Avoiding Communication in Parallel Bidiagonalization of Band Matrices

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SIAM CSE 13

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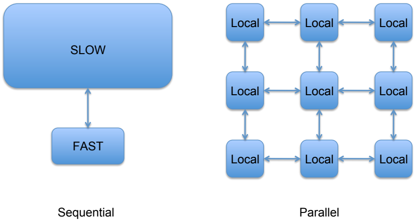
Motivation



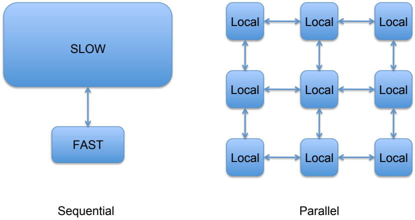
By *communication* we mean

- moving data within memory hierarchy on a sequential computer
- moving data between processors on a parallel computer

Communication is expensive, so our goal is to minimize it

- in many cases we need new algorithms
- in many cases we can prove lower bounds and optimality

Motivation



γ = time per flop

β = time per word moved

α = time per message

F = #flops

BW = #words moved

L = #messages

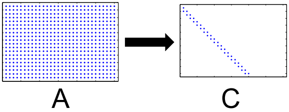
$$\text{Running time } = \gamma \cdot F + \beta \cdot BW + \alpha \cdot L$$

Direct vs Two-Step Bidiagonalization

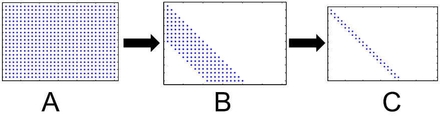
Application: computing the dense SVD via reduction to bidiagonal form (bidiagonalization)

- Conventional approach (e.g. LAPACK) is direct bidiagonalization
- Two-step approach reduces first to band, then band to bidiagonal

Direct:



Two-step:



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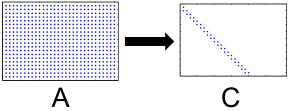

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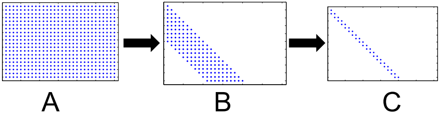
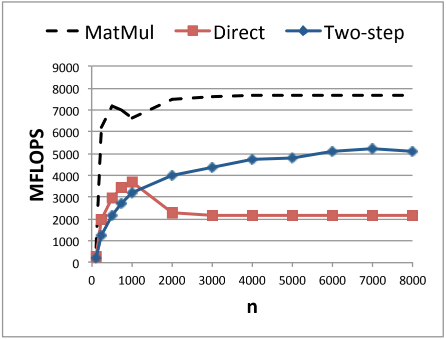
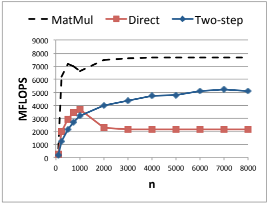




Why is direct bidiagonalization slow?

Communication costs!



Approach		Flops	Words Moved
Direct		$\frac{8}{3}n^3$	$O\left(n^3\right)$
Two-step	(1)	$\frac{8}{3}n^3$	$O\left(\frac{n^3}{\sqrt{M}}\right)$
	(2)	$O\left(n^2\sqrt{M}\right)$	$O\left(n^2\sqrt{M}\right)$

M = fast memory size

- Direct approach achieves $O(1)$ data re-use
- Two-step approach moves fewer words than direct approach
    - using intermediate bandwidth $b = \Theta(\sqrt{M})$
- Full-to-banded step (1) achieves $O(\sqrt{M})$ data re-use
    - this is optimal
- Band reduction step (2) achieves $O(1)$ data re-use
    - **Can we do better?**

Band Reduction via Bulge Chasing

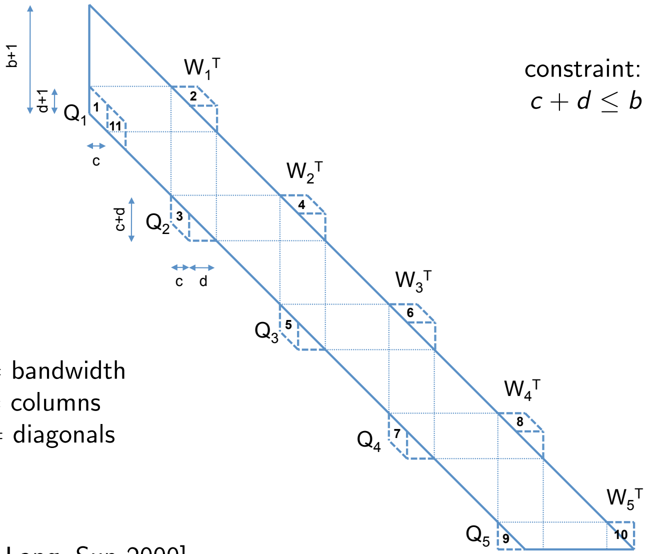
We want to compute and apply orthogonal matrices Q and W to transform a band matrix B to a bidiagonal matrix C:

$$Q^T BW = C$$

The basic procedure for band reduction is known as "bulge chasing"

- main idea is to annihilate entries with orthogonal transformations but maintain band sparsity structure
- there's a big design space, many different approaches
- same ideas work for symmetric band eigenproblem

Successive Band Reduction (bulge-chasing)

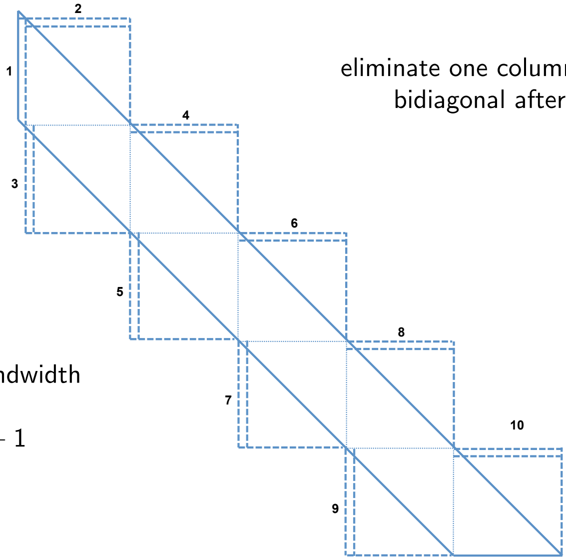


constraint:
$c + d \leq b$

b = bandwidth
c = columns
d = diagonals

[Bischof, Lang, Sun 2000]

SBR - 1 Sweep Approach



eliminate one column at a time
bidiagonal after one sweep

$b =$ bandwidth
$c = 1$
$d = b - 1$

Several Different Scenarios...

- starting with dense matrix OR starting with band matrix
- seeking singular values only OR seeking also singular vectors
  - left AND/OR right singular vectors (some OR all of them)
- sequential machine OR parallel machine
- singular value decomposition OR symmetric eigenproblem

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We'll focus on bidiagonalization of (lower triangular) band matrices for the rest of the talk, considering

- sequential and parallel cases
- values only and values and (left and right) vectors cases

Our main goal will be to find ways to re-use data in band reduction process

Accumulating Orthogonal Transformations

Band reduction:

$$B = QCW^T$$

Bidiagonal SVD:

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

Full SVD:

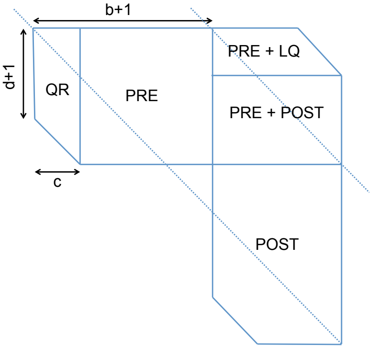
$$B = (QU)\Sigma(WV)^T$$

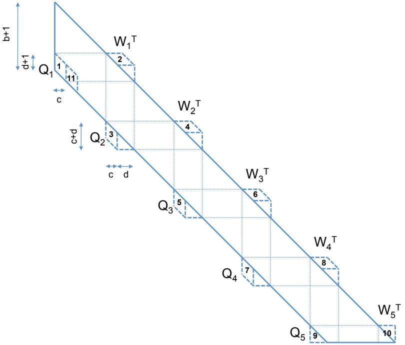
To compute left singular vectors of band matrix B, either

1. form Q explicitly and apply U to Q from right, or
2. store Q implicitly and apply Q to U from left

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





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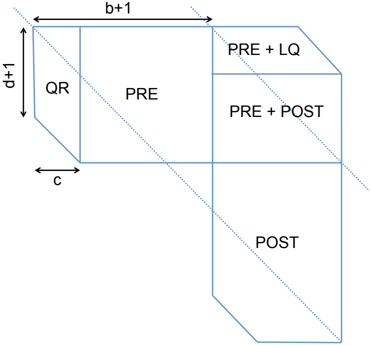

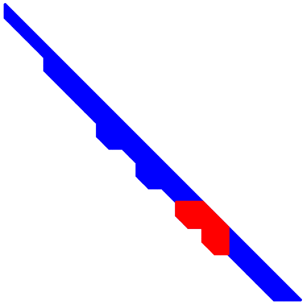

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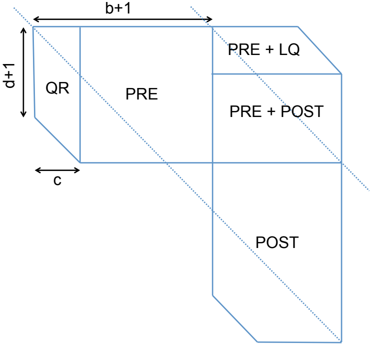

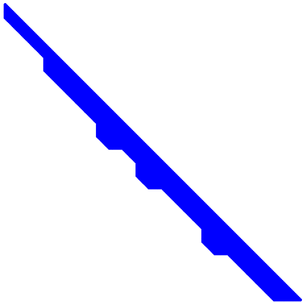

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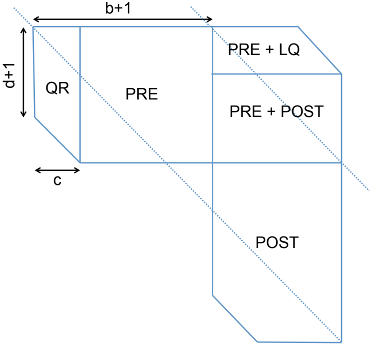

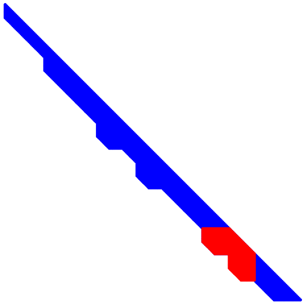

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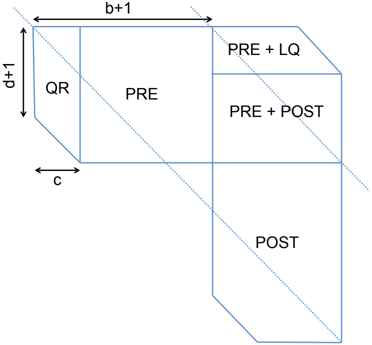

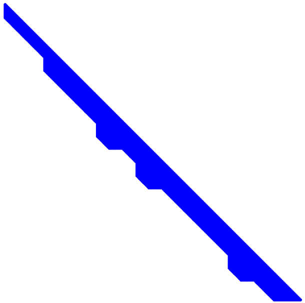

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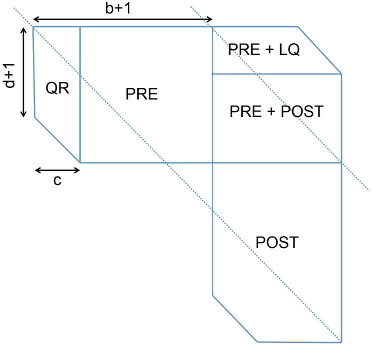

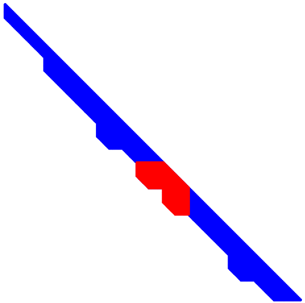

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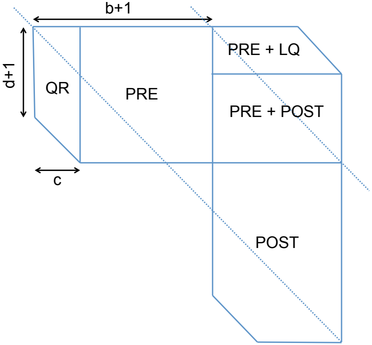

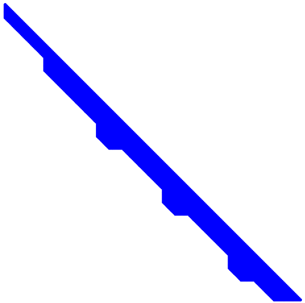

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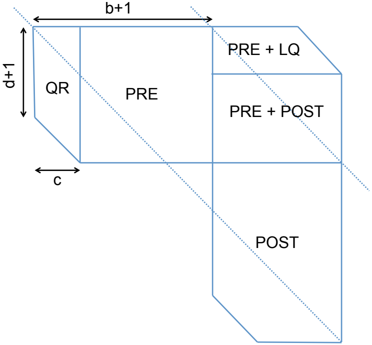

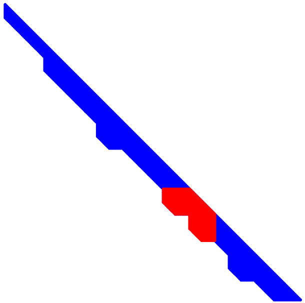

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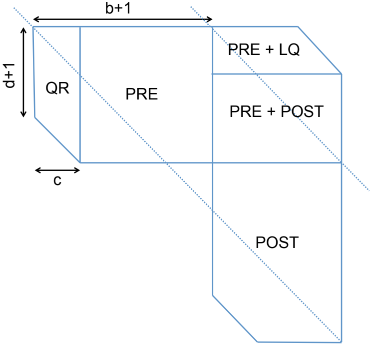

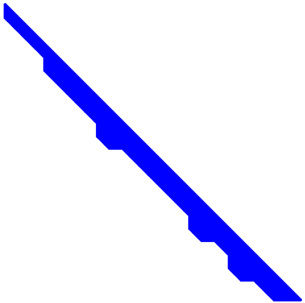

Data access patterns

One bulge at a time

Four bulges at a time

Asymptotics - singular values only - sequential case

Algorithm	Flops	Words	Messages
LAPACK	$4n^2b$	$O(n^2b)$	$O\left(n^2b\right)$
1 Sweep SBR	$8n^2b$	$O(n^2b)$	$O\left(\frac{n^2b}{M}\right)$

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†assuming $1 \leq b \leq \sqrt{M}/3$

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CA-SBR†	$6n^2b$	$O\left(\frac{n^2b^2}{M}\right)$	$O\left(\frac{n^2b^2}{M^2}\right)$

†assuming $1 \leq b \leq \sqrt{M}/3$

CA-SBR cuts remaining bandwidth in half at each sweep

- starts with big c and decreases by half at each sweep
- starts with small ω and doubles at each sweep

What if you want singular vectors too? - sequential case

We've used two optimizations:

1. chase multiple bulges (increase ω)
2. take multiple sweeps (increase c)
   - accumulating orthogonal transformations costs $O(n^3)$ flops per sweep

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1 Sweep SBR	$4n^3$	$O\left(n^2 b + \frac{n^3}{\sqrt{M}}\right)$	$O\left(\frac{n^2 b}{M} + \frac{n^3}{M}\right)$

communication costs: band reduction + orthogonal updates

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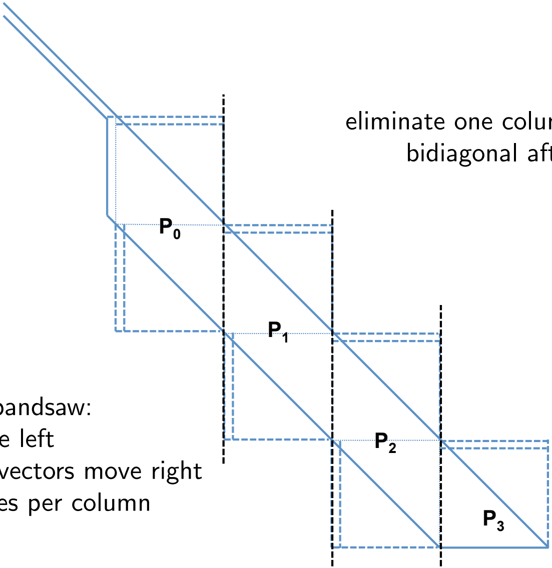
CA-SBR†	$2n^3 \log b$	$O\left(\frac{n^2 b}{\sqrt{M}} + \frac{n^3 \log b}{\sqrt{M}}\right)$	$O\left(\frac{n^2 \log b}{M} + \frac{n^3 \log b}{M^{3/2}}\right)$

communication costs: band reduction + orthogonal updates

†assuming $1 \leq b \leq \sqrt{M}/3$

Parallel 1 Sweep SBR

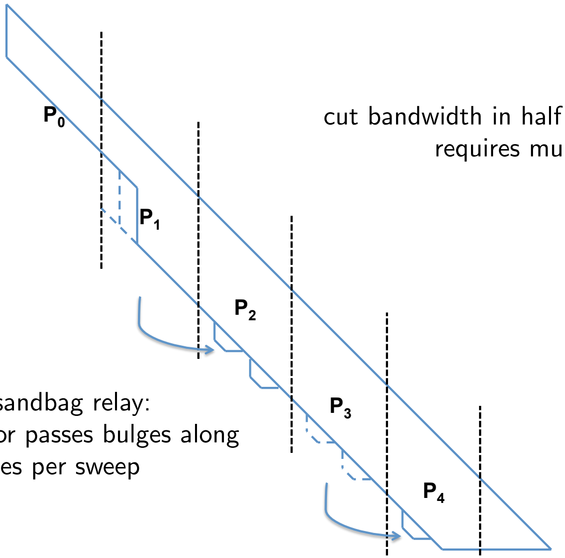
eliminate one column at a time;
bidiagonal after one sweep



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

[Lang 1993]

Parallel CA-SBR



cut bandwidth in half each sweep;
requires multiple sweeps

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

Asymptotics - singular values only - parallel case

Multiple sweeps and chasing multiple bulges reduces latency cost

Algorithm	Flops	Words	Messages
1 Sweep SBR	$O\left(\frac{n^2 b}{p}\right)$	$O(nb)$	$O(n)$
CA-SBR†	$O\left(\frac{n^2 b}{p}\right)$	$O(nb)$	$O(p \log b)$

†assuming $1 \leq b \leq n/(3p)$

What if you want singular vectors too? - parallel case

Run band reduction on $\sqrt{p}$ processors, orthogonal updates on all p

- broadcasting band reduction updates, or
- redundantly computing band reduction

Algorithm	**Flops**	**Words**	**Messages**
1 Sweep SBR*	$\frac{4n^3}{p}$	$O\left(nb + \frac{n^2}{\sqrt{p}}\right)$	$O(n + \log p)$
CA-SBR†	$\frac{2n^3 \log b}{p}$	$O\left(nb + \frac{n^2}{\sqrt{p}} \log b\right)$	$O(\sqrt{p} \log b)$

*[Auckenthaler et al. 2011]
†assuming $1 \le b \le n/(3\sqrt{p})$

Again, latency is reduced at the cost of extra computation

Conclusions and Future Work

We've used two means to improve data re-use in band reduction schemes:

1. taking multiple sweeps (re-using data within a bulge chase)
2. chasing multiple bulges (re-using data among bulge chases)

Asymptotic communication improvements:

1. in sequential case, we can reduce both bandwidth and latency costs
2. in parallel case, we can reduce latency cost

For singular vectors, multiple sweeps results in extra computation

- for subset of vectors, extra computation decreases
- to navigate tradeoff, take $1 \leq \#$ sweeps $\leq \log b$

These ideas can also benefit full SVD case (starting with dense matrix) and symmetric eigenproblem (with different constant factors)

Thank you!

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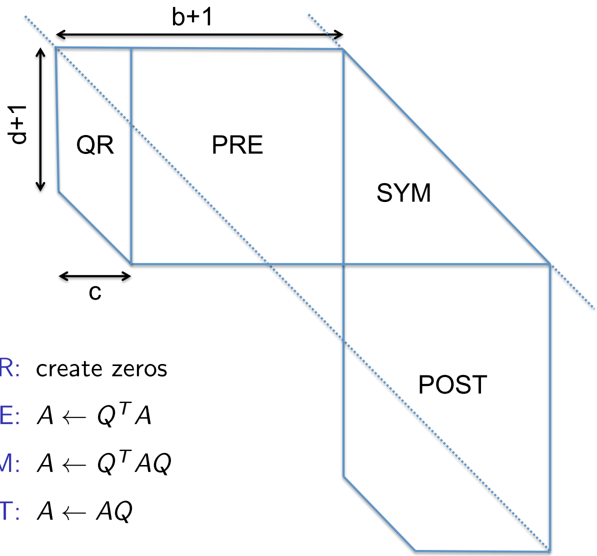
Anatomy of a symmetric bulge-chase



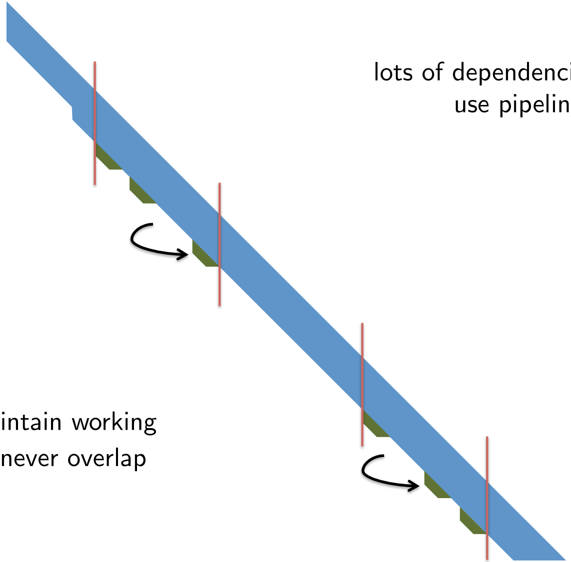
QR: create zeros

PRE: $A \leftarrow Q^T A$

SYM: $A \leftarrow Q^T A Q$

POST: $A \leftarrow AQ$

Shared-Memory Parallel Implementation



lots of dependencies:
use pipelining

threads maintain working
sets which never overlap