Communication-avoiding Krylov subspace methods

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Overview

- Current Krylov methods: *communication-limited*
- Can rearrange them to *avoid communication*
- Can do this in a *numerically stable* way
- Requires rethinking *preconditioning*

Motivation

- Two communication-bound kernels
- Can rearrange *each kernel* to avoid communication, but...
- Data dependency between the two precludes rearrangement...
- *Unless* you rearrange the Krylov method!

Krylov methods: Two communication-bound kernels

- Sparse matrix-vector multiplication (SpMV)
  - Share/communicate source vector w/ neighbors
  - Low computational intensity per processor
- Orthogonalization: $\Theta(1)$ reductions per vector
  - Arnoldi/GMRES:
    - Modified Gram-Schmidt or Householder QR
  - Lanczos/CG:
    - Recurrence orthogonalizes implicitly

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Potential to avoid communication

- SpMV: Matrix powers kernel (Marghoob)
  - Compute $[v, Av, A^2v, \ldots, A^s v]$
  - Tiling to reuse matrix entries
  - Parallel: same latency cost as one SpMV
  - Sequential: only read matrix $O(1)$ times
- Orthogonalization: TSQR (Julien)
  - Just as stable as Householder QR
  - Parallel: same latency cost as one reduction
  - Sequential: only read vectors once

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Problem: Data dependencies limit reuse

- Krylov methods advance one vector at a time
- SpMV, then orthogonalize, then SpMV, ...

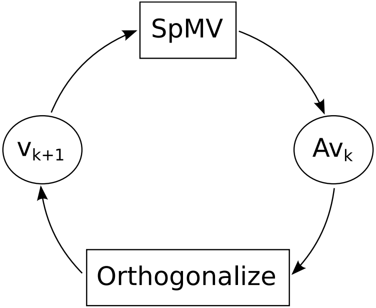

Figure: Data dependencies in Krylov subspace methods.

s-step Krylov methods: break the dependency

- Matrix powers kernel
  - Compute basis of span$\{v, Av, A^2 v, \ldots, A^s v\}$
- TSQR
  - Orthogonalize basis
- Use R factor to reconstruct upper Hessenberg H resp. tridiagonal T
- Solve least squares problem or linear system with H resp. T for coefficients of solution update

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Example: GMRES

Original GMRES

1: **for** $k = 1$ to s **do**
2: $\quad w = Av_{k-1}$
3: $\quad$ Orthogonalize w against $v_0, \ldots, v_{k-1}$ using Modified Gram-Schmidt
4: **end for**
5: Compute solution using H

Version 2: Matrix powers kernel & TSQR

1: $W = [v_0, Av_0, A^2 v_0, \ldots, A^s v_0]$
2: $[Q, R] = TSQR(W)$
3: Compute H using R
4: Compute solution using H

- s powers of A for no extra latency cost
- s steps of QR for one step of latency
- But…

Basis computation not stable

- $v, Av, A^2v, \ldots$ looks familiar…
- It's the power method!
  - *Converges* to principal eigenvector of A
  - Expect increasing linear dependence…
- Basis condition number *exponential* in s

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Version 3: Different basis

- Just like polynomial interpolation
- Use a different basis, e.g.:
  - Newton basis $W = [v, (A - \theta_1 I)v, (A - \theta_2 I)(A - \theta_1 I)v, \dots]$
    - Get shifts θ_i for free – Ritz values
    - Can change shifts with each group of s
  - Chebyshev basis $W = [v, T_1(v), T_2(v), \dots]$
    - Use condition number bounds to scale $T_k(z)$
    - Uncertain sensitivity of $\kappa_2(W)$ to bounds

Basis condition number

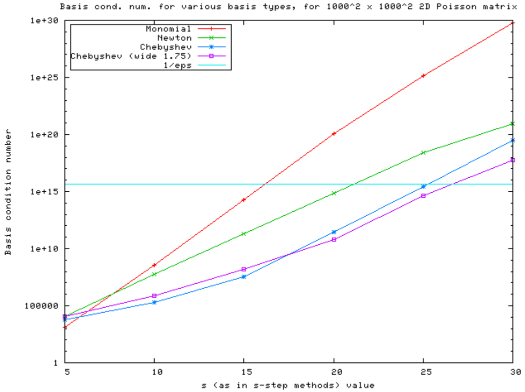

Figure: Condition number of various bases as a function of basis length s. Matrix A is a $10^6 \times 10^6$ 2-D Poisson operator.

Numerical experiments

- Diagonal $10^4 \times 10^4$ matrix, $\kappa_2(A) = 10^8$
- $s = 24$
- Newton: basis condition # about 10^{14}
- Monomial: basis condition # about 10^{16}

Better basis pays off: restarting

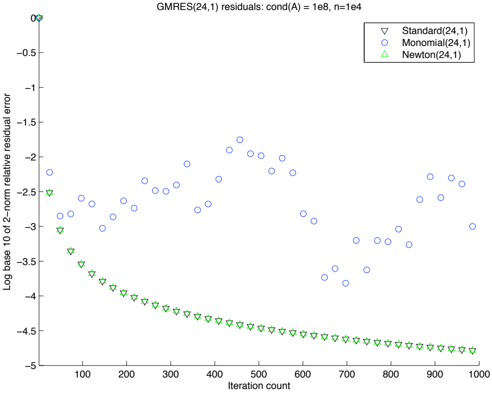

Figure: Restart after every group of *s* steps

Better basis pays off: less restarting

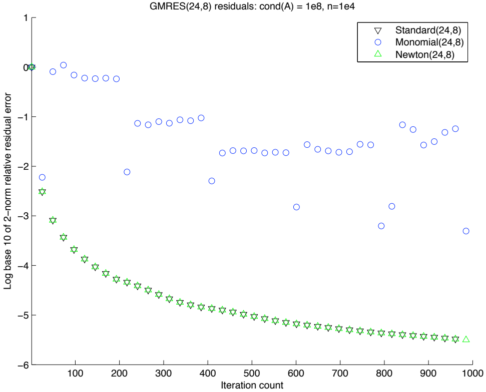

Figure: Restart after 8 groups of $s = 24$ steps.

Krylov methods we can rearrange

- *s*-step Arnoldi / GMRES
- *s*-step symmetric Lanczos / CG
- Need not restart after each group of *s*
  - Just update TSQR factorization

Previous work: s-step CG, part 1

- Van Rosendale 1983, Chronopoulos 1989, ...
  - Compute $W = [v, Av, A^2 v, \ldots, A^s v]$
  - Get solution update coefficients from $W^T W$
- Unstable
  - Monomial basis ($\kappa_2(W)$ is $\Theta(2^s)$)
  - Gram matrix $W^T W$ (squares $\kappa_2(A)$)
- No matrix powers kernel
- No preconditioning

Previous work: *s*-step GMRES

- De Sturler 1991, Bai et al. 1991, et al.
- More stable
  - Newton basis, not monomial
  - QR, not Gram matrix
- No matrix powers kernel
- No preconditioning
- Must restart after each group of *s*

Previous work: s-step CG, part 2

- Toledo 1995 (PhD thesis)
- Developed as part of a matrix powers kernel
  - For (un)structured low-dimensional grids
  - Also for multigrid-like hierarchical graphs
- Based on Chronopoulos 1989
- Suggested change of basis for stability
- Formed Gram matrix $W^T W$ (squares $\kappa_2(A)$)
- No preconditioning

Preconditioning: matrix powers kernel changes

- GMRES with left preconditioning (or any kind)
  - $v, M^{-1}Av, (M^{-1}A)^2 v, \ldots, (M^{-1}A)^s v$
- Symmetric Lanczos / CG with split preconditioning
  - $v, L^{-1}AL^{-T}v, \ldots, (L^{-1}AL^{-T})^s v$
- Symmetric Lanczos / CG with left preconditioning
  - $V = [v, M^{-1}Av, \ldots, (M^{-1}A)^s v]$, and
  - $W = [Av, AM^{-1}Av, \ldots, (AM^{-1})^s Av]$
- Works with any basis

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Effective preconditioning

- Easy to limit communication if connectivity local
- Sparse: “looks like a low-dimensional mesh”
- General: low-rank off-diagonal blocks
  - Rank only grows linearly in s
  - Matrix *and* preconditioner
  - e.g., hierarchical matrices, semiseparable, fast multipole

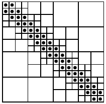

Figure: Discretization of $\log(|x - y|)$ on interval.

Future work

- Preconditioner implementations
- Performance tuning (choosing s)
- Extension to eigensolvers
- Lanczos biorthogonalization (e.g., Bi-CG)
- Combine with block Krylov methods
  - Block methods can already use TSQR
  - Does combining block and s-step pay?

Summary

- s-step Krylov methods incomplete before:
  - Either not stable, not scalable, or both
  - Had to restart between groups of s
  - No preconditioning / not part of optimizations
- Now we have all the pieces!
  - Stable, optimized kernels
  - Can do restarting or not
  - Preconditioning

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Why not use block Krylov methods?

- Solve $Ax = B$ for multiple right-hand sides
- Useful for eigenproblems (original use)
- No extra latency cost
- Bandwidth cost scales linearly w/ # RHS's
- Can use if only one right-hand side

Problems with block methods for $Ax = b$

- If only one right-hand side:
  - Start with one right-hand side
  - After each restart cycle, add error vector to RHS block
  - High startup cost
    - Need s cycles of s until at full block size
    - Whereas, s-step always at full optimization
- More complicated convergence & breakdown conditions

Preconditioning

- Modifications to matrix powers kernel
- Low off-diagonal rank characterization
- Possible preconditioners

Preconditioning and matrix powers

- GMRES or split-preconditioner Lanczos
  - Standard matrix powers kernel
  - Just replace A with preconditioned operator $L^{-1}AL^{-T}$
- Left-preconditioned CG: need new kernel!

New kernel for left-preconditioned CG

- For a basis $p_0, p_1, p_2, \ldots$, define "left shift" operator lshift:
  - In that basis' coordinate system, lshift $e_i = e_{i+1}$ ("multiply by x")
  - $\text{lshift}_A(v)$ means replace x with matrix A
- Left-preconditioned CG: need

$$V_{s+1} = [v, \text{lshift}_{M^{-1}A}(v), \ldots, \text{lshift}^{s}_{M^{-1}A}(v)], \text{and}$$

$$W_s = [Av, \text{lshift}_{AM^{-1}}(Av), \ldots, \text{lshift}^{s-1}_{AM^{-1}}(Av)]$$

Preconditioning and orthogonalization

- GMRES or split-preconditioned CG: no change
- Left-preconditioned CG:
  - $M^{-1}A$ usually nonsymmetric
  - Basis vectors not orthogonal
    - M-orthogonal ("conjugate") instead
    - Can't use QR to orthogonalize
    - Must rely on CG recurrence instead
  - Gram matrix $V_{s+1}^* W_s$ squares $\kappa(A)$ – bad!
  - Avoid by using generalized QR or SVD instead

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Preconditioning: Low off-diagonal rank

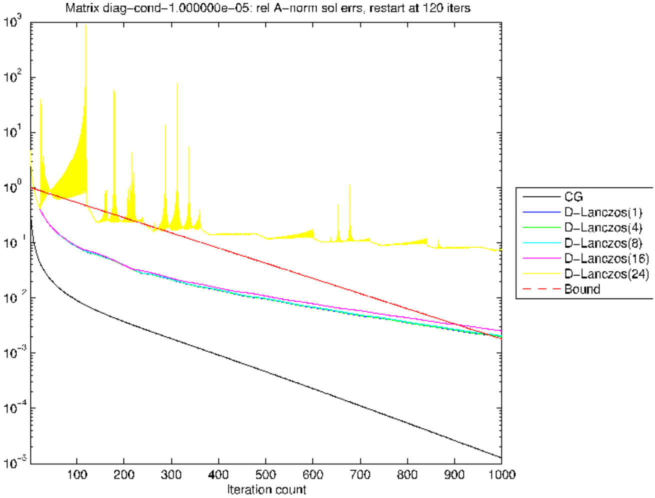
- Matrix powers: depends on boundaries being “lower dimension” than interiors
- Boundary edges of graph are off-diagonal nonzeros
- Generalization: *low-rank off-diagonal blocks*
- Can do matrix powers kernel with SVD-like representation of partitioned matrix

Possible preconditioners

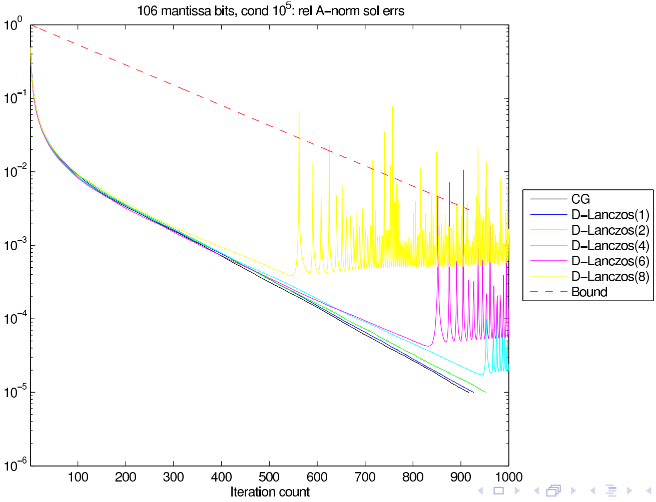
Right generalization: *low-rank off-diagonal blocks*

- Rank 0: block diagonal (a.k.a. block Jacobi)
  - Blocks can be arbitrarily complex
- But effective preconditioning needs some communication!
- Sparse approximate inverse (SPAI) – constrain low off-diag rank
- $\mathcal{H}$, $\mathcal{H}^2$, HSS matrices
  - From integral equations with separable kernels
  - Continuous analogue to discrete “low-rank off-diagonal blocks” condition

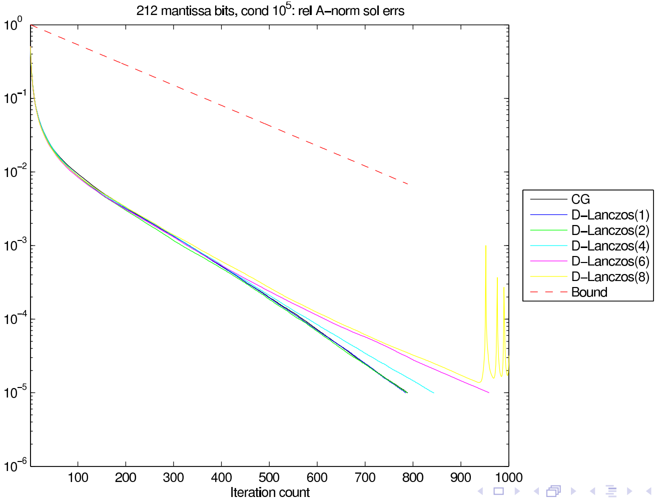
Restarting for stability



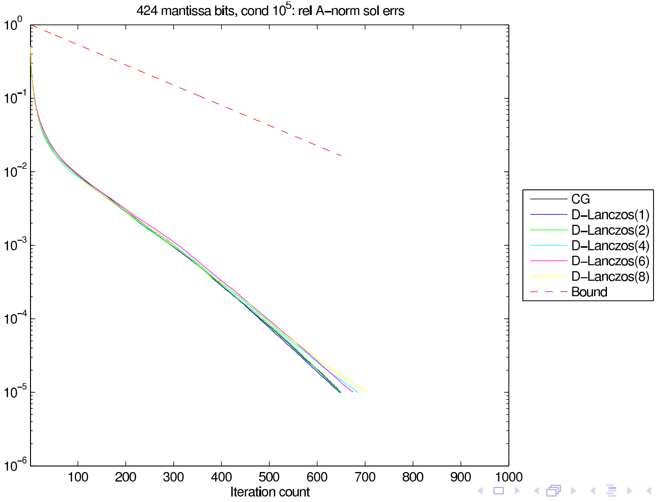
Extra precision for stability (1 of 3)



Extra precision for stability (2 of 3)



Extra precision for stability (3 of 3)



Lanczos(s,t) w/ reorthogonalization

- Get orthogonality estimates from Lanczos recurrence (Paige)
- Each group of s basis vectors is a TSQR Q factor
- Best reorthogonalization:
  - Do TSQR of last group to compute Lanczos coefficients
  - Use Lanczos coeffs in Paige's recurrence
  - If last group not orthogonal w.r.t. previous groups
    - Compute it explicitly
    - Orthogonalize against previous $t-1$ groups
  - Finally take TSQR again of last group
- Converting all groups of s to explicit storage and redoing TSQR on them all is too expensive & unnecessary

Components

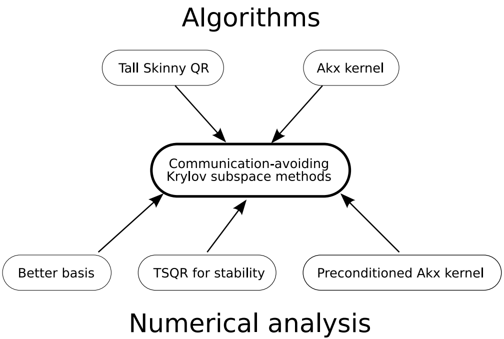


Figure: Components of communication-avoiding Krylov methods.

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