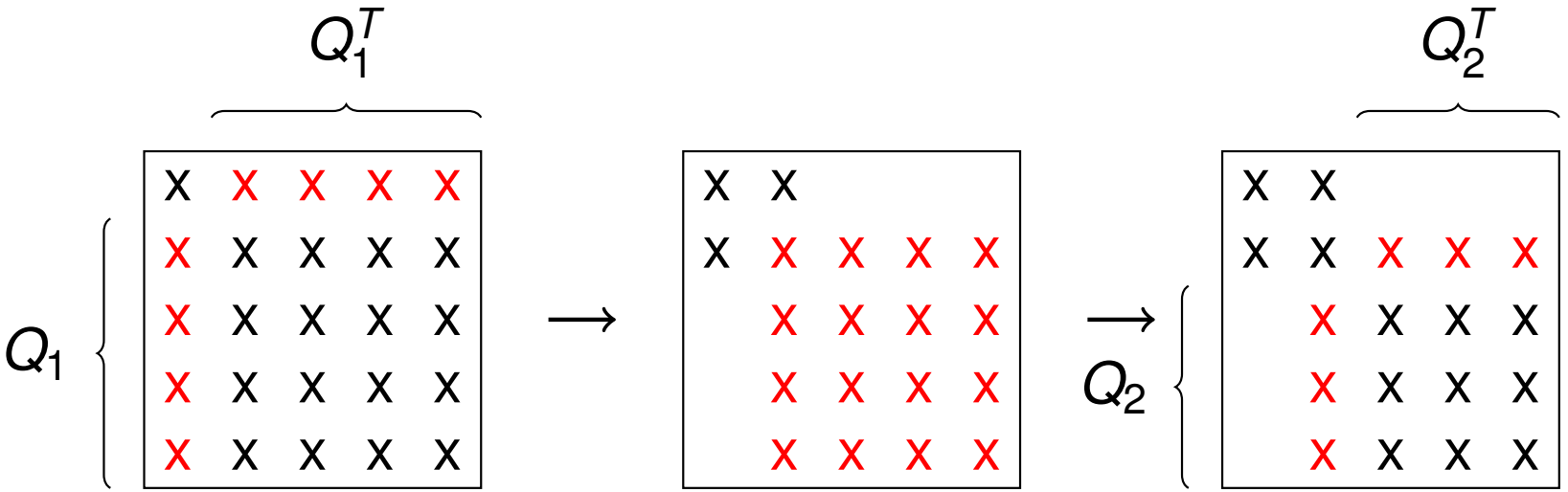
Householder Tridiagonalization



For $i = 1$ **to** $n - 2$

1. compute Householder vector y_i to annihilate column i
2. apply two-sided symmetric update

$$\tilde{A} = (I - \tau_i y_i y_i^T) \cdot A \cdot (I - \tau_i y_i y_i^T)$$

cast as symmetric rank-2 update

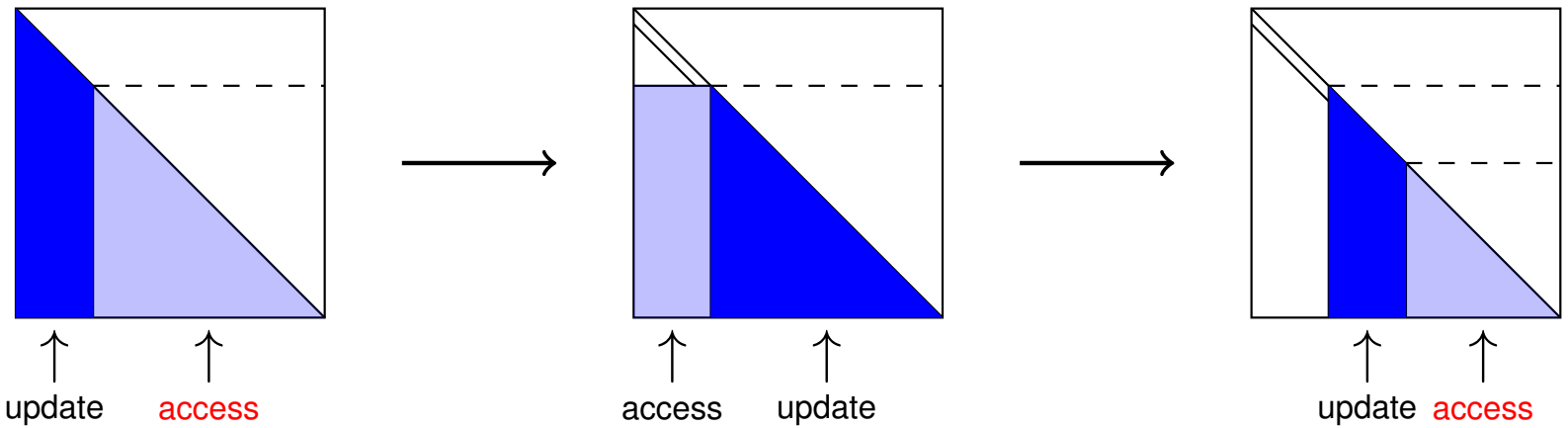
$$\tilde{A} = A - y_i v_i^T - v_i y_i^T \quad \text{(BLAS 2)}$$

End

LAPACK Householder Tridiagonalization

Direct tridiagonalization performed with blocked algorithm:

- panel factorization + (two-sided symmetric) trailing matrix update



- Panel factorization requires BLAS 2 (matrix-vector) operations
  - total of $O(n^3)$ operations
- Trailing matrix update uses BLAS 3 (matrix-matrix) operations
  - total of $O(n^3)$ operations

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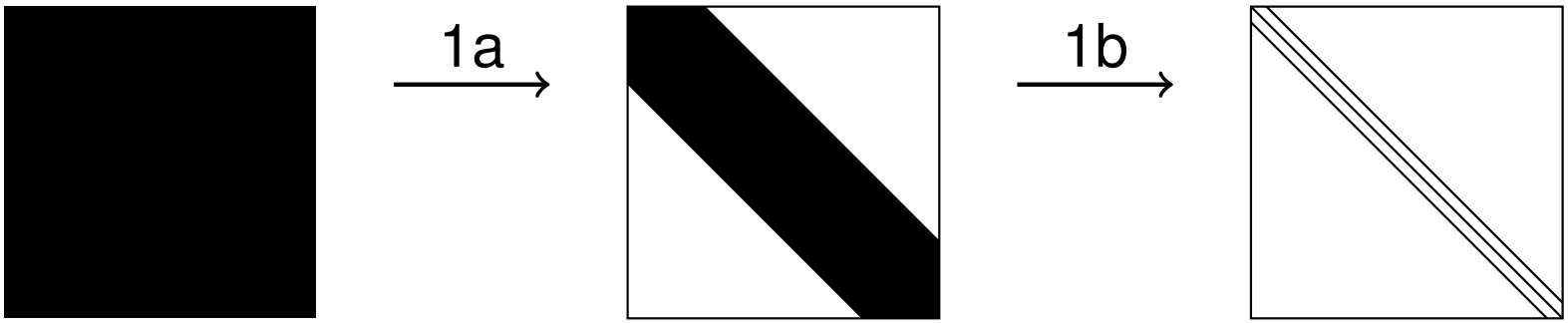
Two-Phase Tridiagonalization (SBR)

Symmetric tridiagonalization can be done over two (or more) phases in procedure known as Successive Band Reduction (SBR) [BLS00]:



1a Full-to-band via orthogonal similarity transformations

1b Band-to-tridiagonal using bulge-chasing transformations

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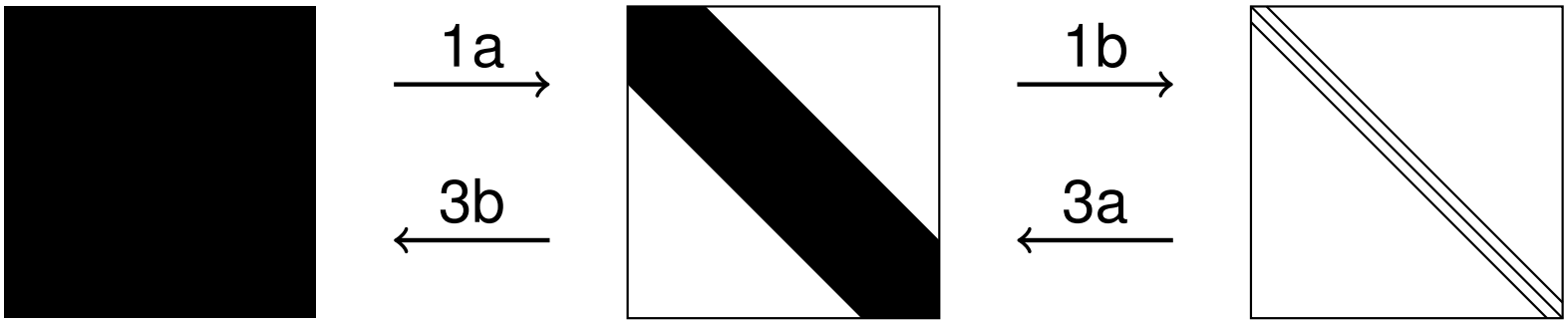


1a Full-to-band via orthogonal similarity transformations

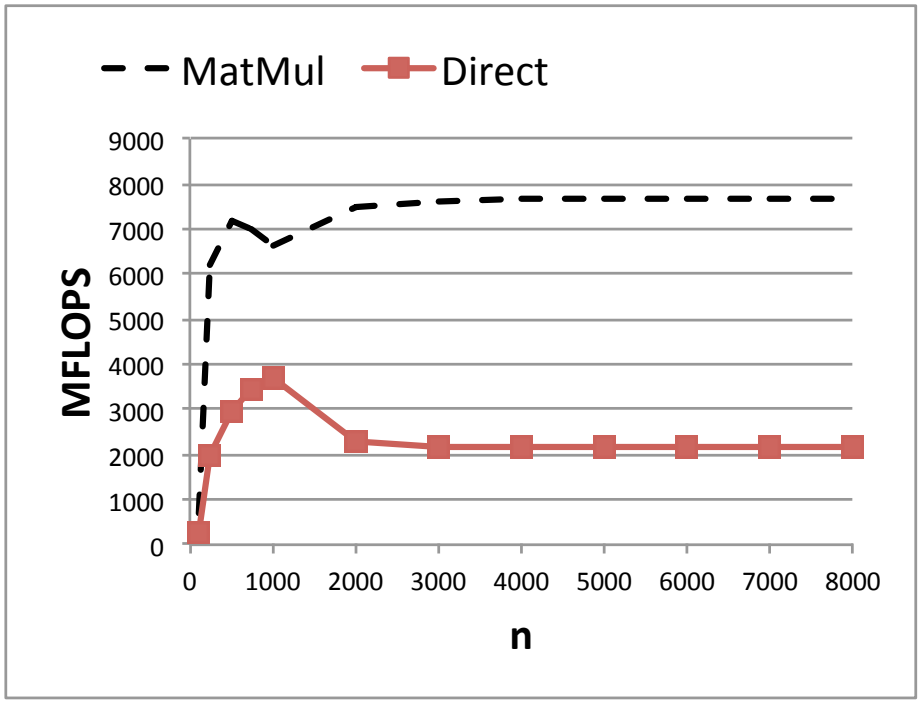
1b Band-to-tridiagonal using bulge-chasing transformations

- Two-phase back-transformation required for eigenvectors

Two-Phase Performance Benefits

Two-phase tridiagonalization avoids communication bottlenecks of direct approach

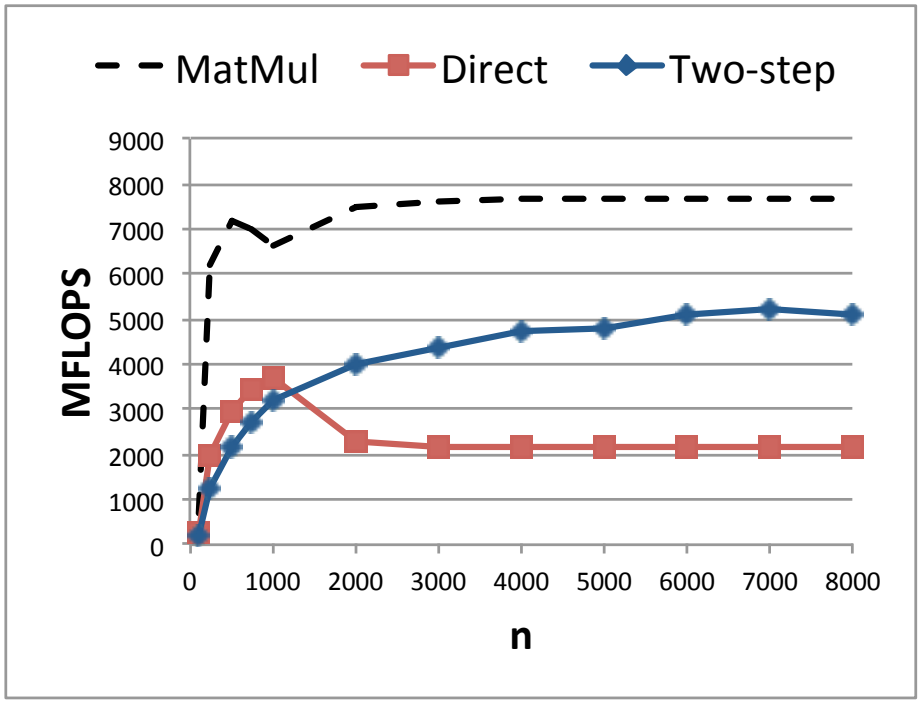
- Sequential performance example
- Direct approach suffers poor cache performance



Two-Phase Performance Benefits

Two-phase tridiagonalization avoids communication bottlenecks of direct approach

- Sequential performance example
- Direct approach suffers poor cache performance
- Two-phase approach already available in MKL



Software for Two-Phase Tridiagonalization

Two-phase tridiagonalization is proven to be effective in practice, achieving better performance than direct tridiagonalization

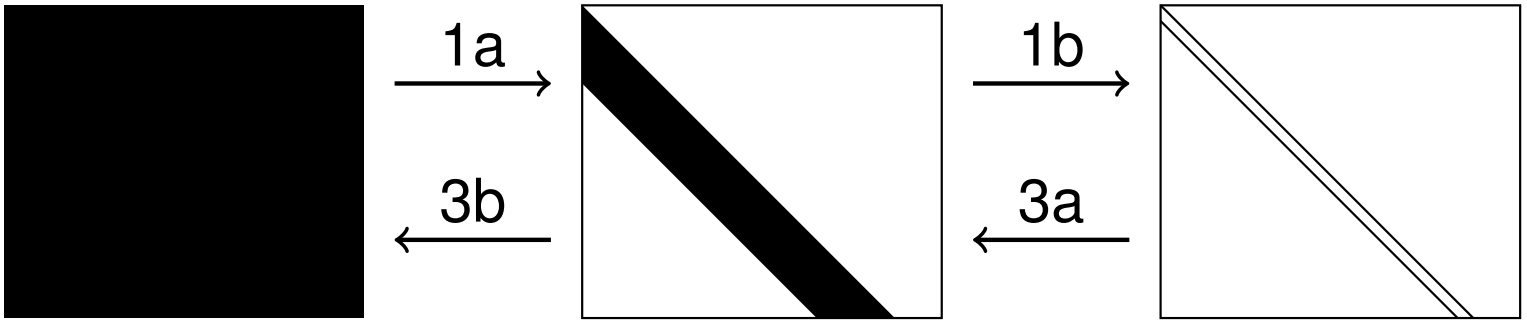
- despite requiring more flops for eigenvectors

- Sequential
  - Successive Band Reduction [BLS00], Intel MKL
- Multicore
  - PLASMA [LLD11], CA-SBR [BDK12]
- GPU
  - MAGMA [HSG+13], Eigen-G [IYM14]
- Distributed-memory parallel
  - ELPA [MBJ+14], Eigen-Exa [IYM11]

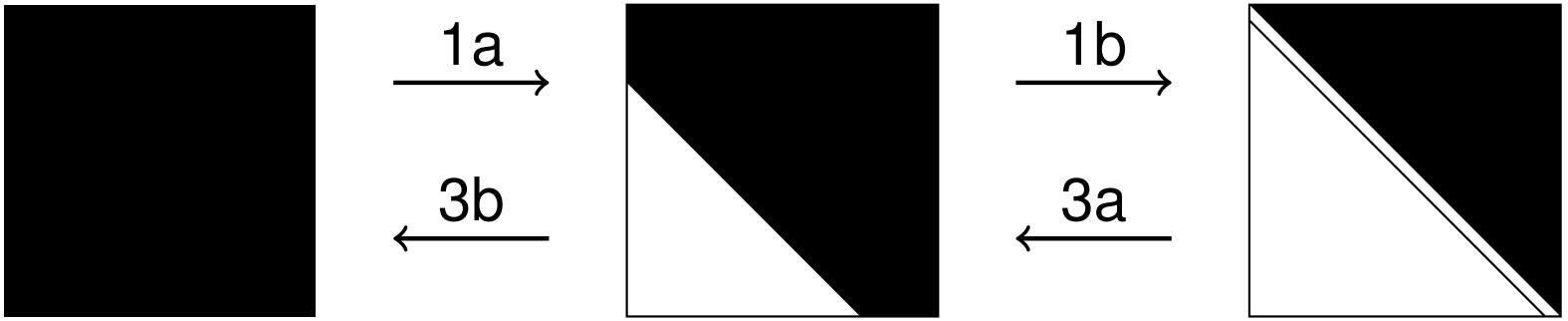
- other work on two-phase reductions for SVD and nonsym. EVD
  - bidiagonal reduction [HKL13], Hessenberg reduction [KK11]

Two-Phase Variants

Bidiagonalization can be done over two phases in a similar procedure:



As can reduction to Hessenberg:



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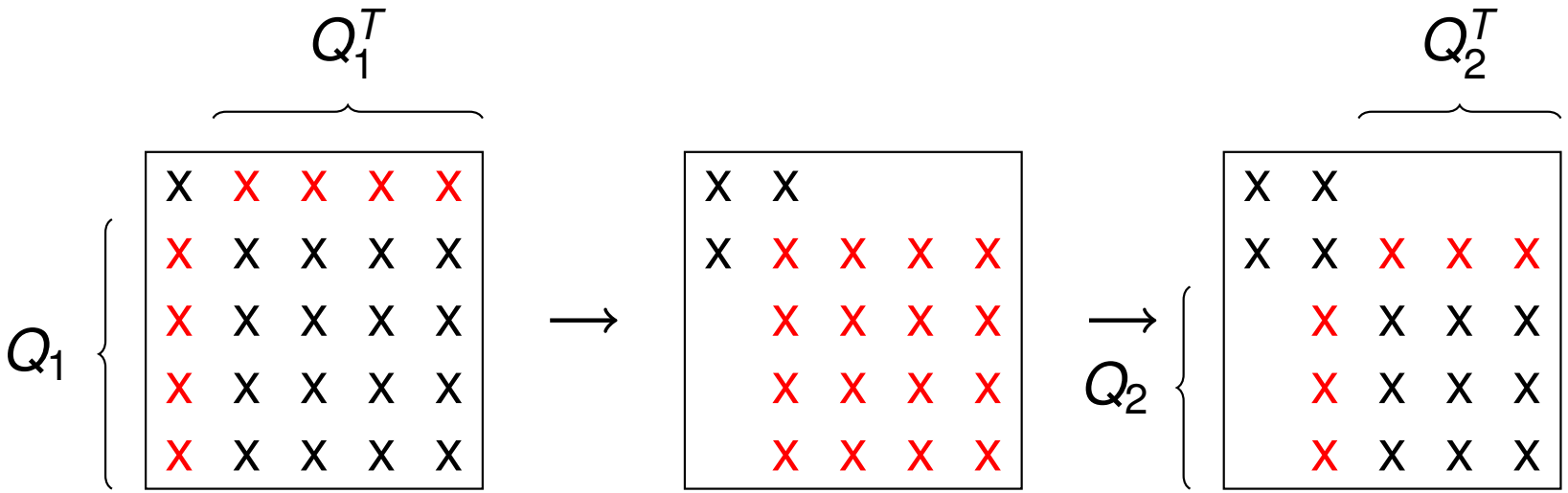
Basic Idea

Start with the Householder tridiagonalization algorithm:



Interpret x's as blocks (submatrices) instead of scalars

Blocked Full-to-Band Algorithm

For $i = 1$ **to** $\frac{n}{b} - 2$

1. QR factorization to generate Y_i and annihilate block column i
2. apply two-sided symmetric update

$$\tilde{A} = (I - Y_i T_i Y_i^T) \cdot A \cdot (I - Y_i T_i^T Y_i^T)$$

cast as symmetric rank-$2b$ update

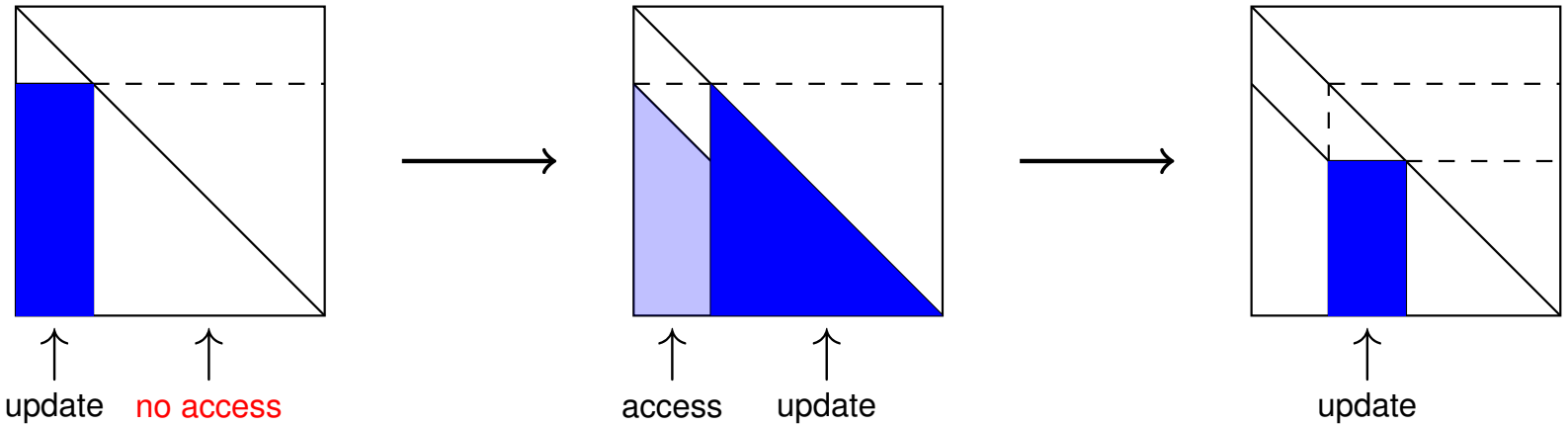
$$\tilde{A} = A - Y_i V_i^T - V_i Y_i^T$$

End

Blocked Full-to-Band Algorithm

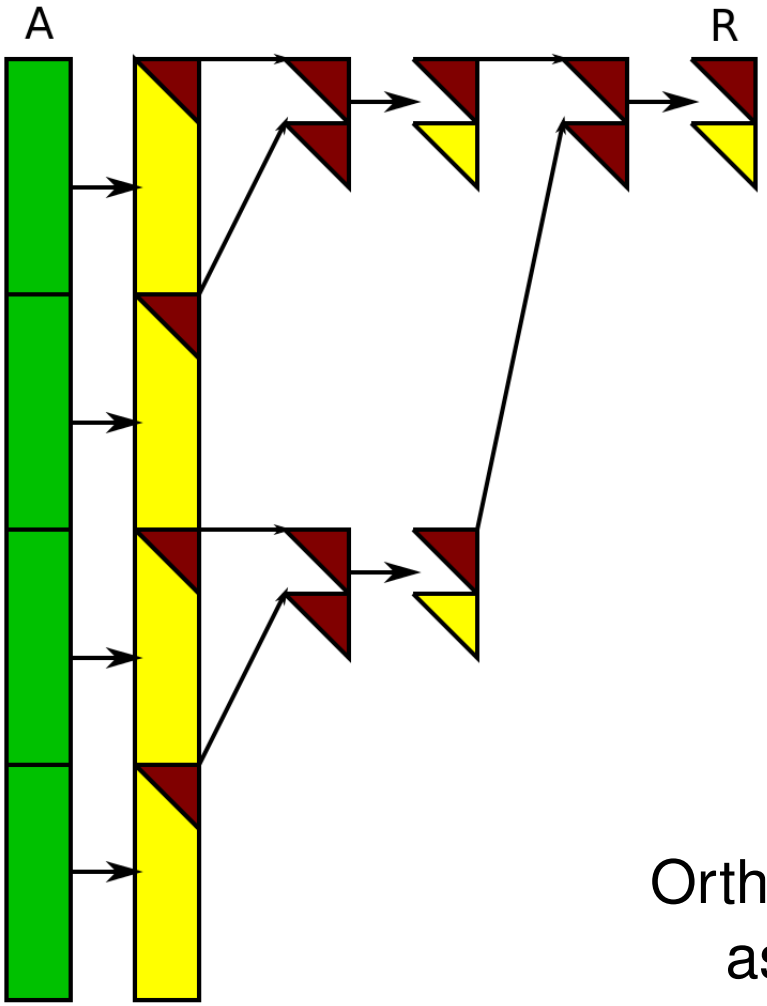
Full-to-band also performed with blocked algorithm:

- panel factorization + (two-sided symmetric) trailing matrix update



- Panel factorization is tall-skinny QR factorization
  - total of $O(n^2 b)$ operations
- Trailing matrix update uses BLAS 3 (matrix-matrix) operations
  - total of $O(n^3)$ operations

Tall-Skinny QR (TSQR) Algorithm [DGHL12]



Key benefit of TSQR:
one parallel reduction

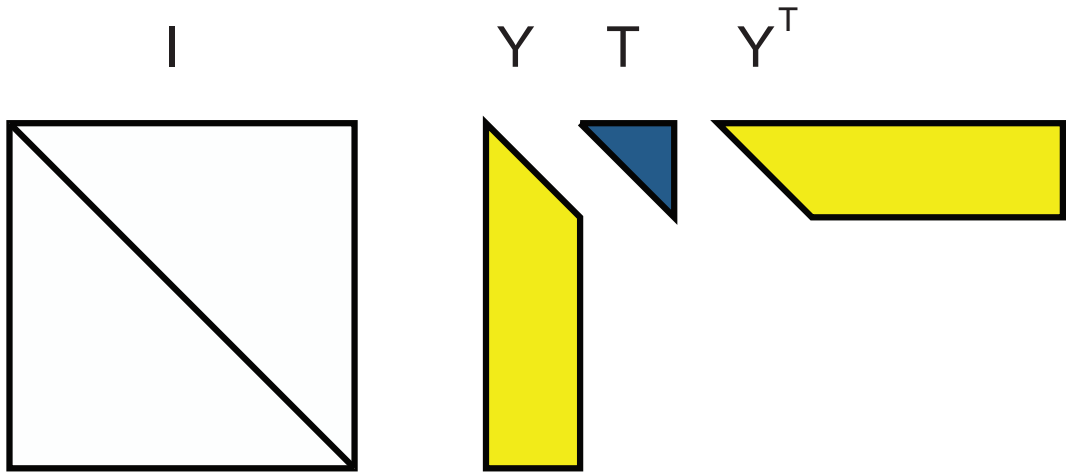
Householder QR:
one reduction *per column*

Orthogonal factor stored implicitly
as tree of Householder vectors

Reconstructing Householder Vectors (TSQR-HR)

1. Perform TSQR
2. Form Q explicitly (tall-skinny orthonormal factor)
3. Perform LU decomposition: $Q - Sgn = LU$
4. Set $Y = L$
5. Set $T = -U \cdot Sgn \cdot Y_1^{-T}$

$$I - YTY^T = I - \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} [T] \begin{bmatrix} Y_1^T & Y_2^T \end{bmatrix}$$



Leading Order Sequential Costs for Full-to-Band

Panel Factorization	Flops	Words	Messages
Householder QR [BLS00]	$\frac{4}{3}n^3$	$O\left(\frac{n^3}{\sqrt{M}}\right)$	$O\left(\frac{n^3}{M^1}\right)$
TSQR [LLD11]			$O\left(\frac{n^3}{M^{3/2}}\right)$
TSQR-HR [BDK15]			$O\left(\frac{n^3}{M^{3/2}}\right)$
Lower Bound [BDHS11]	—	$\Omega\left(\frac{n^3}{\sqrt{M}}\right)$	$\Omega\left(\frac{n^3}{M^{3/2}}\right)$

Sequential costs of full-to-band reduction of $n \times n$ matrix
to band matrix with bandwidth $b \ll n$,
where M is the size of the fast memory.

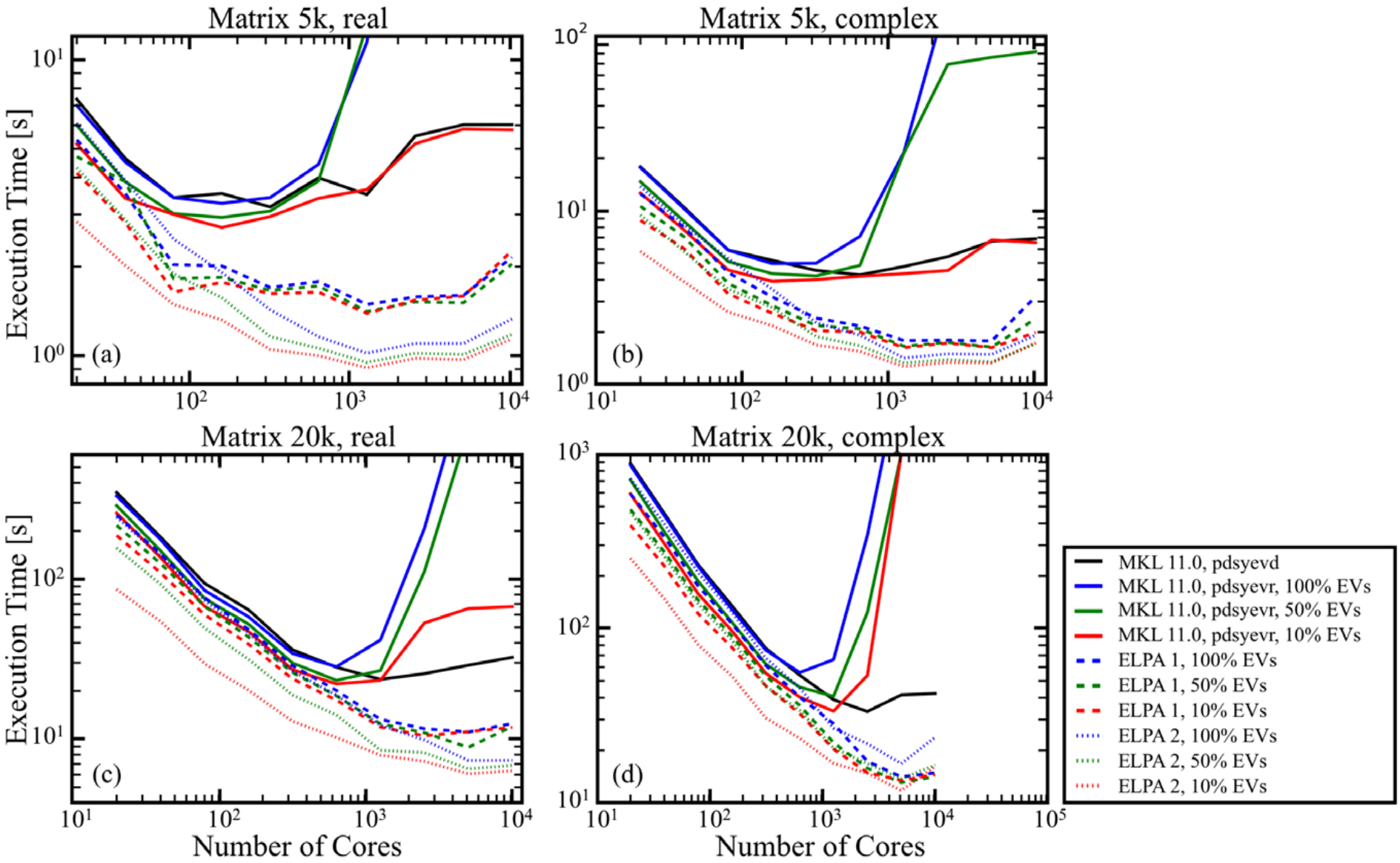
Leading Order Parallel Costs for Full-to-Band

Panel Factorization	Flops	Words	Messages
Householder QR [MBJ+14]	$\frac{4}{3}\frac{n^3}{p}$	$O\left(\frac{n^2}{\sqrt{p}}\right)$	$O\left(n \log p\right)$
TSQR		$O\left(\frac{n^2}{\sqrt{p}} \log p\right)$	$O\left(\sqrt{p} \log^3 p\right)$
TSQR-HR [BDK15]		$O\left(\frac{n^2}{\sqrt{p}}\right)$	$O\left(\sqrt{p} \log^2 p\right)$
Lower Bound* [BDHS11]	—	$\Omega\left(\frac{n^2}{\sqrt{p}}\right)$	$\Omega\left(\sqrt{p}\right)$

Parallel costs of full-to-band reduction of $n \times n$ matrix
to band matrix with bandwidth $b \ll n$
distributed over p processors in 2D fashion.

* assumes local memory restricted to $O(n^2/p)$

ELPA Library Parallel Performance [MBJ+14]



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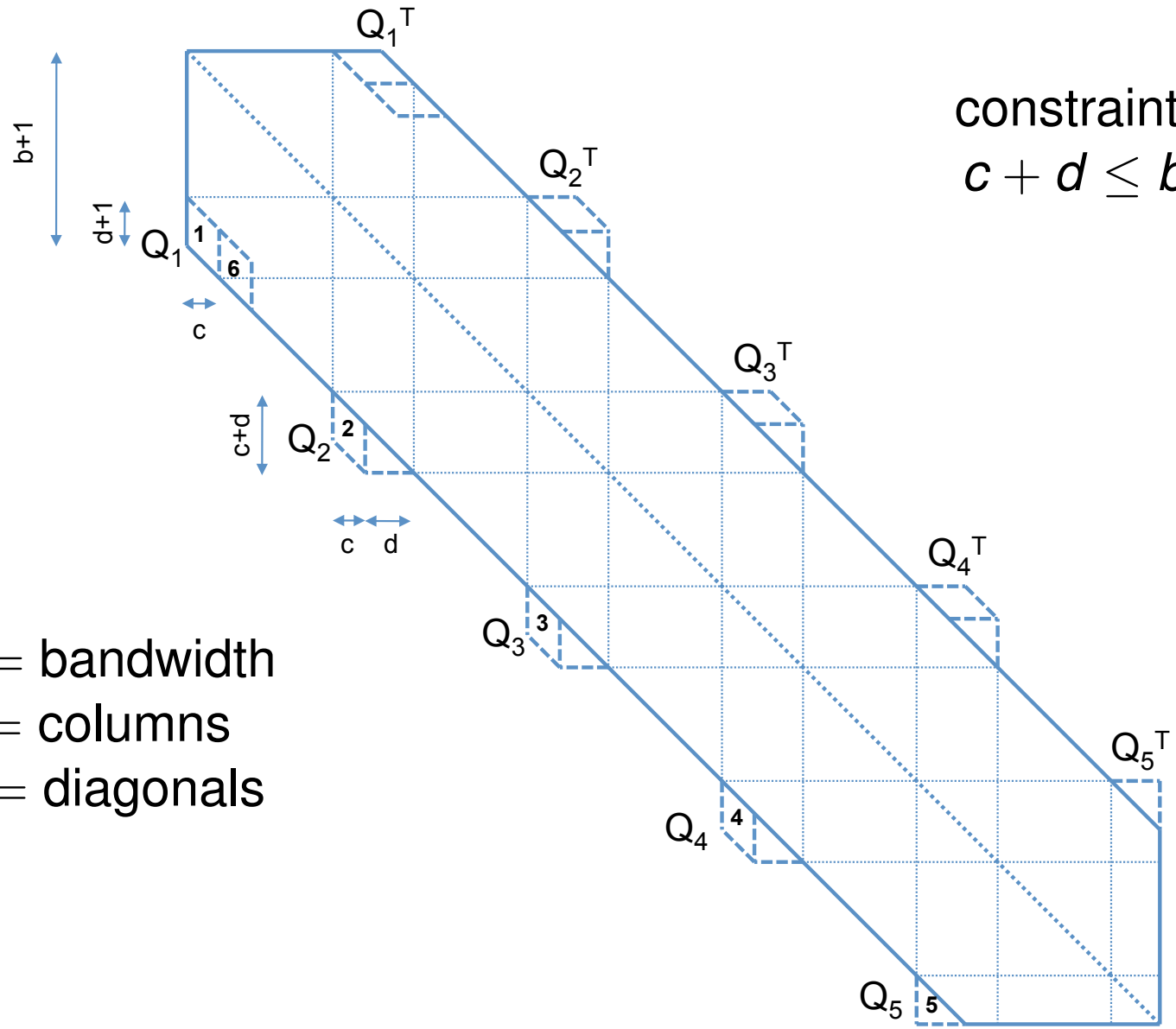
Band-to-Tridiagonal Reduction

Maintaining band structure during orthogonal similarity transformations is trickier than with full-to-band phase

- Annihilating entries within band causes fill-in outside the band
- Bulge-chasing process is required to maintain band structure

- Ideas go back a long way:
  - Rutishauser [Rut63]
  - Schwarz [Sch63]
  - Murata and Horikoshi [MH75]
  - Kaufman [Kau84]
  - Bischof, Lang, and Sun [BLS00]

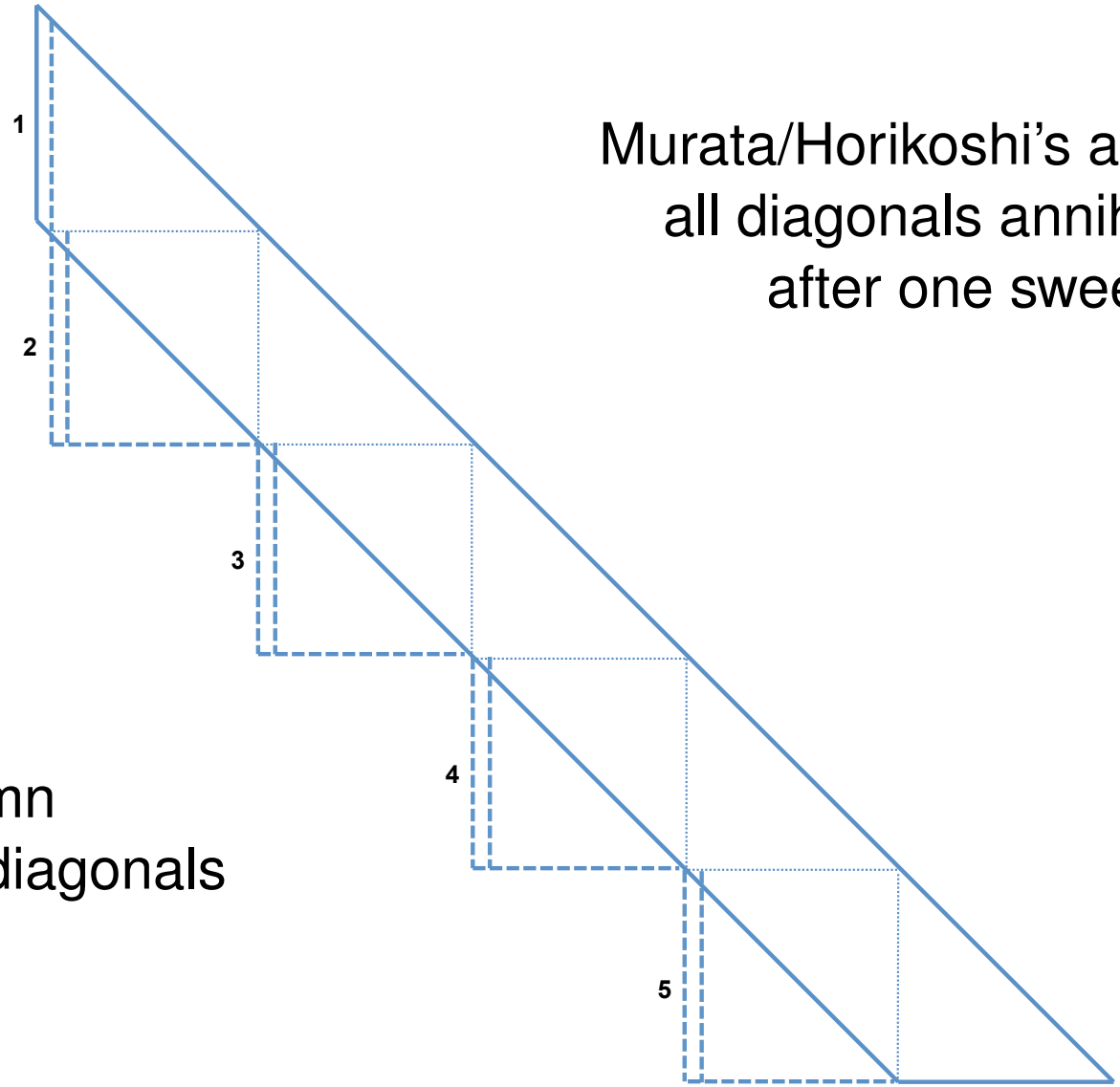
Band-to-Tridiagonal Bulge Chasing



constraint:
$c + d \leq b$

$b =$ bandwidth
$c =$ columns
$d =$ diagonals

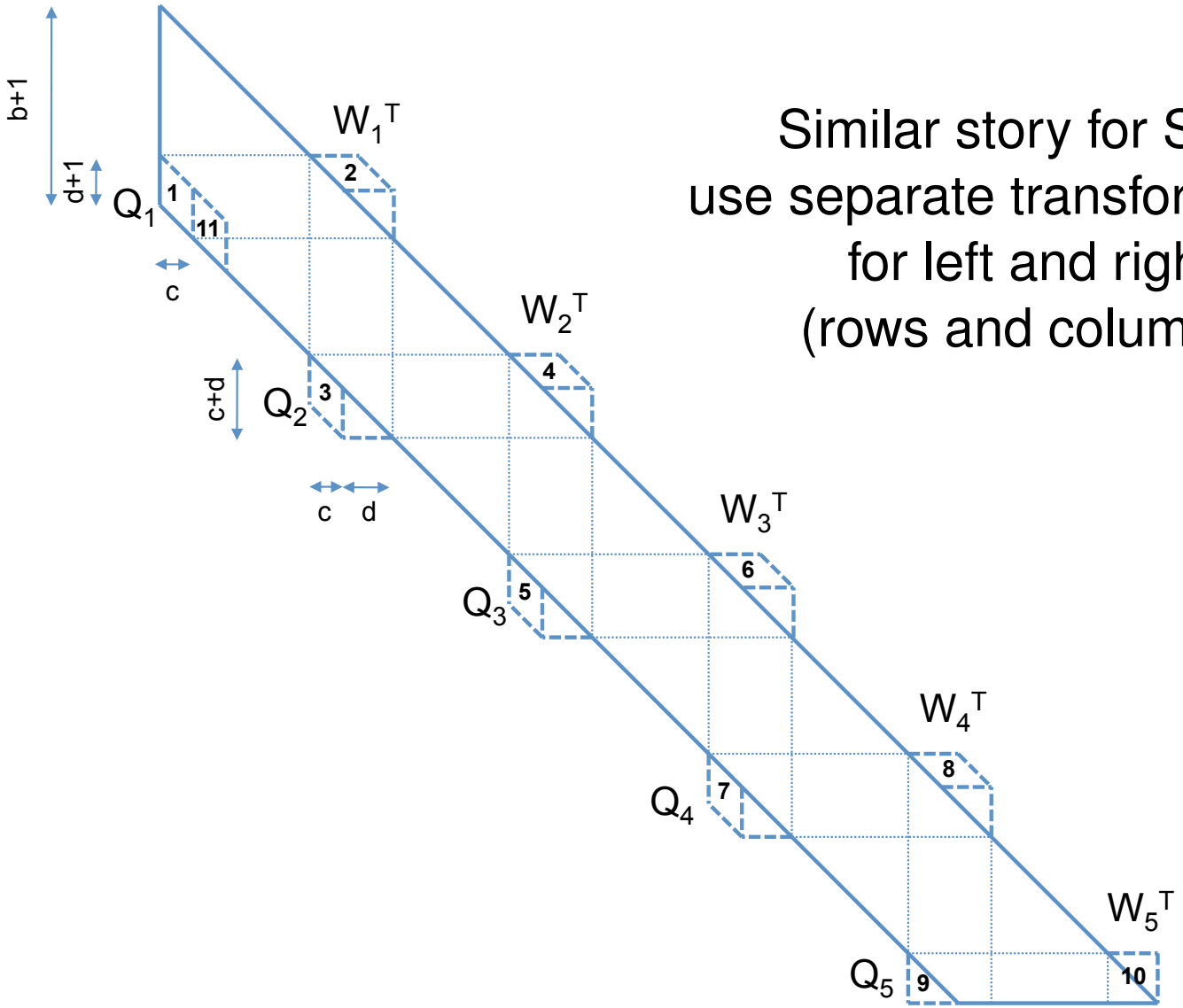
1-Sweep Band-to-Tridiagonal [MH75]



Murata/Horikoshi's algorithm:
all diagonals annihilated
after one sweep

$c = 1$ column
$d = b - 1$ diagonals

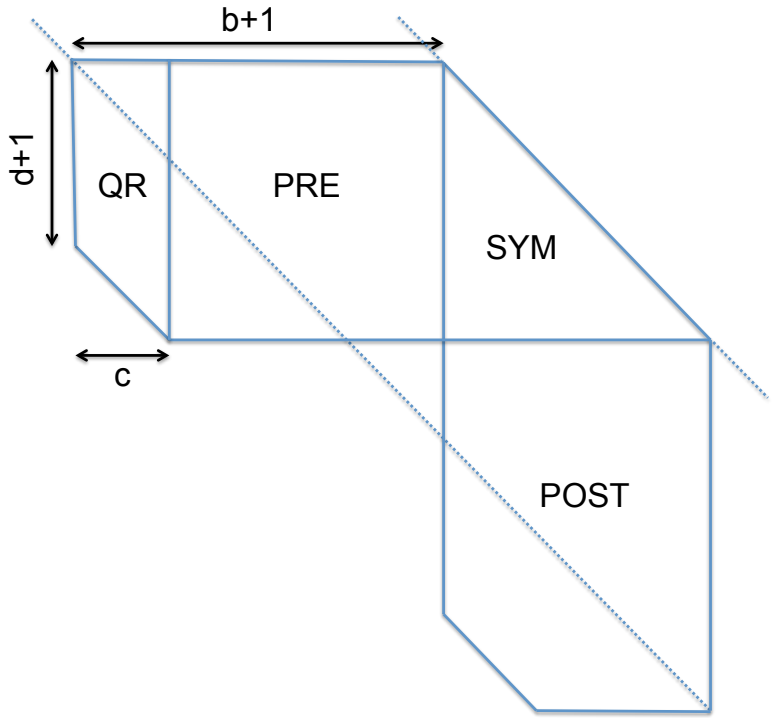
Band-to-Bidiagonal Bulge Chasing

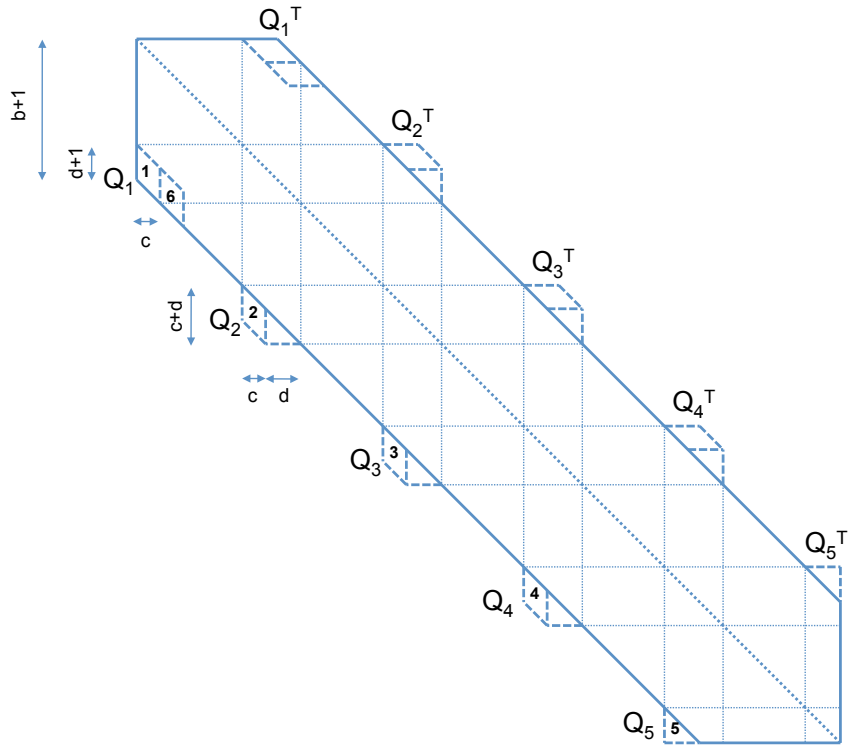


Similar story for SVD:
use separate transformations
for left and right
(rows and columns)

How do we get data re-use?

1. Increase number of columns in parallelogram (c)
   - permits blocking Householder updates: $O(c)$ re-use
   - constraint $c + d \leq b \implies$ trade-off between re-use and progress
   - requires multiple "sweeps"
2. Chase multiple bulges at a time (ω)
   - apply several updates to band while it's in local memory: $O(\omega)$ re-use
   - bulges cannot overlap, need working set to fit in local memory





Communication-Avoiding SBR

CA-SBR balances the two techniques for getting data re-use

Theoretically optimal approach: cut bandwidth in half at every sweep

- $\log b$ sweeps

Sequential and shared-memory implementation exist [BDK12]

- number of sweeps is tuning parameter

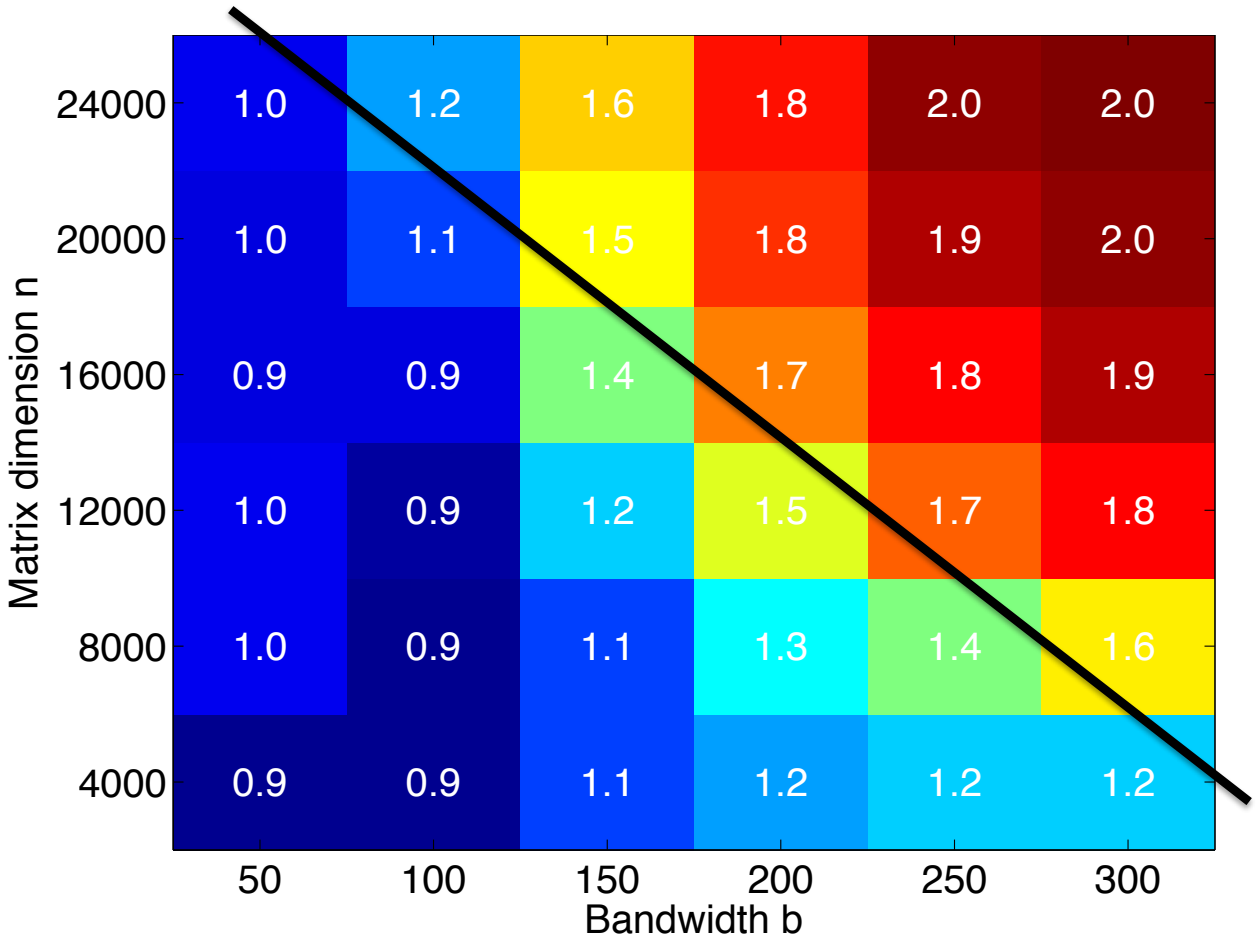
Leading Order Costs for Seq. Band-to-Tridiagonal

Algorithm	Flops	Words	Messages
LAPACK [Kau00]	$4n^2b$	$O(n^2b)$	$O(n^2b)$
CA-SBR	$5n^2b$	$O\left(\frac{n^2b^2}{M}\right)$	$O\left(\frac{n^2b^2}{M^2}\right)$
Lower Bound	—	?	?

Sequential costs of band-to-tridiagonal reduction of $n \times n$ band matrix with bandwidth $b < \sqrt{M}/3$, where M is the size of the fast memory.

Performance Results in Shared Memory

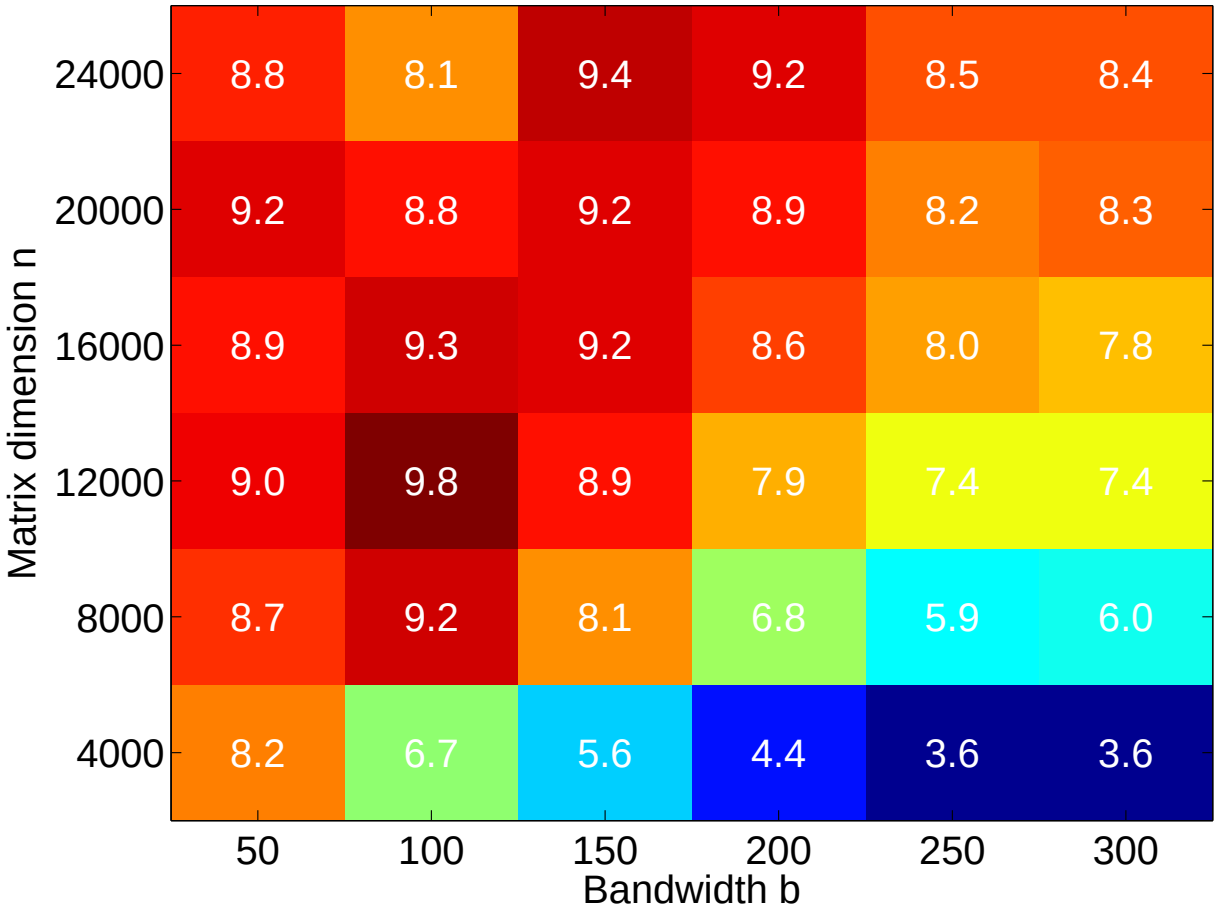
Speedup of sequential CASBR over Intel's Math Kernel Library



Benchmarked on 10-core Intel Westmere [BDK12]

Performance Results in Shared Memory

Speedup of parallel CASBR (10 threads) over sequential CASBR



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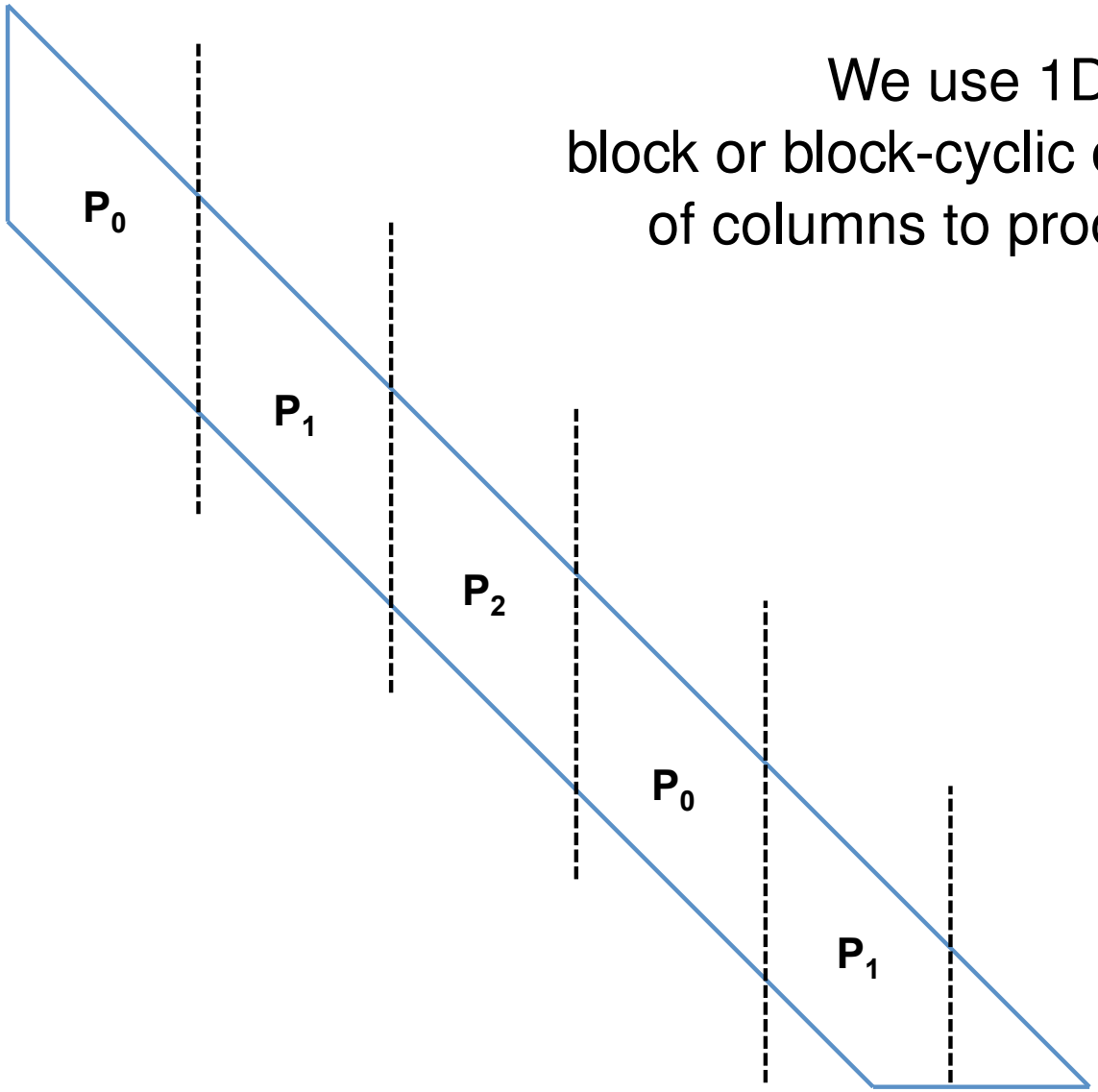
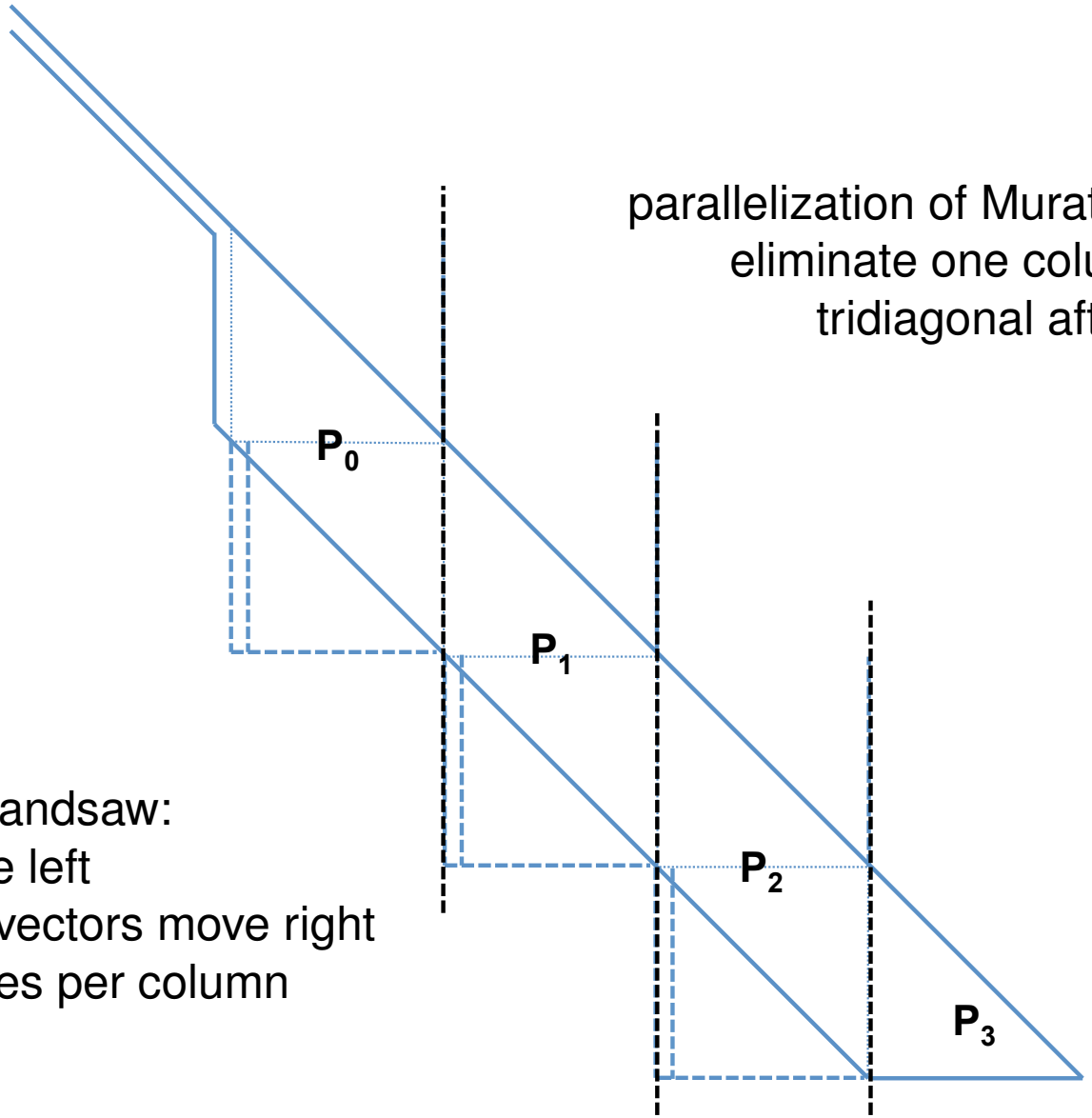
Distributed-Memory Parallel Distribution



We use 1D
block or block-cyclic distribution
of columns to processors

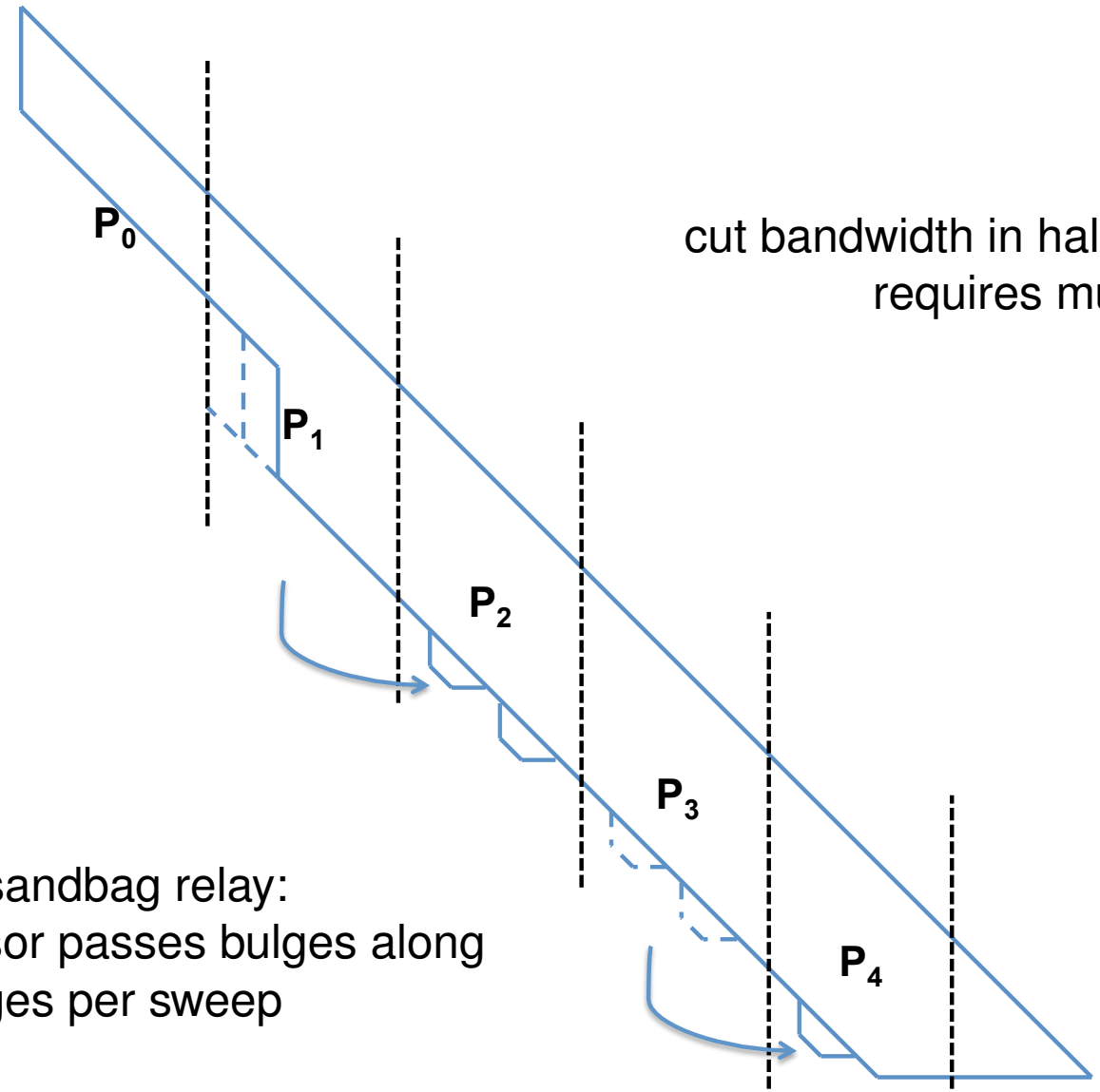
Lang's Algorithm [Lan93, Auc12]



parallelization of Murata/Horikoshi's:
eliminate one column at a time,
tridiagonal after one sweep

works like a bandsaw:
columns move left
Householder vectors move right
$O(1)$ messages per column

Communication-Avoiding SBR [BDK15]



cut bandwidth in half each sweep;
requires multiple sweeps

works like a sandbag relay:
each processor passes bulges along
$O(p)$ messages per sweep

Leading Order Costs for Parallel Band-to-Tridiagonal

Algorithm	Flops	Words	Messages
Lang's [Lan93, Auc12]	$O\left(\frac{n^2 b}{p}\right)$	$O(nb)$	$O(n)$
CA-SBR [BDK15]			$O(p \log b)$
Lower Bound	—	?	?

Costs of band-to-tridiagonal reduction of $n \times n$ band matrix with bandwidth $b \ll n$ distributed over p processors in 1D fashion.

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Back-Transformation for Eigenvectors

If only eigenvalues are desired, CA-SBR gives a theoretical net win, but . . .

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. . . what if we want eigenvectors?

- we must accumulate all the orthogonal transformations from the band-to-tridiagonal reduction
- we generate $O(n^2)$ data per sweep
- naively, we need $O(n^3)$ computation per sweep

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- naively, we need $O(n^3)$ computation per sweep

In order to achieve $O(p \log b) \ll O(n)$ messages,
we need to take $O(\log b)$ sweeps instead of 1 sweep

- tradeoff between latency cost and flops/bandwidth cost

Open Mathematical Problem

In two-phase tridiagonalization, we compute the following matrices:

$$A = Q_1 B {Q_1}^T = Q_1 (Q_2 T Q_2^T) Q_1^T = Q_1 Q_2 (V \Lambda V^T) {Q_2}^T Q_1^T$$

where A is dense, B is band, T is tridiagonal, Λ is diagonal

We can compute A, B, T, Λ, V stably and efficiently, we seek $Q_1 Q_2 V$

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where A is dense, B is band, T is tridiagonal, Λ is diagonal

We can compute A, B, T, Λ, V stably and efficiently, we seek $Q_1 Q_2 V$

Can we compute

- $Q_1 Q_2$ from A and T; or
- Q_2 from B and T

stably (as stable as direct tridiagonalization) and efficiently ($\ll O(n)$ messages)?

Open Mathematical Problem

Problem: Given A and (similar) T, compute Q such that $A = QTQ^T$

Householder reconstruction established a connection between $A = QR$ and $A = LU$

Is there an analogous connection between $A = QTQ^T$ and $A = L\tilde{T}L^T$ (or $A = LDL^T$)?

- $\tilde{T}$ is tridiagonal from Aasen's factorization
- D is block-diagonal from Bunch-Kaufman's factorization

Open CA Problem

Two-phase tridiagonalization attains the communication lower bound assuming local memory of $O(n^2/p)$

Can you exploit the memory-communication tradeoff in the case of EVD/SVD (like 2.5D matrix multiplication)?

We're currently working on this

Open Implementation Problems

Communication-optimal algorithms have not all been implemented

Shared-memory parallel implementation of CA band reduction showed promising results

There are preliminary implementations of Householder reconstruction for full-to-band in distributed memory

CA band reduction not implemented in distributed memory

Even less work on two-phase SVD and nonsymmetric EVD

For more details:

Avoiding Communication in Successive Band Reduction
Grey Ballard, Jim Demmel, and Nick Knight
ACM Transactions on Parallel Computing 2015
http://doi.acm.org/10.1145/2686877

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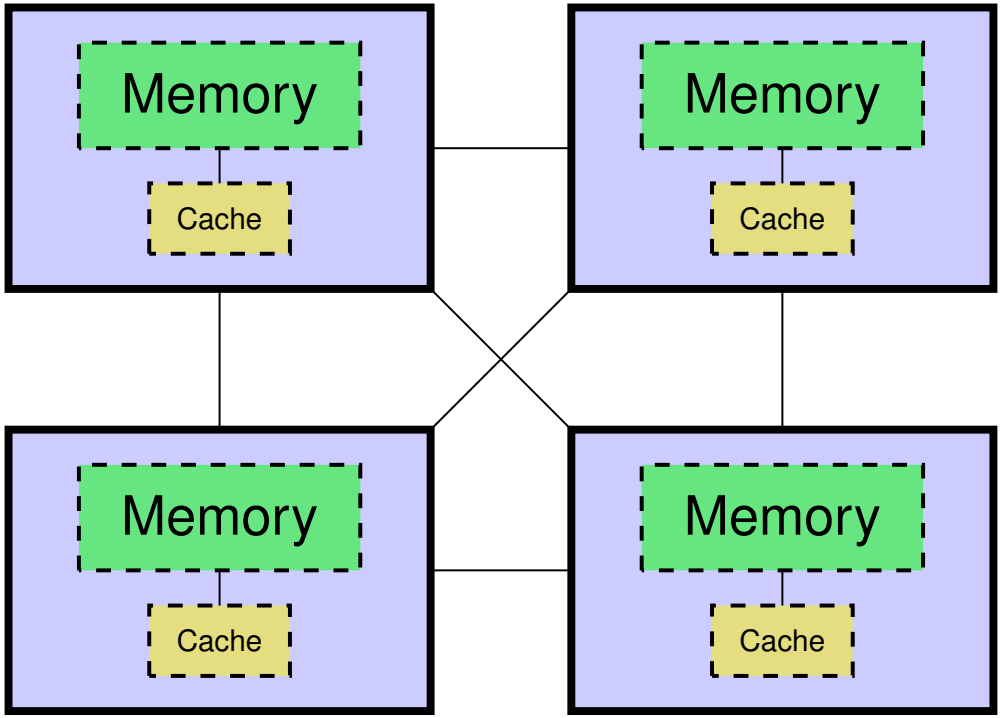
Model of Distributed-Memory Parallel Computation



To analyze algorithms, we are interested in the following quantities

- **flops** — floating point operations
- **memory bandwidth cost** — words moved between memory and cache
- **interprocessor bandwidth cost** — words communicated between processors
- **latency cost** — messages communicated between processors