GMRES Acceleration Analysis for a Convection Diffusion Model Problem

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Outline

1. The convection diffusion model problem

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3. Analysis of the second phase of convergence

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1. The convection diffusion model problem

We consider, as in for example [Liesen, Strakoš - 2004],

$$\begin{aligned} -\nu \nabla^2 u + w \cdot \nabla u = 0 \quad & \text{in} \quad \Omega = (0,1) \times (0,1), \\ u = g \quad & \text{on} \quad \partial\Omega, \end{aligned}$$

- ν: scalar diffusion coefficient
- $w = [0,1]^T$: vector velocity field
- g : given by the boundary conditions

$$\begin{aligned} u(x,0) = u(1,y) = 1 \quad & \text{for} \quad \frac{1}{2} \leq x \leq 1 \quad \text{and} \quad 0 \leq y < 1, \\ u(x,y) = 0 \quad & \text{elsewhere on } \partial\Omega \end{aligned}$$

We use

- A 35×35 grid
- SUPG discretization (see for example [Brooks, Hughes - 1990])
- Discrete sine transformation [Liesen, Strakoš - 2004]
- The zero initial guess

This yields a linear system with a $35^2 \times 35^2$ block diagonal matrix $\mathbf{A}$ with tridiagonal Toeplitz blocks of dimension 35×35 :

$$\mathbf{A}\,x = \begin{pmatrix} \mathbf{T}_1 & & & & \\ & \mathbf{T}_2 & & & \\ & & \ddots & & \\ & & & \mathbf{T}_{34} & \\ & & & & \mathbf{T}_{35} \end{pmatrix} x = \begin{pmatrix} b^{(1)} \\ b^{(2)} \\ \vdots \\ b^{(34)} \\ b^{(35)} \end{pmatrix} = b,$$

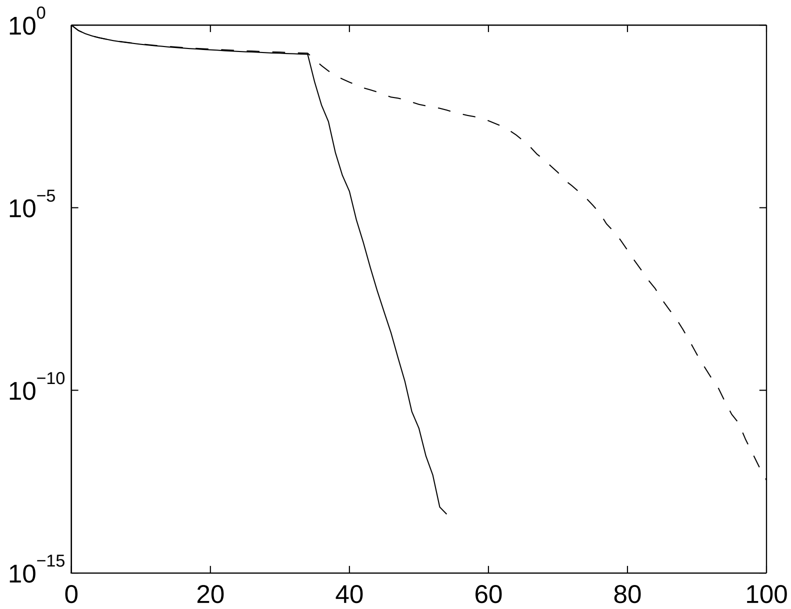
where b is partitioned according to the block-diagonal structure and

$$\mathbf{T}_i = \begin{pmatrix} \gamma_i\tau_i & \gamma_i\zeta_i & & & \\ \gamma_i & \gamma_i\tau_i & \gamma_i\zeta_i & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_i & \gamma_i\tau_i & \gamma_i\zeta_i \\ & & & \gamma_i & \gamma_i\tau_i \end{pmatrix} = \gamma_i \left(\mathbf{S} + \tau_i \mathbf{I} + \zeta_i \mathbf{S}^T \right),$$

and where $\mathbf{I}$ is the identity matrix and $\mathbf{S}$ is the downshift matrix $\mathbf{S} = (e_2, \ldots, e_{35}, 0)$.

- For very small ν the operator is highly non-normal [Reddy, Trefethen - 1994]
- We consider two cases: $\nu = 0.05$ and $\nu = 0.0005$

GMRES norm reduction for the discretized convection diffusion model problem



Dashed line: $\nu = 0.0005$ - Solid line: $\nu = 0.05$.

2. Analysis of the initial phase of convergence

The kth GMRES residual norm $\|r_k\| = \|b - \mathbf{A}x_k\|$ is given by

$$\|r_k\| = \min_{p \in \mathcal{P}_k} \|p(\mathbf{A})b\|,$$

where $\mathcal{P}_k$ denotes the polynomials of maximal degree k with the value 1 at the origin. Slow initial convergence is explained by

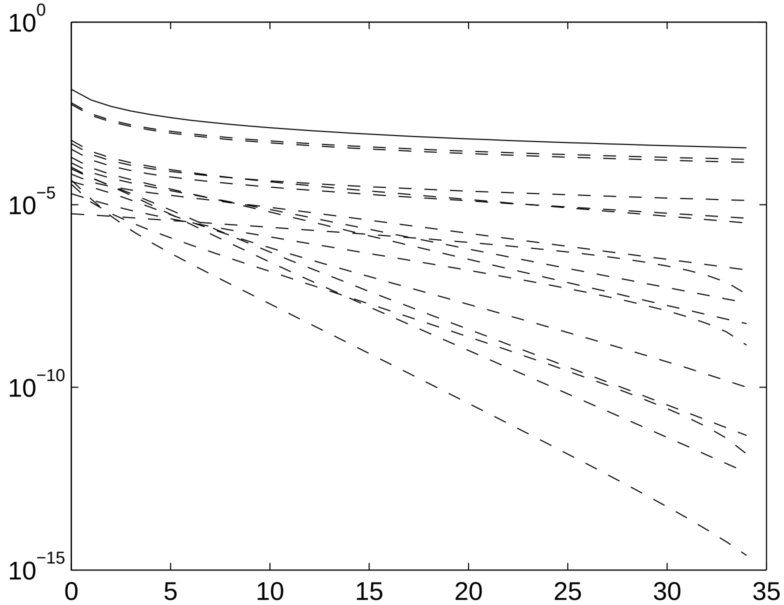
$$\|r_k\|^2 = \min_{p \in \mathcal{P}_k} \|p\,(\mathbf{A})\,b\|^2 = \min_{p \in \mathcal{P}_k} \sum_{i=1}^{N} \|p\,(\mathbf{T}_i)\,b^{(i)}\|^2 \geq \sum_{i=1}^{N} \min_{p \in \mathcal{P}_k} \|p\,(\mathbf{T}_i)\,b^{(i)}\|^2.$$

We bound from below by residual norms for the block problems

$$\mathbf{T}_i\,x^{(i)} = b^{(i)}, \qquad i = 1, 2, \ldots, 35.$$

Note that for $k \geq 35$ the bound is useless.

The 35 initial squared GMRES residual norms



Dashed lines: Block 35×35 problems
Solid line: Large $35^2 \times 35^2$ problem

In [Liesen, Strakoš - 2004] we find an analysis of GMRES convergence behavior for the ith block problem with matrix

$$\mathbf{T}_i = \gamma_i \, (\mathbf{S} + \tau_i \mathbf{I} + \zeta_i \, \mathbf{S}^T).$$

It is based on the result that when $[b^{(i)}, \mathbf{T}_i b^{(i)}, \ldots, \mathbf{T}_i^k b^{(i)}]$ has full column rank, then

$$(r_k^{(i)})^T = \|r_k^{(i)}\|^2 [1, -\tau_i, \ldots, (-\tau_i)^k] [b^{(i)}, (\mathbf{S}+\zeta_i \mathbf{S}^T) b^{(i)}, \ldots, (\mathbf{S}+\zeta_i \mathbf{S}^T)^k b^{(i)}]^+ \,,$$

where $[\mathbf{X}]^+$ denotes the Moore-Penrose pseudoinverse of the matrix $\mathbf{X}$.

Taking norms,

$$\begin{aligned}\|r_k^{(i)}\| &= \left\| [1, -\tau_i, \ldots, (-\tau_i)^k][b^{(i)}, (\mathbf{S} + \zeta_i \mathbf{S}^T) b^{(i)}, \ldots, (\mathbf{S} + \zeta_i \mathbf{S}^T)^k b^{(i)}]^+ \right\|^{-1} \\ &\geq \left(\sum_{j=0}^{k} (-\tau_i)^{2j} \right)^{-\frac{1}{2}} \sigma_{\min}\Big([b^{(i)}, (\mathbf{S} + \zeta_i \mathbf{S}^T) b^{(i)}, \ldots, (\mathbf{S} + \zeta_i \mathbf{S}^T)^k b^{(i)}] \Big) .\end{aligned}$$

Slow initial convergence can be quantified by the large values of this lower bound for some dominating blocks $\mathbf{T}_i$.

Acceleration of convergence after the 35th iteration needs to be described be an upper bound that couples the influence of the individual blocks.

3. Analysis of the second phase of convergence

The identity for GMRES residual vectors for tridiagonal Toeplitz blocks in [Liesen, Strakoš - 2004] can be generalized as

Theorem: *Let us consider the residual vectors generated by GMRES applied to* $\mathbf{C}y = d$ *and assume that* $[d, \mathbf{C}d, \ldots, \mathbf{C}^k d]$ *has full column rank. If* $\mathbf{C} = \mathbf{B} + \mathbf{U}$ *with* $\mathbf{UB} = \mathbf{BU}$ *and* $\mathbf{U}d = \tau d$*, then*

$$r_k^T = \|r_k\|^2 \, [1, -\tau, \ldots, (-\tau)^k] \cdot \left[d, \mathbf{B}d, \ldots, \mathbf{B}^k d\right]^+ .$$

We will apply this result with $\mathbf{C} \equiv \mathbf{A}$, $d \equiv b$ and $\mathbf{U} \equiv \tau \mathbf{I}$, hence $\mathbf{A} = \mathbf{B} + \tau \mathbf{I}$ for some appropriate diagonal translation $\tau \mathbf{I}$.

Recall that we consider a block diagonal system matrix with blocks

$$\mathbf{T}_i = \begin{pmatrix} \gamma_i\tau_i & \gamma_i\zeta_i & & & \\ \gamma_i & \gamma_i\tau_i & \gamma_i\zeta_i & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_i & \gamma_i\tau_i & \gamma_i\zeta_i \\ & & & \gamma_i & \gamma_i\tau_i \end{pmatrix}, \qquad i = 1, \ldots 35.$$

All $|\gamma_i\zeta_i| << 1$ and all $\gamma_i\tau_i$ are close. Hence for a diagonal translation τ close to all $\gamma_i\tau_i$, the matrix $\mathbf{B} = \mathbf{A} - \tau\mathbf{I}$ has blocks

$$\tilde{\mathbf{T}}_i = \mathbf{T}_i - \tau\mathbf{I} \approx \begin{pmatrix} 0 & 0 & & & \\ \gamma_i & 0 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_i & 0 & 0 \\ & & & \gamma_i & 0 \end{pmatrix}, \qquad i = 1, \ldots 35.$$

Because of

$$\mathbf{B}b = \begin{pmatrix} \tilde{\mathbf{T}}_1 & & & & \\ & \tilde{\mathbf{T}}_2 & & & \\ & & \ddots & & \\ & & & \tilde{\mathbf{T}}_{34} & \\ & & & & \tilde{\mathbf{T}}_{35} \end{pmatrix} \begin{pmatrix} b^{(1)} \\ b^{(2)} \\ \vdots \\ b^{(34)} \\ b^{(35)} \end{pmatrix}, \quad \tilde{\mathbf{T}}_i \approx \begin{pmatrix} 0 & 0 & & & \\ \gamma_i & 0 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_i & 0 & 0 \\ & & & \gamma_i & 0 \end{pmatrix},$$

application of $\mathbf{B}$ to b shifts down one position all entries of all $b^{(i)}$. Hence $\mathbf{B}^{35}b \approx \mathbf{0}$. Now our equality

$$\|r_k\| = \frac{1}{\| [1, -\tau, \ldots, (-\tau)^k] \, [b, \mathbf{B}b, \ldots, \mathbf{B}^k b]^+ \|}$$

yields the upper bound

$$\|r_k\| \quad \le \quad \frac{\|\mathbf{B}^k b\|}{|\tau|^k},$$

which quantifies the acceleration of convergence.

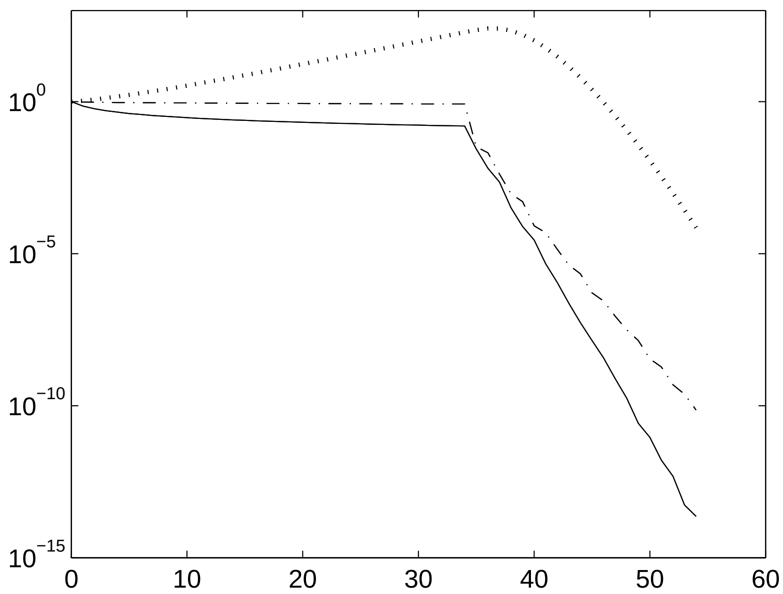
4. Numerical examples

For $\nu = 0.05$:

- The diagonal values $\gamma_i \tau_i$ are particularly close.
- The norms $\|b^{(1)}\|, \|b^{(2)}\| >> \|b^{(i)}\|$ for $i \geq 3$

The choices $\tau = (\gamma_1 \tau_1 + \gamma_2 \tau_2)/2$ and $\tau = (\sum_{i=1}^{35} \gamma_i \tau_i)/35$ yield

Convergence curve and upper bounds for $\nu = 0.05$



Solid line: GMRES residual norm reduction

Dotted line: Upper bound with $\tau = (\gamma_1\tau_1 + \gamma_2\tau_2)/2$

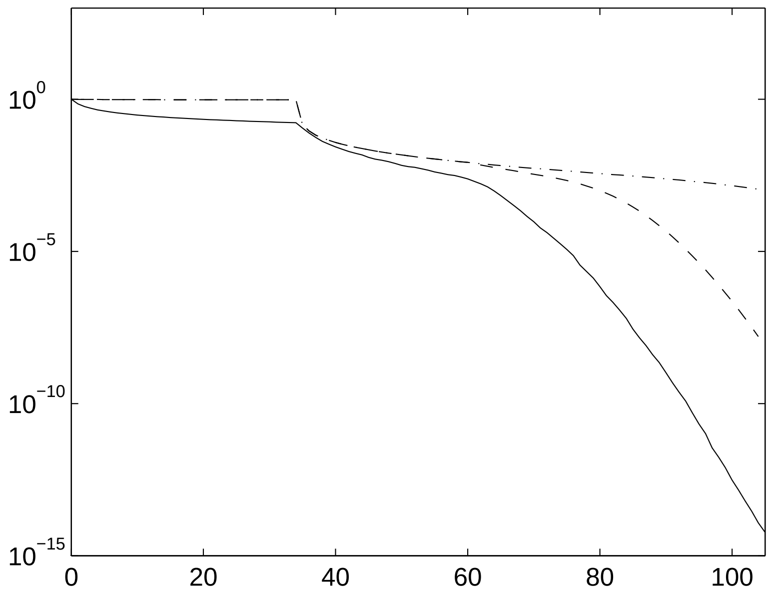
Dash-dotted line: Upper bound with $\tau = (\sum_{i=1}^{35} \gamma_i\tau_i)/35$

For $\nu = 0.0005$:

- The diagonal values $\gamma_i \tau_i$ are less close than for $\nu = 0.05$.
- The upper-diagonal values $|\gamma_i \zeta_i|$ are particularly small
- Again, the norms $\|b^{(1)}\|, \|b^{(2)}\| >> \|b^{(i)}\|$ for $i \geq 3$

The choice $\tau = (\gamma_1 \tau_1 + \gamma_2 \tau_2)/2$ yields the dash-dotted line in the following graph:

Convergence curve and upper bounds for $\nu = 0.0005$



Solid line: GMRES residual norm reduction

Dash-dotted line: Upper bound with $\tau = (\gamma_1\tau_1 + \gamma_2\tau_2)/2$

Dashed line: Extended upper bound (details in Proceedings)

Thank you for your attention.

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