Spectral Properties of Saddle Point Linear Systems and Iterative Solvers

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The problem

$$\begin{bmatrix} F & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

- Computational Fluid Dynamics (see, e.g., Elman, Silvester, Wathen 2005)
- Elasticity problems
- Mixed (FE) formulations of II and IV order elliptic PDEs
- Linearly Constrained Programs
- Linear Regression in Statistics
- Image restoration
- ... Survey: Benzi, Golub and Liesen, Acta Num 2005

The problem

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Hypotheses:

- $\star$ $F \in \mathbb{R}^{n\times n}$ (often: F positive definite in Ker(B))
- $\star$ B^T tall, possibly rank deficient
- $\star$ C symmetric positive (semi)definite
- $\star$ $g = 0$ in some cases

More hypotheses later...

A possible setting

The variational problem:

$$u = \arg\min_{v \in V} a(v,v) - 2F(v) \quad \text{subject to} \quad b(v,q) = G(q),\; q \in Q,$$

where F, G, a, b are bounded (bi)linear functionals in Hilbert spaces

a is symmetric and positive semi-definite

The associated saddle point system:

Find $(u,p) \in V \times Q$ such that

$$\begin{aligned} a(u,v) + b(v,p) &= F(v) \quad v \in V \\ b(u,q) &= G(q) \quad q \in Q \end{aligned}$$

Why are we interested in a spectral analysis?

- To detect “sensitive” blocks in the coeff. matrix
  (guidelines for preconditioning strategies)

- To “tune” the regularization parameter (matrix C)

- To predict convergence behavior of the iterative solver

Iterative solver. Convergence considerations.

$$\mathcal{M}x = b$$

$\mathcal{M}$ is symmetric and indefinite $\quad\longrightarrow\quad$ MINRES

$$x_k \in x_0 + K_k(\mathcal{M}, r_0), \quad \text{s.t.} \qquad \min \|b - \mathcal{M}x_k\|$$

$r_k = b - \mathcal{M}x_k$, $k = 0, 1, \ldots$, x_0 starting guess

If $\mu(\mathcal{M}) \subset [-a, -b] \cup [c, d]$, with $|b - a| = |d - c|$, then

$$\|b - \mathcal{M}x_{2k}\| \leq 2 \left(\frac{\sqrt{ad} - \sqrt{bc}}{\sqrt{ad} + \sqrt{bc}} \right)^k \|b - \mathcal{M}x_0\|$$

Note: more general but less tractable bounds available

Spectral properties

$A := F$ for F symmetric

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & O \end{bmatrix} \qquad \begin{array}{ll} 0 < \lambda_n \leq \cdots \leq \lambda_1 & \text{eigs of } A \\ 0 < \sigma_m \leq \cdots \leq \sigma_1 & \text{sing. vals of } B \end{array}$$

$\sigma(\mathcal{M})$ subset of (Rusten & Winther 1992)

$$\left[\frac{1}{2}(\lambda_n - \sqrt{\lambda_n^2 + 4\sigma_1^2}), \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\sigma_m^2})\right] \quad \cup \quad \left[\lambda_n, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

A nonsingular

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Generalizations:

- A spd in Ker(B)
- A indefinite

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B full rank

Spectral properties

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \qquad \begin{array}{ll} 0 < \lambda_n \leq \cdots \leq \lambda_1 & \text{eigs of } A \\ 0 = \sigma_m \leq \cdots \leq \sigma_1 & \text{sing. vals of } B \end{array}$$

$\sigma(\mathcal{M})$ subset of

$$\left[\frac{1}{2}(-\gamma_1 + \lambda_n - \sqrt{(\gamma_1 + \lambda_n)^2 + 4\sigma_1^2})\ , \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\theta})\right] \cup \left[\lambda_n, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

B rank deficient, but $\quad \theta = \lambda_{\min}(BB^T + C)$ full rank

$$\gamma_1 = \lambda_{\max}(C)$$

In some cases, C regularization matrix, used also for B full row rank

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Good (= slim) spectrum: $\lambda_1 \approx \lambda_n, \quad \sigma_1 \approx \sigma_m$

e.g.

$$\mathcal{M} = \begin{bmatrix} I & U^T \\ U & O \end{bmatrix}, \quad UU^T = I$$

General preconditioning strategy

- Find $\mathcal{P}$ such that

$$\mathcal{M}\mathcal{P}^{-1}\hat{u} = b \qquad \hat{u} = \mathcal{P}u$$

  is easier (faster) to solve than $\mathcal{M}u = b$

- A look at efficiency:
  - Dealing with $\mathcal{P}$ should be cheap
  - Storage requirements for $\mathcal{P}$ should be low
  - Properties (algebraic/functional) should be exploited

  Mesh/parameter independence

Structure preserving preconditioners

Block diagonal Preconditioner

$\star$ A nonsing., $C = 0$:

$$\mathcal{P}_0 = \begin{bmatrix} A & 0 \\ 0 & BA^{-1}B^T \end{bmatrix}$$

$$\Rightarrow \qquad \mathcal{P}_0^{-\frac{1}{2}} \mathcal{M} \mathcal{P}_0^{-\frac{1}{2}} = \begin{bmatrix} I & A^{-\frac{1}{2}} B^T (BA^{-1}B^T)^{-\frac{1}{2}} \\ (BA^{-1}B^T)^{-\frac{1}{2}} BA^{-\frac{1}{2}} & 0 \end{bmatrix}$$

MINRES converges in at most 3 iterations. $\sigma(\mathcal{P}_0^{-\frac{1}{2}} \mathcal{M} \mathcal{P}_0^{-\frac{1}{2}}) = \{1, 1/2 \pm \sqrt{5}/2\}$

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A more practical choice:

$$\mathcal{P} = \begin{bmatrix} \widetilde{A} & 0 \\ 0 & \widetilde{S} \end{bmatrix} \qquad \text{spd.} \quad \widetilde{A} \approx A \qquad \widetilde{S} \approx BA^{-1}B^T$$

eigs in $\quad [-a, -b] \cup [c, d], \qquad a, b, c, d > 0$

still an Indefinite Problem

An example. Stokes problem

$$\begin{bmatrix} -\Delta & -\mathrm{grad} \\ \mathrm{div} & \end{bmatrix} \approx \begin{bmatrix} -\widetilde{\Delta} & \\ & I \end{bmatrix}$$

In algebraic terms:

$I \to$ mass matrix

$-\widetilde{\Delta} \to$ Algebraic MG

(spectrally equivalent matrix)

(cf. K.-A. Mardal & R. Winther

to appear in JNLAA)

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2D. Final residual norm $< 10^{-6}$

size($\mathcal{M}$)	its	Time (secs)
578	26	0.04
217	26	0.14
8450	26	0.50
132098	26	11.17

Giving up symmetry ...

- Change the preconditioner: *Mimic the LU factors*

$$\mathcal{M} = \begin{bmatrix} I & O \\ BA^{-1} & I \end{bmatrix} \begin{bmatrix} A & B^T \\ O & BA^{-1}B^T + C \end{bmatrix} \quad \Rightarrow \mathcal{P} \approx \begin{bmatrix} A & B^T \\ O & BA^{-1}B^T + C \end{bmatrix}$$

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- Change the preconditioner: *Mimic the Structure*

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \quad \Rightarrow \mathcal{P} = \begin{bmatrix} \widetilde{A} & B^T \\ B & -\widetilde{C} \end{bmatrix}$$

(Constraint Preconditioning)

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(Constraint Preconditioning)

- Change the matrix: *Eliminate indef.* $\quad \mathcal{M}_- = \begin{bmatrix} A & B^T \\ -B & C \end{bmatrix}$

Triangular preconditioner

$$A \text{ spd}, \quad \mathcal{P} = \begin{bmatrix} \widetilde{A} & B^T \\ 0 & -\widetilde{C} \end{bmatrix} \qquad \widetilde{A} \approx A, \quad \widetilde{C} \approx BA^{-1}B^T + C$$

Ideal case: $\widetilde{A} = A,\ \widetilde{C} = BA^{-1}B^T + C \quad \Rightarrow \quad \mathcal{M}\mathcal{P}^{-1} = \begin{bmatrix} I & 0 \\ BA^{-1} & I \end{bmatrix}$

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A particular choice. Augmented block preconditioner:

$$\mathcal{P} = \begin{bmatrix} A + B^T W^{-1} B & B^T \\ O & W \end{bmatrix}$$

The "minus-signed" Problem

$$\mathcal{M}_- = \begin{bmatrix} A & B^T \\ -B & C \end{bmatrix} \qquad \text{nonsym}$$

B full rank $\Rightarrow \mathcal{M}_-$ positive stable $\Rightarrow$ eigs in $\mathbb{C}^+$

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Some facts

- $\mathcal{M}_-$ has always at least $n - m$ real eigs
- If $2\|B\| < \lambda_{\min}(A) - \lambda_{\max}(C) \Rightarrow$ all eigs real and positive

  for $C = 0$, condition simplifies: $\lambda_{\min}(A) > 4\lambda_{\max}(B^T A^{-1} B)$
- If B full rank and $\lambda_{\min}(A) > \lambda_{\max}(C)$

  apon scaling all eigs real and positive

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Splitting precond.: Hermitian-Skew-Hermitian preconditioners

General nonsymmetric problem

$$\mathcal{M} = \begin{bmatrix} F & B^\top \\ B & -\beta C \end{bmatrix} \qquad F \quad \text{nonsymmetric}$$

Preconditioning strategies (other alternatives are possible):

$$\mathcal{P}_{tr} = \begin{bmatrix} \widetilde{F} & B \\ & \pm\widetilde{C} \end{bmatrix} \qquad \mathcal{P}_d = \begin{bmatrix} \widetilde{F} & \\ & \pm\widetilde{C} \end{bmatrix} \text{ with } \widetilde{C} > 0$$

- $\widetilde{F} \approx F$
- $\widetilde{F} \approx F + B^\top \widetilde{C}^{-1} B$ (augmentation block precond.)

For $+\widetilde{C}$: $\qquad \mathcal{M}\mathcal{P}^{-1}$ indefinite

Questions

⋆ Which formulation/preconditioner for which iterative solver?

⋆ Is the theoretical spectral information useful in practice?

⋆ Are the imposed “constraints” needed?

The standard solvers

Krylov subspace iterative solvers for $\mathcal{M}x = b$:

- $\mathcal{M}$ symmetric and positive definite $\Rightarrow$ (P)CG
- $\mathcal{M}$ symmetric indefinite $\Rightarrow$ (P)MINRES, (P)SYMLQ
- $\mathcal{M}$ nonsymmetric $\Rightarrow$ (P)GMRES, (P)BiCGSTAB(ℓ), (P)IDR(s)

A wasted effort: an H-sym constraint preconditioner

$$\mathcal{P} = \begin{bmatrix} I & O \\ B\widehat{A}^{-1} & I \end{bmatrix} \begin{bmatrix} \widehat{A} & O \\ O & -S \end{bmatrix} \begin{bmatrix} I & \widehat{A}^{-1}B^T \\ O & I \end{bmatrix}$$

where $\widehat{A} \approx A$, $\quad S \approx B\widehat{A}^{-1}B^T$

Two alternatives:

$\star$ Use $\mathcal{P}$ with nonsymmetric solver

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Two alternatives:

⋆ Use $\mathcal{P}$ with nonsymmetric solver

⋆ Enforce constraints on $\widehat{A}$, S to derive H-symmetric CG:

$\mathcal{P}^{-1}\mathcal{M}$ is H-symmetric with

$$H = \begin{bmatrix} \widehat{A} - A & O \\ O & B\widehat{A}^{-1}B^T - S \end{bmatrix} > 0$$

A wasted effort: an H-sym constraint preconditioner. Stokes problem.

Preconditioner: $\widehat{A}$: $\texttt{cholinc}(A, 10^{-2})$ $\quad S$: $\texttt{cholinc}(B\widehat{A}^{-1}B^T, 10^{-2})$

Preconditioner forcing H-symmetry: $\widetilde{A} = \widehat{A} + \tau I$, s.t. $\lambda_{\min}(\widetilde{A} - A) \approx 2.74$

$\widehat{S}$: from $\texttt{cholinc}(B\widetilde{A}^{-1}B, 10^{-2})$ scaled s.t. $\lambda_{\min}(B\widetilde{A}^{-1}B^T - \widehat{S}) \approx 0.07$

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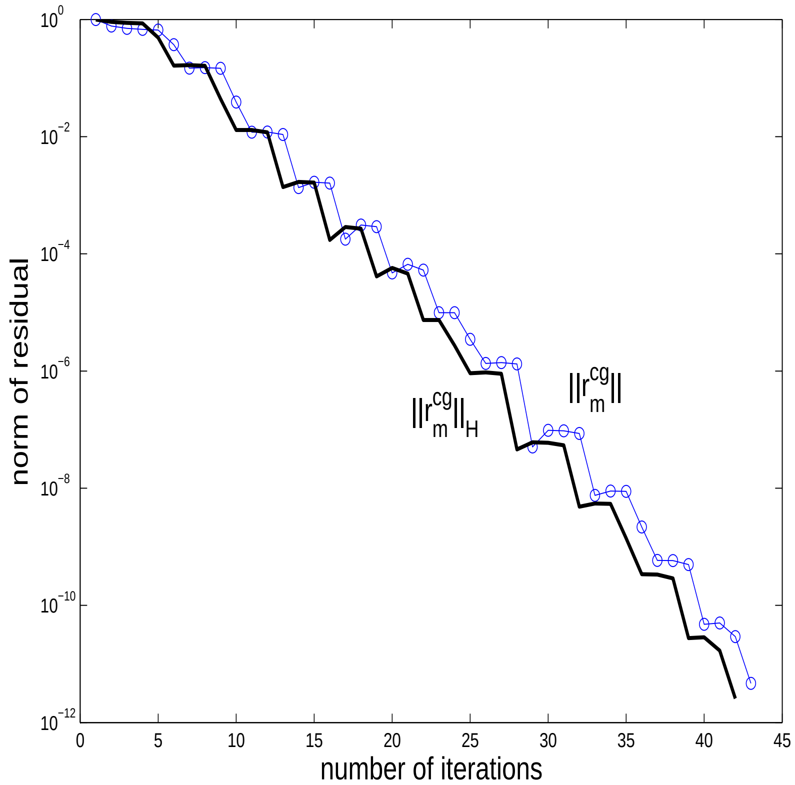

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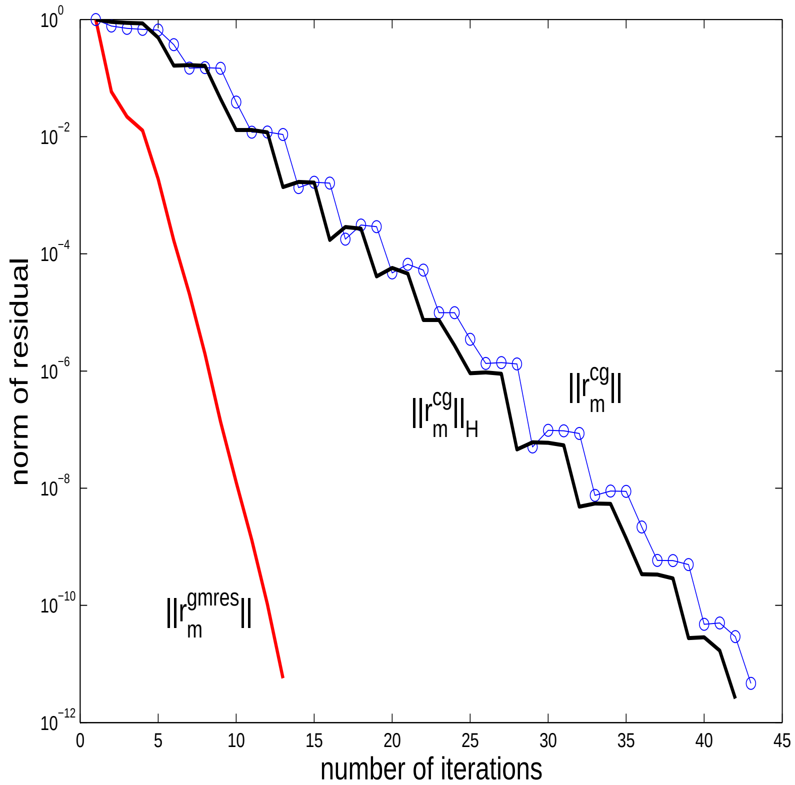
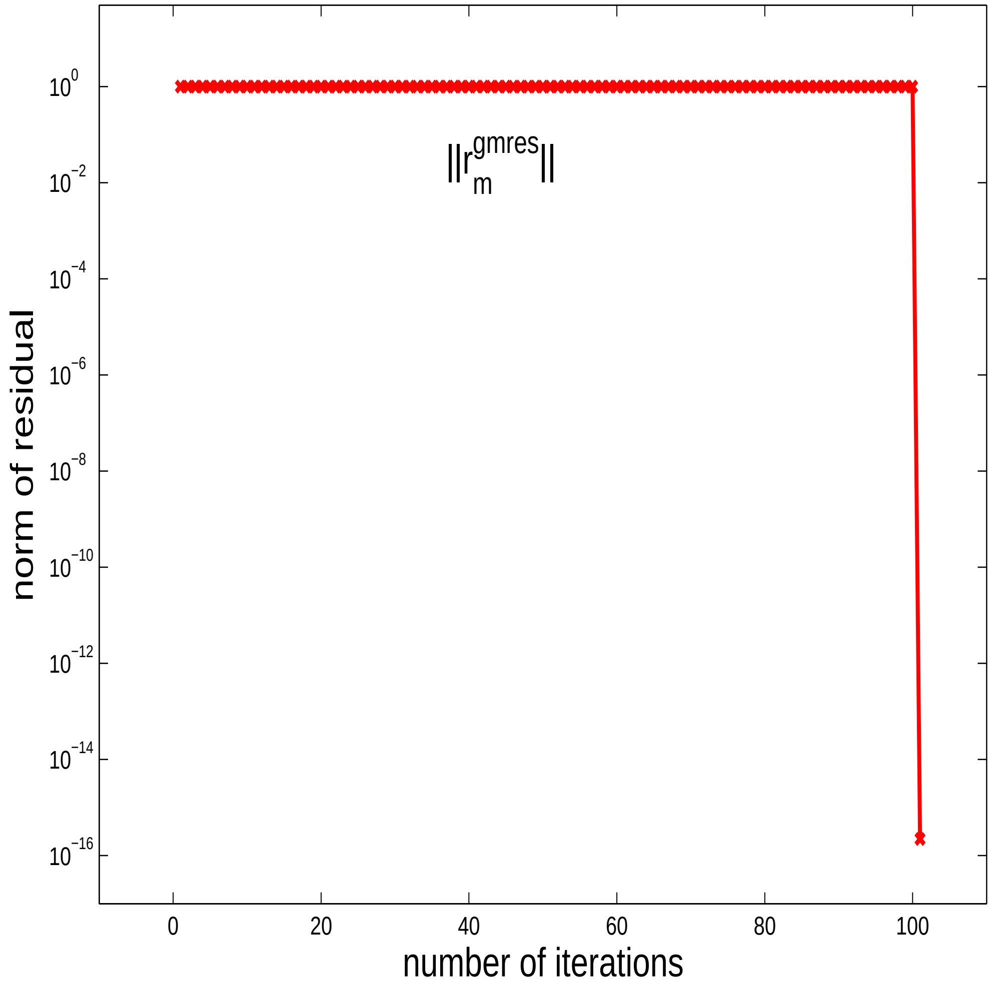


Stagnation of GMRES

A is 100×100



Conditions for non-Stagnation of GMRES

If $\alpha = \lambda_{\min}(\frac{1}{2}(\mathcal{M} + \mathcal{M}^T)) > 0$ (!!!), then

$$\|r_k\| \leq \left(1 - \frac{\alpha^2}{\|\mathcal{M}\|^2}\right)^{\frac{k}{2}} \|b\| < \|b\|$$

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New condition: Let $H = \frac{1}{2}(\mathcal{M} + \mathcal{M}^T)$, $\quad S = \frac{1}{2}(\mathcal{M} - \mathcal{M}^T)$

If H is nonsingular and $\|SH^{-1}\| < 1$ then

$$\|r_2\| \le \left(1 - \frac{\theta_{\min}^2}{\|\mathcal{M}^2\|^2}\right)^{\frac{1}{2}} \|r_0\| \quad \theta_{\min} = \lambda_{\min}(\tfrac{1}{2}(\mathcal{M}^2 + (\mathcal{M}^2)^\top)) > 0$$

The same relation holds at every other iteration

(same result for S nonsingular and $\|HS^{-1}\| < 1$)

Example. Navier-Stokes problem

IFISS Package (Elman, Ramage, Silvester)

"Flow over a step". Uniform grid, Q1-P0 elements

Mesh independence

$$P_{tr,aug} = \begin{bmatrix} F & B \\ & +\widetilde{C} \end{bmatrix} \text{ (2,2) block: } \widetilde{C} = \beta C + BF^{-1}B^\top,$$

n	m	$\lambda_{\min}(H)$	$\|SH^{-1}\|$	# its
418	176	-3.8091	0.9672	14
1538	704	-3.7057	0.9662	15
5890	2816	-3.6710	0.9660	13

Beyond non-stagnation. Indefinite vs. Definite

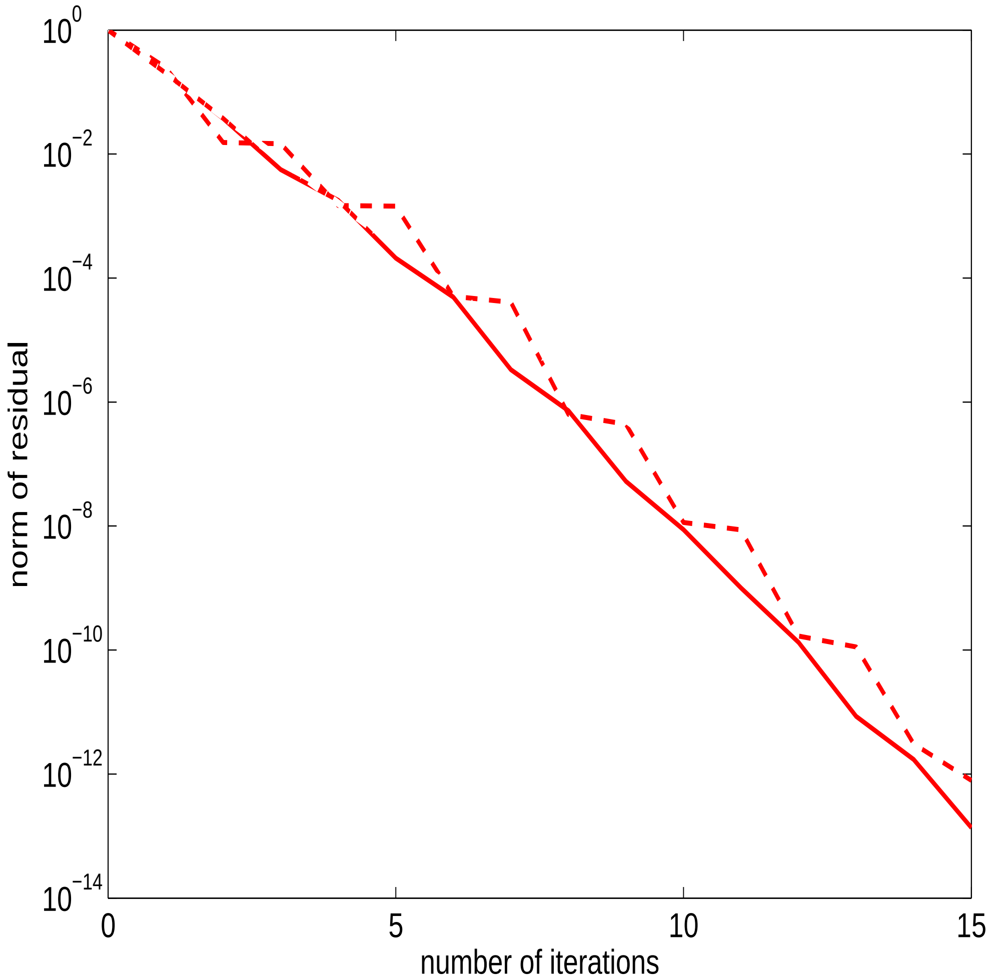
$$\mathcal{P}_{tr,+} = \begin{bmatrix} \widetilde{F} & B \\ & +\widetilde{C} \end{bmatrix} \qquad \mathcal{P}_{tr,-} = \begin{bmatrix} \widetilde{F} & B \\ & -\widetilde{C} \end{bmatrix}$$

$\mathcal{M}\mathcal{P}_{tr,+}^{-1}$ Indefinite

$\mathcal{M}\mathcal{P}_{tr,-}^{-1}$ Positive definite

Should $\mathcal{M}\mathcal{P}_{tr,+}^{-1}$ be discarded?

GMRES Convergence history: $\mathcal{P}_{tr,+}, \mathcal{P}_{tr,-}$



Some important (but not included) issues

- Stopping criterion in a “natural” norm for the problem;
- Cheap error estimates (in a “natural” norm)