A subspace-conjugate gradient method for linear matrix equations

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From joint work with Martina Iannacito and Davide Palitta

Large linear systems

Given a PDE and your preferred discretization strategy,

$$\mathcal{A}x = b, \quad \mathcal{A} \in \mathbb{R}^{n \times n}$$

- Krylov subspace methods (CG, MINRES, GMRES, BiCGSTAB, etc.)

$$x \approx x_m = \mathcal{V}_m y_m$$

where $\mathcal{V}_m$ has (orthonormal) columns spanning $\mathbb{K}_m(\mathcal{A}, b) = \mathrm{span}\{b, \mathcal{A}b, \ldots, \mathcal{A}^{m-1}b\}$

- Preconditioners: find P such that

$$\mathcal{A}P^{-1}\widetilde{x} = b \qquad x = P^{-1}\widetilde{x}$$

where $\mathcal{A}P^{-1}$ is "easier" to solve with.

Comfort zone

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Heterogeneous variable setting

The differential problem may depend on space variable and

- Time (high quality soln of heat-, wave-type equations, dynamical systems generally)
- Parameters (e.g., coefficients with uncertainty, model tuning)

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Approximation space during the discretization phase: tensor space

$$\mathcal{H} \times \mathcal{S}$$

with ♣ $\mathcal{H}$: spatial variables
♣ $\mathcal{S}$: time/parameter variables

Algebraic system: $\mathcal{A}$ mixes all components, e.g.,

$$\mathcal{A} = I \otimes A + G^T \otimes I$$

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Identity-preserving algebraic formulations

$$\mathcal{A}x = b, \qquad \mathcal{A} = I \otimes A + G^T \otimes I \qquad \mathcal{A} \in \mathbb{R}^{n \times n}, \text{ with } n = n_A n_G$$

$$\Downarrow$$

$$AX + XG = B, \qquad x = \mathrm{vec}(X), \qquad b = \mathrm{vec}(B), \quad X \in \mathbb{R}^{n_A \times n_G}$$

Pros:

- ✓ Matrices of Smaller dimension $\Rightarrow$ Reach more complex problems
- ✓ No mixing – Preserve properties of continuous problem
- ✓ Exploit algebraic structure (symmetries, rank properties...)

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Exploiting rank structure

Assume B can be well represented by a low rank matrix.

$$x \in \mathbb{R}^{n_A n_G \times 1} \quad \rightarrow \quad X \approx \widetilde{X} = \begin{bmatrix} X_1 \end{bmatrix} \begin{bmatrix} X_2^T \end{bmatrix}$$

with $X_1 \in \mathbb{R}^{n_A \times k}, X_2 \in \mathbb{R}^{n_G \times k}$ tall, $k \ll n_a, n_G$

Uncover low rank approximate representation!

- Save memory allocations while approximating!
- Different interpretation: approximate soln snapshots (MOR style)
- Recognize roles at the algebraic level: use different approximations for X_1, X_2

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Numerical solution of the Sylvester equation

$$AX + XG^T = B$$

Various settings:

- Tiny A and G: Kron will do!
- Small A and G: Bartels-Stewart algorithm (Computes the Schur form of A and G)
- Large A and G: Iterative solution (B low rank)
  - Projection methods
  - ADI (Alternating Direction Iteration)
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Projection-type methods

Assume $B = B_1 B_2^T$.
Given two low dimensional approx spaces $\mathcal{K}_A$, $\mathcal{K}_G$, and V_m, W_m their orthonormal bases let $X_m := V_m Y_m W_m^T$, $X_m \approx X$

Galerkin condition: $R := AX_m + X_m G^T - B_1 B_2^T \quad \perp \quad \mathcal{K}_A \otimes \mathcal{K}_G$

$$V_m^\top R W_m = 0$$

Note: $\mathcal{K}_A$, $\mathcal{K}_G$ tiny wrto $\mathbb{K}(\mathcal{A}, b)$

Projected Sylvester equation:

$$\begin{aligned} V_m^\top (AV_m Y_m W_m^\top + V_m Y_m W_m^\top G^\top &- B_1 B_2^\top) W_m = 0 \\ (V_m^\top A V_m) Y_m + Y_m (V_m^\top G^\top V_m) &- V_m^\top B_1 B_2^\top W_m = 0 \end{aligned}$$

Early contributions: Saad '90, Jaimoukha & Kasenally '94, for $\mathrm{range}(V_m) = \mathcal{K}_A = \mathrm{Range}([B_1, AB_1, \ldots, A^{m-1} B_1])$

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More recent options as approximation space

Enrich space to decrease space dimension

- Extended Krylov subspace

  (Druskin & Knizhnerman '98, Simoncini '07)

- Rational Krylov subspace

$$\mathcal{K}_A = \mathbb{K}_A := \mathrm{Range}([B_1, (A - s_1 I)^{-1} B_1, \ldots, \prod_{j=1}^{m-1} (A - s_j I)^{-1} B_1])$$

  usually, $\{s_1, \ldots, s_{m-1}\} \subset \mathbb{C}^+$ chosen either a-priori or dynamically
  (form matrix equations, Druskin & Simoncini '11)

In both cases, for $\mathrm{Range}(V_m) = \mathcal{K}_A$, $\mathrm{Range}(W_m) = \mathcal{K}_{G^T}$ projected Lyapunov equation:

$$(V_m^T A V_m) Y_m + Y_m (W_m^T G^T W_m) - V_m^T B_1 B_2^T W_m = 0 \qquad X_m = V_m Y_m W_m^T$$

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Multiterm linear matrix equation

$$A_1 \boldsymbol{X} B_1 + A_2 \boldsymbol{X} B_2 + \ldots + A_\ell \boldsymbol{X} B_\ell = C \tag{1}$$

$A_i \in \mathbb{R}^{n \times n}$, $B_i \in \mathbb{R}^{m \times m}$, $\boldsymbol{X}$ unknown matrix

Possibly large dimensions, structured coefficient matrices

> *The problem in its full generality is far from tractable, although the transformation to a matrix-vector equation [...] allows us to use the considerable arsenal of numerical weapons currently available for the solution of such problems.*

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- Projection-type methods $\Rightarrow$ low rank approximation
- Ad-hoc problem-dependent procedures
- etc.

A sample of these methodologies on different problems:

- Stochastic PDEs
- PDEs on polygonal domains, IGA, spectral methods, etc
- Space-time PDEs
- All-at-once PDE-constrained optimization problem
- Bilinear control problems
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Multiterm linear matrix equation. Classical device

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Kronecker formulation

$$\left(B_1^\top \otimes A_1 + \ldots + B_\ell^\top \otimes A_\ell\right) \boldsymbol{x} = c \qquad \Leftrightarrow \qquad \mathcal{A}\boldsymbol{x} = c$$

Iterative methods: matrix-matrix multiplications and rank truncation

(Benner, Bioli, Breiten, Bouhamidi, Chehab, Damm, Grasedyck, Jbilou, Kressner, Kuerschner, Matthies, Nagy, Onwunta, Palitta, Raydan, Robol, Stoll, Tobler, Wedderburn, Zander, ...)

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CG matricization and truncation

⋆ **Matricization.** Typically,

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)} \in \mathbb{R}^{n^2} \qquad \Rightarrow \quad X^{(k+1)} = X^{(k)} + \alpha_k P^{(k)} \in \mathbb{R}^{n \times n}$$

⋆ **Truncation.** If $X^{(k)} = X_1^{(k)} (X_1^{(k)})^\top$ with $X_1^{(k)}$ low rank, and similarly for $P^{(k)}$, then

$$X^{(k+1)} = X_1^{(k)} (X_1^{(k)})^\top + \alpha_k P_1^{(k)} (P_1^{(k)})^\top$$

- $X^{(k+1)}$ low rank:

$$X^{(k+1)} = [X_1^{(k)}, \sqrt{\alpha_k} P_1^{(k)}] \, [X_1^{(k)}, \sqrt{\alpha_k} P_1^{(k)}]^\top \tag{2}$$

  (but generally larger than at iteration k)

- Cure: Rank shrinking $[X_1^{(k)}, \sqrt{\alpha_k} P_1^{(k)}] \Rightarrow X_1^{(k+1)} \qquad X^{(k+1)} \approx X_1^{(k+1)} (X_1^{(k+1)})^\top$

  Implementation: $\mathcal{T}(X^{(k+1)})$ acts on the QR-SVD of factor in (2)

Alternative truncation criteria:

♣ Fix lower threshold tolerance ♣ Fix maximum allowed rank

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Truncated matrix-oriented CG (TCG) for Kronecker form

Input: $\mathcal{L}(\boldsymbol{X}) = A_1 \boldsymbol{X} B_1 + A_2 \boldsymbol{X} B_2 + \ldots + A_\ell \boldsymbol{X} B_\ell$, right-hand side $C \in \mathbb{R}^{n \times n}$ in low-rank format. Truncation operator $\mathcal{T}$.
Output: Matrix $X \in \mathbb{R}^{n \times n}$ in low-rank format s.t. $||\mathcal{L}(X) - C||_F / ||C||_F \leq tol$

1. $X_0 = 0$, $R_0 = C$, $P_0 = R_0$, $Q_0 = \mathcal{L}(P_0)$
2. $\xi_0 = \langle P_0, Q_0 \rangle$, $k = 0$ $\qquad\qquad \langle X, Y \rangle = \mathrm{tr}(X^\top Y)$
3. While $||R_k||_F > tol$
4. $\quad \alpha_k = \langle R_k, P_k \rangle / \xi_k$
5. $\quad X_{k+1} = X_k + \alpha_k P_k,$ $\qquad X_{k+1} \leftarrow \mathcal{T}(X_{k+1})$
6. $\quad R_{k+1} = C - \mathcal{L}(X_{k+1}),$ $\qquad$ Optionally: $R_{k+1} \leftarrow \mathcal{T}(R_{k+1})$
7. $\quad \beta_k = -\langle R_{k+1}, Q_k \rangle / \xi_k$
8. $\quad P_{k+1} = R_{k+1} + \beta_k P_k,$ $\qquad P_{k+1} \leftarrow \mathcal{T}(P_{k+1})$
9. $\quad Q_{k+1} = \mathcal{L}(P_{k+1}),$ $\qquad$ Optionally: $Q_{k+1} \leftarrow \mathcal{T}(Q_{k+1})$
10. $\quad \xi_{k+1} = \langle P_{k+1}, Q_{k+1} \rangle$
11. $\quad k = k + 1$
12. end while

♣ Iterates kept in factored form! Kressner and Tobler, '11

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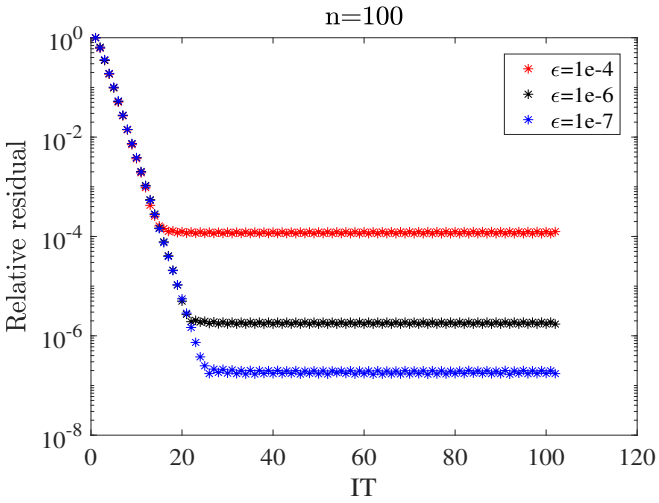
4. $\quad \alpha_k = \langle R_k, P_k\rangle/\xi_k$
5. $\quad X_{k+1} = X_k + \alpha_k P_k$, $\qquad X_{k+1} \leftarrow \mathcal{T}(X_{k+1})$
6. $\quad R_{k+1} = C - \mathcal{L}(X_{k+1})$, $\qquad$ Optionally: $R_{k+1} \leftarrow \mathcal{T}(R_{k+1})$
7. $\quad \beta_k = -\langle R_{k+1}, Q_k\rangle/\xi_k$
8. $\quad P_{k+1} = R_{k+1} + \beta_k P_k$, $\qquad P_{k+1} \leftarrow \mathcal{T}(P_{k+1})$
9. $\quad Q_{k+1} = \mathcal{L}(P_{k+1})$, $\qquad$ Optionally: $Q_{k+1} \leftarrow \mathcal{T}(Q_{k+1})$
10. $\quad \xi_{k+1} = \langle P_{k+1}, Q_{k+1}\rangle$
11. $\quad k = k + 1$
12. end while

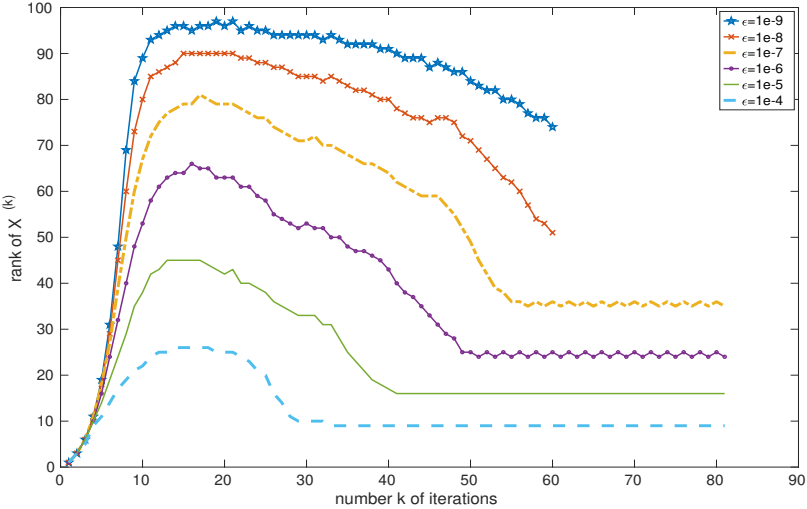
♣ Iterates kept in factored form! Kressner and Tobler, '11

Typical convergence behavior



(Hao, '20, personal comm.)

Typical iterate rank behavior



(Simoncini & Hao, '22)

Within the CG framework, can we do better?

Considerations:

1. At best, convergence as for Kronecker problem
2. Rank of iterates hard to control to maintain convergence
3. Coeffs α, β under exploited

$$\boldsymbol{p}_k = \mathrm{vec}(P_k), \boldsymbol{r}_k = \mathrm{vec}(R_k) \quad \Rightarrow \quad \{\boldsymbol{r}_0, \ldots, \boldsymbol{r}_k\}, \{\boldsymbol{p}_0, \ldots, \boldsymbol{p}_k\} \quad \text{orth prop}$$

Recalling CG basics: $\mathcal{A}\boldsymbol{x} = \boldsymbol{b}$

Problem: Minimize the convex function

$$\Phi(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T \mathcal{A}\boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x}$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k, \qquad \alpha_k \, s.t. \, \min_{\alpha} \Phi(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)$$

with residual and direction updates:

$$\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \mathcal{A}\boldsymbol{p}_k \alpha_k, \quad \boldsymbol{p}_{k+1} = \boldsymbol{r}_{k+1} + \boldsymbol{p}_k \beta_k.$$

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The new **subspace**-CG

Warning: For the sake of the presentation, we assume a simplified form:

$$\mathcal{L}(\boldsymbol{X}) = \mathcal{L}(\boldsymbol{X})^T, \qquad \text{for any} \quad \boldsymbol{X} = \boldsymbol{X}^T$$

This assumption allows us to write a square $\boldsymbol{X}$ as $\boldsymbol{X} = XX^T$

In practice, the whole derivation holds for $\mathcal{A} = B_1 \otimes A_1 + \cdots + B_\ell \otimes A_\ell$ spd
(that is, $\mathcal{L}$ spd in the matrix inner product)
so that

$$\boldsymbol{X} \in \mathbb{R}^{n_l \times n_r}, \qquad \boldsymbol{X} = X^l (X^r)^T$$

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We define $\Phi : \mathbb{R}^{n\times n} \to \mathbb{R}$,

$$\Phi(\boldsymbol{X}) = \frac{1}{2}\langle \boldsymbol{X}, \mathcal{L}(\boldsymbol{X})\rangle - \langle \boldsymbol{X}, \boldsymbol{C}\rangle$$

The new minimization problem: *Find* $\boldsymbol{X} \in \mathbb{R}^{n\times n}$ *such that*

$$\boldsymbol{X} = \arg \min_{\boldsymbol{X}\in\mathbb{R}^{n\times n}} \Phi(\boldsymbol{X})$$

with iteration

$$\boldsymbol{X}_{k+1} = \boldsymbol{X}_k + P_k \boldsymbol{\alpha}_k P_k^T$$

where $\boldsymbol{\alpha}_k \in \mathbb{R}^{s_k\times s_k}$ and $P_k \in \mathbb{R}^{n\times s_k}$

Residual and direction computation:

$$\boldsymbol{R}_{k+1} = \boldsymbol{R}_k - \mathcal{L}(P_k \boldsymbol{\alpha}_k P_k^T), \qquad \boldsymbol{P}_{k+1} = \boldsymbol{R}_{k+1} + P_k \boldsymbol{\beta}_k P_k^T,$$

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Defining the coefficients. I

At the kth iteration:

1. Construct $\boldsymbol{\alpha}_k$ so that

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{s_k \times s_k}} \Phi(\boldsymbol{X}_k + P_k \boldsymbol{\alpha} P_k^T)$$

2. Impose a descent direction requirement for $\boldsymbol{P}_k = P_k P_k^T$:

$$\langle \nabla \Phi(\boldsymbol{X}_k), \boldsymbol{P}_k \rangle < 0$$

3. Construct β_k so that the new direction $\boldsymbol{P}_{k+1}$ is $\mathcal{L}$-orthogonal with respect to the previous ones:

$$(P_k \otimes P_k)^T \mathrm{vec}(\mathcal{L}(\boldsymbol{P}_{k+1})) = 0$$

Defining the coefficients. II

Let $\widetilde{A}_k^{(i)} = P_k^T A_i P_k, \widetilde{B}_k^{(i)} = P_k^T B_i P_k$, $i = 1, \ldots, \ell$

- Construction of $\boldsymbol{\alpha}_k$:
  $\boldsymbol{\alpha}_k$ is the unique solution of

$$\widetilde{A}_k^{(1)} \boldsymbol{\alpha} \widetilde{B}_k^{(1)} + \ldots + \widetilde{A}_k^{(\ell)} \boldsymbol{\alpha} \widetilde{B}_k^{(\ell)} = P_k^T \boldsymbol{R}_k P_k$$

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Making the idea practical

$$\begin{aligned} \boldsymbol{X}_{k+1} &= X_k \boldsymbol{\tau}_k X_k^T + P_k \boldsymbol{\alpha}_k P_k^T = [X_k, P_k] \boldsymbol{\tau}_{k+1} [X_k, P_k]^T \\ \boldsymbol{R}_{k+1} &= [R_0, \boldsymbol{A}_\star \bullet X_{k+1}] \boldsymbol{\rho}_{k+1} [R_0, \boldsymbol{B}_\star \bullet X_{k+1}]^T \end{aligned}$$

where $\boldsymbol{A}_\star \bullet R = [A_1 R, \ldots, A_\ell R]$

- All terms are kept in factored form
- The rank grows

Rank truncation

- Computing $\boldsymbol{R}_{k+1}$ becomes too expensive (CPU time and memory)

Randomized range finder

Given a target rank `maxrankR` and a Gaussian matrix $G^l \in \mathbb{R}^{n_B \times \texttt{maxrankR}}$:

$$\boldsymbol{R}_{k+1} G^l = C_1 (C_2^T G^l) - \sum_{i=1}^{\ell} A_i (X^l_{k+1} \boldsymbol{\tau}_{k+1} ((X^r_{k+1})^T (B_i G^l)))$$

(Analogously for $\boldsymbol{R}_{k+1}^T$)
Then proceed with a cheap evaluation of the reduced residual matrix

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A computational experiment. I

Parameterized diffusion equation (Biolietal, tech.rep.2024)

$$-\nabla \cdot (k \nabla u) = 0 \qquad \text{in} \quad (0,1)^2$$

with homogeneous boundary conditions and semi-separable diffusion coefficient:

$$k(x,y) = \sum_{j=1}^{\ell_k} \delta_j k_{j,x}(x) k_{j,y}(y) = 1 + \sum_{j=1}^{\ell_k - 1} \frac{10^j}{j!} x^j y^j, \qquad \ell_k = 4$$

This gives

$$\sum_{j=1}^{\ell_k} \delta_j (A_{j,x} \boldsymbol{X} D_{j,y} + D_{j,y} \boldsymbol{X} A_{j,y}) = \boldsymbol{C}$$

with $\boldsymbol{C}$ rank-four nonsym matrix accounting for b.c. (total of $\ell = 8$ terms)

Algorithms to be compared:
* SS-CG-determ: new method, residual matrix computed sequentially;
* SS-CG-rand'zed: new method, residual matrix computed using Randfinder
* TPCG: truncated matrix-oriented preconditioned CG (Kressner, Tobler, 2011, and others)
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A computational experiment. II

n type	Precond	maxrank	R-NLCG	TPCG	SS–CG determ.	SS–CG rand'zed
10000	$\mathcal{P}_1$	20	– (100)	– (100)	– (100)	– (100)
	$\mathcal{P}_1$	40	– (100)	– (100)	1.08 (5)	**0.92** (5)
	$\mathcal{P}_1$	60	– (100)	– (100)	2.47 (5)	**2.34** (5)
	$\mathcal{P}_2$	20	**11.25 (36)**	11.42 (38)	– (100)	– (100)
	$\mathcal{P}_2$	40	*42.97 (36)	**15.54** (33)	– (100)	– (100)
	$\mathcal{P}_2$	60	*98.62 (35)	32.39 (28)	9.59 (5)	**8.37** (5)
102400	$\mathcal{P}_1$	20	– (100)	– (100)	– (100)	– (100)
	$\mathcal{P}_1$	40	†	– (100)	18.17 (6)	**8.74** (6)
	$\mathcal{P}_1$	60	†	– (100)	23.50 (5)	**16.93** (5)
	$\mathcal{P}_2$	20	**183.44** (41)	– (100)	– (100)	– (100)
	$\mathcal{P}_2$	40	†	446.94 (47)	– (100)	– (100)
	$\mathcal{P}_2$	60	†	884.20 (26)	115.73 (3)	**101.91** (3)

– no conv. * Lower final residual norm than other methods † Out of Memory

Running time in seconds (# iter's)
Stopping tolerance $\texttt{tol} = 5 \cdot 10^{-6}$ True residual norm at termination

$\mathcal{P}_1$: one-term precond, cheap $\mathcal{P}_2$: two-term precond, expensive (fixed ADI iters)

What is left

What I have not told you about:

- Orthogonality properties of residuals and directions
- Optimality and finite termination properties
- Preconditioning
- More experiments on a variety of application problems

Outlook:

- Experiments are very promising
- The idea can be generalized to other Krylov methods
- Tensor version under investigation

Reference

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A subspace-conjugate gradient method for linear matrix equations
pp. 1-25, Jan 2025. ArXiv 2501.02938

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