Preconditioning, weighting and deflation applied to non-symmetric linear systems

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Consider applying GMRES to:

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \text{ with non-singular } \mathbf{A}.$$

Two Questions

- How fast does GMRES converge ?
- How can convergence be accelerated ?

Consider three accelerators

- **Preconditioner**,
- **Weighted norm**,
  $\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbf{W}} = \mathbf{y}^* \mathbf{W} \mathbf{x}$,
  $\|\mathbf{x}\|_{\mathbf{W}} = \sqrt{\mathbf{x}^* \mathbf{W} \mathbf{x}}$,
- **Deflation**.

Objective

Choose a **combination** of the three accelerators that ensures fast convergence with respect to a (new?) **convergence bound**.

High performance computing

We have domain decomposition preconditioners and scalability in mind.

GMRES

Generalized Minimal Residual Method

- First introduced by Saad and Schultz [1986]
- Iterative algorithm. Starts with an initial guess $\mathbf{x}_0 \in \mathbb{C}^n$.
- At iteration k:
  - $\mathbf{x}_k$ (approximate solution) characterized by:

$$\mathbf{x}_k = \text{argmin}_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)} \{\|\mathbf{b} - \mathbf{A}\mathbf{x}\|\},$$

where $\begin{cases} \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \text{span}\left\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{k-1}\mathbf{r}_0\right\} \text{ (Krylov subspace)}, \\ \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0 \text{ (initial residual)}. \end{cases}$

  - $\mathbf{x}_k$ and $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$ not computed at each iteration.
  - Instead, orthonormal basis for $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$ computed by updating the orthonormal basis for $\mathcal{K}_{k-1}(\mathbf{A}, \mathbf{r}_0)$ (Arnoldi).
  - Residual $\|\mathbf{b} - \mathbf{A}\mathbf{x}_k\|$ can be monitored. At convergence, $\mathbf{x}_k$ computed (least squares).

Fundamental Questions

- How fast does GMRES converge ?
- How can convergence be accelerated ?

Convergence of GMRES for $\mathbf{Ax} = \mathbf{b}$

Characterization of approximate solution $\mathbf{x}_k$ at iteration k

$$
\begin{aligned}
\|\mathbf{r}_k\| &= \|\mathbf{b} - \mathbf{A}\mathbf{x}_k\| \\
&= \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|, \text{ where } \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \operatorname{span}\left\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{k-1}\mathbf{r}_0\right\} \\
&= \min_{\mathbf{y} \in \mathbf{r}_0 + A\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)} \|\mathbf{y}\|, \text{ where } \mathbf{r}_0 + A\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) = \mathbf{r}_0 + \operatorname{span}\left\{\mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^k\mathbf{r}_0\right\} \\
&= \min_{p \in \mathbb{P}_k;\, p(0)=1} \|p(\mathbf{A})\mathbf{r}_0\| \text{ where } \mathbb{P}_k\text{: polynomials of degree at most } k.
\end{aligned} \tag{1}
$$

Convergence estimate by worst case GMRES for non-singular A

$$
\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} \leqslant \min_{p \in \mathbb{P}_k;\, p(0)=1} \|p(\mathbf{A})\|; \quad \|p(\mathbf{A})\| = \max_{\mathbf{y} \in \mathbb{C}^n} \|p(\mathbf{A})\mathbf{x}\| / \|\mathbf{x}\|. \tag{2}
$$

“By passing from [(1) to (2)] we disentangle this matrix essence of the process from the distracting effects of the initial vector and end up with [an] elegant mathematical problem in the bargain.”

[Greenbaum, Trefethen, SIAM Review, 1998]

Does convergence of GMRES depend on the spectrum of $\mathbf{A}$?

Why am I raising this point ?

- I come from symmetric positive definite problems,
- For these, convergence depends only on the spectrum of $\mathbf{A}$.
- The strategy for accelerating convergence is clear:

  $\rightarrow$ cluster the spectrum away from zero.
- Sidenote: conjugate gradient method rather than GMRES (short recurrence).

For non symmetric problems working on the spectrum is not sufficient.
Fundamental result by [Greenbaum, Pták, Strakoš (1996)]

Let $r_0 \geqslant r_1 \geqslant r_2 \geqslant \cdots \geqslant r_{n-1} > 0$. There exists an $n \times n$ matrix $\mathbf{A}$ and a vector $\mathbf{b}$ such that, the norm of the k-th residual of GMRES applied to $\mathbf{Ax} = \mathbf{b}$ is r_k.
Moreover, the matrix $\mathbf{A}$ can be chosen to have any desired eigenvalues.

Other bounds for GMRES

See [Embree, *How descriptive are GMRES convergence bounds ?* 2023] for overview and comparison.

Elman estimate [Eisenstat, Elman, Schultz, 1983]:

$$\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} \leqslant \left[1 - \frac{d(0, \mathrm{FOV}(\mathbf{A}))^2}{\|\mathbf{A}\|^2}\right]^{k/2}, \text{ where } \underbrace{\mathrm{FOV}(\mathbf{A}) := \left\{\frac{\langle \mathbf{Au}, \mathbf{u}\rangle}{\langle \mathbf{u}, \mathbf{u}\rangle}; \mathbf{u} \in \mathbb{C}^n \setminus \{0\}\right\}}_{\text{Field of values of } \mathbf{A} \text{ (aka numerical range)}}.$$

Pseudo-spectral bound:

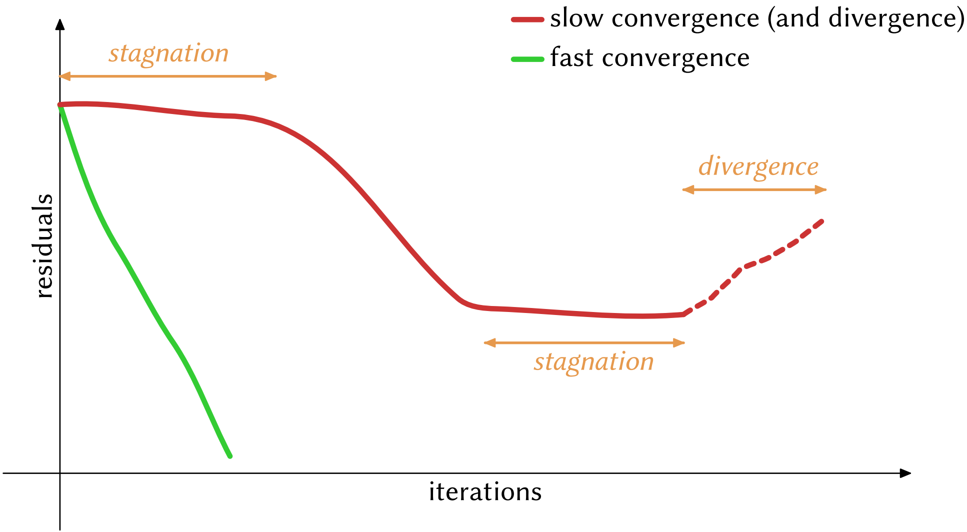
$$\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} \leqslant \frac{\mathcal{L}(\Gamma_\epsilon)}{2\pi\epsilon} \min_{p \in \mathbb{P}_k;\, p(0)=1} \max_{z \in \sigma_\epsilon(\mathbf{A})} |p(z)|,$$

where $\mathcal{L}(\Gamma_\epsilon)$ is the contour-length of the boundary Γ_ϵ of $\sigma_\epsilon(\mathbf{A})$, and

$\sigma_\epsilon(\mathbf{A}) := \{z \in \mathbb{C}; s \text{ is an eigenvalue of } \mathbf{A} + \mathbf{E} \text{ and} \|\mathbf{E}\| < \epsilon\}$ is the ϵ-pseudospectrum of $\mathbf{A}$.

Applied in [Marchand, Galkowski, Spence and Spence, 2022] to GMRES for Helmholtz.

Slow and fast convergence of GMRES, an illustration



1. GMRES
2. Preconditioning (by $\mathbf{H}$) and Weighting (by $\mathbf{W}$)
3. $\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H}$, $\mathbf{A}$ pd
4. Spectral deflation
5. Numerics
6. Prescribe simultaneous convergence curves

Preconditioning (by H) and Weighting (by W)

GMRES for $\mathbf{Ax} = \mathbf{b}$ preconditioned by $(\mathbf{H}_L, \mathbf{H}_R)$

Solve $\mathbf{H}_L\mathbf{A}\mathbf{H}_R\mathbf{u} = \mathbf{H}_L\mathbf{b}$ followed by $\mathbf{x} = \mathbf{H}_R\mathbf{u}$.

At iteration k, $\mathbf{r}_k := \mathbf{b} - \mathbf{A}\mathbf{x}_k$ satisfies:

$$\|\mathbf{H}_L\mathbf{r}_k\| = \min_{\mathbf{y}\in\mathbf{r}_0+\mathbf{A}\mathcal{K}_k(\mathbf{HA},\mathbf{Hr}_0)} \|\mathbf{H}_L\mathbf{y}\| = \min_{q\in\mathbb{P}_k;\, q(0)=1} \|\mathbf{H}_L q(\mathbf{AH})\mathbf{r}_0\| \quad ,$$

- $\mathbf{H} = \mathbf{H}_R\mathbf{H}_L$ is the combined preconditioner,
- $\mathcal{K}_k(\mathbf{HA}, \mathbf{Hr}_0) := \operatorname{span}\{\mathbf{Hr}_0, \mathbf{HAr}_0, \dots, (\mathbf{HA})^{k-1}\mathbf{r}_0\}$ is the Krylov subspace,
- A good choice of preconditioner reduces the iteration count.
- A good preconditioner is not too costly to apply.

GMRES for $\mathbf{Ax} = \mathbf{b}$ preconditioned by $(\mathbf{H}_L, \mathbf{H}_R)$ and weighted by $\mathbf{W}$ (a hpd matrix)

Solve $\mathbf{H}_L\mathbf{A}\mathbf{H}_R\mathbf{u} = \mathbf{H}_L\mathbf{b}$ followed by $\mathbf{x} = \mathbf{H}_R\mathbf{u}$.

At iteration k, $\mathbf{r}_k := \mathbf{b} - \mathbf{A}\mathbf{x}_k$ satisfies:

$$\|\mathbf{H}_L\mathbf{r}_k\|_{\mathbf{W}} = \min_{\mathbf{y}\in\mathbf{r}_0+\mathbf{A}\mathcal{K}_k(\mathbf{HA},\mathbf{H}\mathbf{r}_0)} \|\mathbf{H}_L\mathbf{y}\|_{\mathbf{W}} = \min_{q\in\mathbb{P}_k;\, q(0)=1} \|\mathbf{H}_L q(\mathbf{AH})\mathbf{r}_0\|_{\mathbf{W}},$$

- $\mathbf{H} = \mathbf{H}_R\mathbf{H}_L$ is the combined preconditioner,
- $\mathcal{K}_k(\mathbf{HA}, \mathbf{H}\mathbf{r}_0) := \operatorname{span}\{\mathbf{H}\mathbf{r}_0, \mathbf{HA}\mathbf{r}_0, \dots, (\mathbf{HA})^{k-1}\mathbf{r}_0\}$ is the Krylov subspace,
- A good choice of preconditioner reduces the iteration count.
- A good preconditioner is not too costly to apply.
- $\mathbf{W}$ induces $\langle \mathbf{x}, \mathbf{y}\rangle_{\mathbf{W}} = \mathbf{y}^*\mathbf{W}\mathbf{x}$ and $\|\cdot\|_{\mathbf{W}}$. all $\langle\cdot,\cdot\rangle$ in GMRES replaced by $\langle\cdot,\cdot\rangle_{\mathbf{W}}$.

References

- [Cai (1989)] [Cai and Widlund (1992)] [Essai's thesis w/ Brezinski (1998)]
- [Sarkis, Szyld (2007)], [Pestana, Wathen (2013)], [Güttel, Pestana (2013)], [Embree, Morgan, Nguyen (2017)], [Embree (2023)], [S, Matalon (2025)]

A short interlude (in connection with my poster)

I asked AI if attendees of DD29 precondition on the left or on the right.

- **Chat GPT**: *In summary: At DD29, the overwhelming majority of talks and tutorials on domain-decomposition preconditioners assume right-preconditioning by default, especially in the context of flexible or adaptable iterative solvers.* i
- **Perplexity AI**: *There is no indication that one approach is universally preferred over the other at the DD29 conference; rather, both are actively used and studied by participants.*

I asked *you* if you precondition on the left or on the right? (56 replies)

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I asked *you* if you precondition on the left or on the right? (56 replies)

left	right	split	only PCG	It varies/ I don't know	I don't precondition
24	14	1	4	8	5

And does it matter? (37 replies)

yes	no
27	10

You can still vote.

Final results during P. Matalon's talk (Thursday 14:40 – CT01).

Redundancy between (left,right) preconditioning and weighting

GMRES for $\mathbf{Ax} = \mathbf{b}$ preconditioned by $(\mathbf{H}_L, \mathbf{H}_R)$ and weighted by $\mathbf{W}$ (a hpd matrix)

At iteration k, $\mathbf{r}_k := \mathbf{b} - \mathbf{Ax}_k$ satisfies:

$$\|\mathbf{H}_L \mathbf{r}_k\|_{\mathbf{W}} = \min_{q \in \mathbb{P}_k;\, q(0)=1} \|\mathbf{H}_L q(\mathbf{AH})\mathbf{r}_0\|_{\mathbf{W}}$$

- $\mathbf{H} = \mathbf{H}_R \mathbf{H}_L$ is the combined preconditioner,

Redundancy between (left,right) preconditioning and weighting

GMRES for Ax = b preconditioned by $(\mathbf{H}_\mathrm{L}, \mathbf{H}_\mathrm{R})$ and weighted by W (a hpd matrix)

At iteration k, $\mathbf{r}_k := \mathbf{b} - \mathbf{A}\mathbf{x}_k$ satisfies:

$$\|\mathbf{r}_k\|_{\mathbf{H}_\mathrm{L}{}^*\mathbf{W}\mathbf{H}_\mathrm{L}} \leqslant \|\mathbf{H}_\mathrm{L}\mathbf{r}_k\|_\mathbf{W} = \min_{q\in\mathbb{P}_k;\, q(0)=1} \|\mathbf{H}_\mathrm{L} q(\mathbf{A}\mathbf{H})\mathbf{r}_0\|_\mathbf{W} = \min_{q\in\mathbb{P}_k;\, q(0)=1} \|q(\mathbf{A}\mathbf{H})\mathbf{r}_0\|_{\mathbf{H}_\mathrm{L}{}^*\mathbf{W}\mathbf{H}_\mathrm{L}}.$$

- $\mathbf{H} = \mathbf{H}_\mathrm{R}\mathbf{H}_\mathrm{L}$ is the combined preconditioner,
- There is a redundancy between (left,right) preconditioning and weighting.
- Weighting is *Preconditioning by similarity transform*

[Gutknecht and Loher, Abstract for a talk, 2001]

Without loss of generality, assume right preconditioned weighted GMRES:

$$\frac{\|\mathbf{r}_k\|_\mathbf{W}}{\|\mathbf{r}_0\|_\mathbf{W}} \leqslant \min_{q\in\mathbb{P}_k;\, q(0)=1} \|q(\mathbf{A}\mathbf{H})\|_\mathbf{W}; \quad \|q(\mathbf{A}\mathbf{H})\|_\mathbf{W} = \max_{y\in\mathbb{C}^n} \|p(\mathbf{A}\mathbf{H})\mathbf{x}\|_\mathbf{W}/\|\mathbf{x}\|_\mathbf{W}.$$

Crouzeix and Palencia theory

The field of values is a $(1+\sqrt{2})$-spectral set. [Crouzeix, Palencia, 2017]

Theorem

For any matrix $\mathbf{B} \in \mathbb{C}^{n\times n}$ and polynomial q,

$$\|q(\mathbf{B})\|_{\mathbf{W}} \leqslant (1+\sqrt{2}) \max_{z \in \mathrm{FOV}^{\mathbf{W}}(\mathbf{B})} |q(z)|,$$

where, $\mathrm{FOV}^{\mathbf{W}}(\mathbf{B}) := \left\{ \frac{\langle \mathbf{B}\mathbf{z}, \mathbf{z}\rangle_{\mathbf{W}}}{\langle \mathbf{z}, \mathbf{z}\rangle_{\mathbf{W}}}; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\}$ is the $\mathbf{W}$-field of values of $\mathbf{B}$.

Crouzeix and Palencia theory

The field of values is a $(1+\sqrt{2})$-spectral set. [Crouzeix, Palencia, 2017]

Theorem

For any matrix $\mathbf{B} \in \mathbb{C}^{n\times n}$ and polynomial q,

$$\|q(\mathbf{B})\|_{\mathbf{W}} \leqslant (1+\sqrt{2}) \max_{z \in \mathrm{FOV}^{\mathbf{W}}(\mathbf{B})} |q(z)|,$$

$$\text{where, } \mathrm{FOV}^{\mathbf{W}}(\mathbf{B}) := \left\{ \frac{\langle \mathbf{B}\mathbf{z}, \mathbf{z}\rangle_{\mathbf{W}}}{\langle \mathbf{z}, \mathbf{z}\rangle_{\mathbf{W}}};\ \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\} \text{ is the } \mathbf{W}\text{-field of values of } \mathbf{B}.$$

Hence, W-GMRES preconditioned on the right by H converges as:

$$\frac{\|\mathbf{r}_k\|_{\mathbf{W}}}{\|\mathbf{r}_0\|_{\mathbf{W}}} \leqslant (1+\sqrt{2}) \min_{q \in \mathbb{P}_k;\, q(0)=1} \max_{z \in \mathrm{FOV}^{\mathbf{W}}(\mathbf{AH})} |q(z)|.$$

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$\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H}$, $\mathbf{A}$ pd

With loss of generality, assume that:

- $\mathbf{H}$ is Hermitian positive definite (hpd),
- $\mathbf{W} = \mathbf{H}$,
- $\mathbf{A}$ is positive definite (pd).

Same setting as:

- [Starke, 1997]
  [Klawonn and Starke, 1999]
- [Chan, Chow, Saad, and Yeung, 1999]

Advantages:

- The min-max problem is posed over

$$\mathrm{FOV}^{\mathbf{H}}(\mathbf{AH}) = \left\{ \frac{\langle \mathbf{HAHz}, \mathbf{z} \rangle}{\langle \mathbf{Hz}, \mathbf{z} \rangle} ; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\} .$$

- No extra application of $\mathbf{H}$ at each iteration.

Continue with $\mathbf{H}$ hpd and $\mathbf{W} = \mathbf{H}$

Let $\mathbf{M} := \dfrac{\mathbf{A}+\mathbf{A}^*}{2}$ and $\mathbf{N} := \dfrac{\mathbf{A}-\mathbf{A}^*}{2}$ (Hermitian + skew-Hermitian splitting).

- Convergence Bounds

$$\mathrm{FOV}^{\mathbf{H}}(\mathbf{AH}) \subset \underbrace{\left\{ \frac{\langle \mathbf{HMHz}, \mathbf{z}\rangle}{\langle \mathbf{Hz}, \mathbf{z}\rangle}; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\}}_{\in \mathbb{R}} + \underbrace{\left\{ \frac{\langle \mathbf{HNHz}, \mathbf{z}\rangle}{\langle \mathbf{Hz}, \mathbf{z}\rangle}; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\}}_{\in i\mathbb{R}}$$

$$\subset [\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + i[-\rho(\mathbf{NH}), \rho(\mathbf{NH})]$$

$\lambda_{\min}$ and $\lambda_{\max}$: min and max of the (real) eigenvalues,

ρ: spectral radius *i.e.* module of eigenvalue of maximal module.

- Fast convergence if
  - $\mathbf{H}$ is a good preconditioner for both $\mathbf{M}$ and $\mathbf{N}$.

Continue with $\mathbf{H}$ hpd and $\mathbf{W} = \mathbf{H}$

Let $\mathbf{M} := \dfrac{\mathbf{A} + \mathbf{A}^*}{2}$ and $\mathbf{N} := \dfrac{\mathbf{A} - \mathbf{A}^*}{2}$ (Hermitian + skew-Hermitian splitting).

- Convergence Bounds

$$\mathrm{FOV}^{\mathbf{H}}(\mathbf{AH}) \subset \underbrace{\left\{ \frac{\langle \mathbf{HMHz}, \mathbf{z}\rangle}{\langle \mathbf{Hz}, \mathbf{z}\rangle}; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\}}_{\in\mathbb{R}} + \underbrace{\left\{ \frac{\langle \mathbf{HNHz}, \mathbf{z}\rangle}{\langle \mathbf{Hz}, \mathbf{z}\rangle}; \mathbf{z} \in \mathbb{C}^n \setminus \{0\} \right\}}_{\in \mathrm{i}\mathbb{R}}$$

$$\subset [\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + \mathrm{i}[-\rho(\mathbf{NH}), \rho(\mathbf{NH})]$$

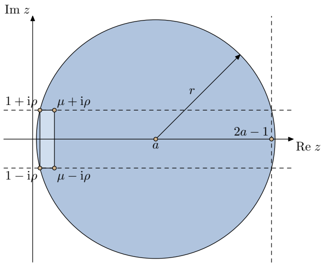
$$\subset [\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + \mathrm{i}[-\rho(\mathbf{M}^{-1}\mathbf{N})\lambda_{\max}(\mathbf{HM}), \rho(\mathbf{M}^{-1}\mathbf{N})\lambda_{\max}(\mathbf{HM})].$$

$\lambda_{\min}$ and $\lambda_{\max}$: min and max of the (real) eigenvalues,

ρ: spectral radius *i.e.* module of eigenvalue of maximal module.

- Fast convergence if
  - $\mathbf{H}$ is a good preconditioner for both $\mathbf{M}$ and $\mathbf{N}$.
  - or, $\mathbf{H}$ is a good preconditioner for $\mathbf{M}$ and problem is mildly non-Hermitian.

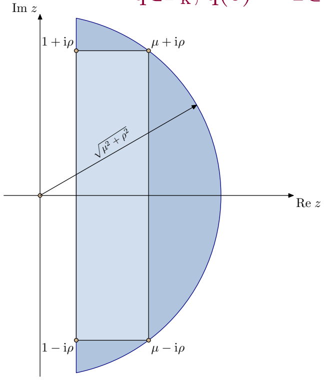
Min-max problem on a rectangle: $M_k := \min_{q \in \mathbb{P}_k;\, q(0)=1} \max_{z \in [1,\mu]+i[-\rho,\rho]} |q(z)|$



$$M_k \leqslant \left[\frac{\rho}{\sqrt{1+\rho^2}} \right]^k$$

as long as $\mu \leqslant 2\rho^2 + 1$.

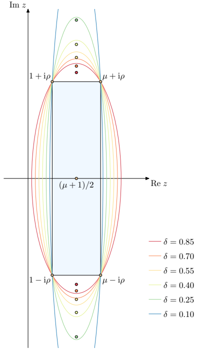
[Opfer, Schober, 1984]



$$M_k \leqslant \min \left\{ 2 + \gamma_\beta, \frac{2}{1-\gamma_\beta^{k+1}} \right\} \gamma_\beta^k,$$

γ_β depends on $\mu^2 + \rho^2$.

[Beckermann, Goreinov, Tyrtyshnikov, 2006]



$$M_k \leqslant C_k\left(\frac{a}{d}\right) \left| C_k\left(\frac{c}{d}\right) \right|^{-1}.$$

(a, c, d) define ellipse,
C_k: Chebyshev polynomial

[Saad, 2003]

Min-max problem on a rectangle: $M_k := \min_{q \in \mathbb{P}_k;\, q(0)=1} \max_{z \in [1,\mu]+i[-\rho,\rho]} |q(z)|$

Conformal Mapping **[Beckermann, Goreinov, Tyrtyshnikov, 2006]**

Let ϕ denote the Riemann conformal mapping from $\overline{\mathbb{C}} \setminus [1,\mu] + i[-\rho,\rho]$ onto the exterior of the closed unit disk with $\phi(\infty) = \infty$, then

$$M_k \leqslant \min \left\{ 2 + \gamma, \frac{2}{1 - \gamma^{k+1}} \right\} \gamma^k, \quad \gamma := \frac{1}{\phi(0)}.$$

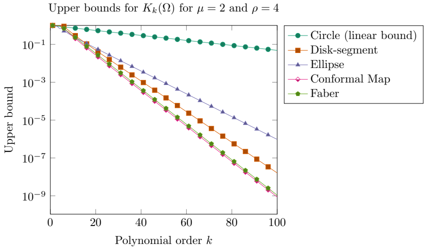
Faber Polynomial **[Beckermann, 2005]**

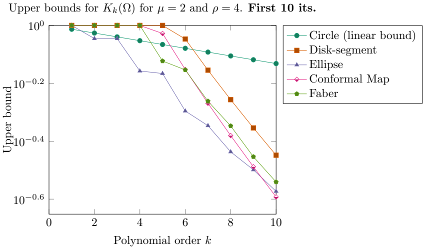
Let F_k be the k-th Faber polynomial for $[1,\mu] + i[-\rho,\rho]$, then

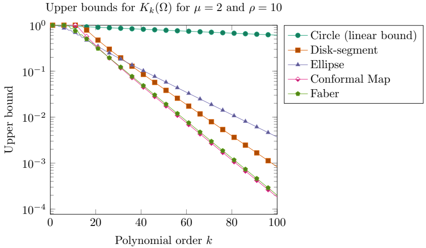
$$M_k \leqslant \frac{2}{|F_k(0)\,|}.$$

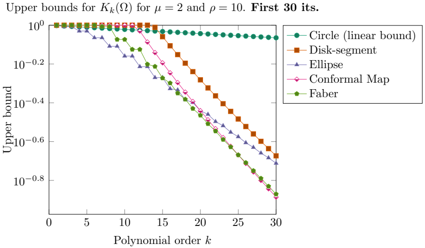
Both computed by Matlab's Schwarz-Christoffel Toolbox by [Driscoll, Trefethen].

Min-max problem $\min_{q\in\mathbb{P}_k;\, q(0)=1} \max_{z\in\Omega} |q(z)|$ on rectangle









Advection-Diffusion-Reaction : What to expect ?

Lagrange Finite Element discretization of

$$\underbrace{\int_\Omega ((c_0 + \frac{1}{2}\operatorname{div}\mathbf{a})uv + \nu \nabla u \cdot \nabla v)}_{\text{"}\mathbf{M}\text{"}} + \underbrace{\int_\Omega (\frac{1}{2}\mathbf{a}\cdot\nabla uv - \frac{1}{2}\mathbf{a}\cdot\nabla vu)}_{\text{"}\mathbf{N}\text{"}} = \int_\Omega fv.$$

Convergence bound wrt min-max on
$[1, \kappa(\mathbf{HM})] + i[-\rho(\mathbf{M}^{-1}\mathbf{N})\kappa(\mathbf{HM}), \rho(\mathbf{M}^{-1}\mathbf{N})\kappa(\mathbf{HM})]$.

Bound for $\rho(M^{-1}N)$ (Proof uses [Bonazzoli, Claeys, Nataf, Tournier (2021)])

$$\rho(\mathbf{M}^{-1}\mathbf{N}) \leqslant \|\mathbf{M}^{-1}\mathbf{N}\|_{\mathbf{M}} \leqslant \frac{1}{2}\frac{\|\mathbf{a}\|_{L^\infty(\Omega)}}{\sqrt{\inf(\nu)\inf(c_0 + \frac{1}{2}\operatorname{div}(\mathbf{a}))}}.$$

If H is Domain Decomposition for M with GenEO coarse space

[S., Dolean, Hauret, Nataf, Pechstein, and Scheichl, 2013]

$\kappa(\mathbf{HM})$ does not depend on:

- discretization step h
- number of subdomains or processors on a supercomputer.

Scalability without deflation

- Freefem++ with ffddm developed by Tournier, Hecht, Jolivet, Nataf.
- Weighted GMRES with (DD + GenEO) preconditioner of **M**.

```
-ffddm_schwarz_method asm
-ffddm_geneo_threshold 0.15
-ffddm_schwarz_coarse_correction BNN.
```

- $\int_\Omega ((c_0 + \frac{1}{2}\operatorname{div}\mathbf{a})uv + \nu\nabla u \cdot \nabla v) + \int_\Omega (\frac{1}{2}\mathbf{a} \cdot \nabla uv - \frac{1}{2}\mathbf{a} \cdot \nabla vu) = \int_\Omega fv.$
  - $\mathbf{a} = 2\pi[-(y - 0.1), x - 0.5]$
  - $c_0 = \nu = 1$

Iteration count when number of subdomains and h vary

Number of subdomains	4	8	16	32
$h = 1/200$	19	20	20	20
$h = 1/500$	18	19	19	20

$\rightarrow$ Scalability and h-independence BUT degrades when $\rho(\mathbf{M}^{-1}\mathbf{N})$ increases.

Bibliography : origins of non symmetric DD

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- X.-C. Cai and O. B. Widlund, *Domain decomposition algorithms for indefinite elliptic problems*, SIAM J. Sci. Stat. Comput., 13 (1992).
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- M. Bonazzoli, X. Claeys, F. Nataf, and P.-H. Tournier, *Analysis of the SORAS domain decomposition preconditioner for non-self-adjoint or indefinite problems*, J. Sci. Comput., 89 (2021).
- N. Bootland, V. Dolean, I. G. Graham, C. Ma, and R. Scheichl, *Overlapping Schwarz methods with GenEO coarse spaces for indefinite and nonself-adjoint problems*, IMA J. Numer. Anal., 43 (2023).

Looking forward to MS7 to learn more

This afternoon and tomorrow morning.

Bibliography: methods that most resemble our work

- Exploit the splitting $\mathbf{A} = \mathbf{M} + \mathbf{N}$:

Z.-Z. Bai, G. H. Golub, and M. K. Ng, *Hermitian and skew-Hermitian splitting methods for non-Hermitian positive definite linear systems*, SIAM J. Matrix Anal. Appl., 24 (2003), pp. 603–626.

- Solve $(\mathbf{A} + \mathbf{E})\mathbf{x} = \mathbf{b}$ with $\mathbf{A}$ spd.
  Later Called CSPD for Coarse Grid + spd preconditioning.

J. Xu and X.-C. Cai, *A preconditioned GMRES method for nonsymmetric or indefinite problems*, Math. Comput., 59 (1992), pp. 311–319.

- See also:

X.-C. Cai, W. D. Gropp, and D. E. Keyes, *A comparison of some domain decomposition algorithms for nonsymmetric elliptic problems*, in Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations, Philadelphia, PA, 1992.

J. Xu, *A new class of iterative methods for nonselfadjoint or indefinite problems*, SIAM J. Numer. Anal., 29(2), 1992.

1. GMRES
2. Preconditioning (by $\mathbf{H}$) and Weighting (by $\mathbf{W}$)
3. $\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H}$, $\mathbf{A}$ pd
4. Spectral deflation
5. Numerics
6. Prescribe simultaneous convergence curves

Spectral deflation

Deflation

Following [Tang, Nabben, Vuik, Erlangga (2009)] [García Ramos, Kehl, Nabben (2020)]

- Choose $\mathbf{Y}, \mathbf{Z} \in \mathbb{K}^{n \times m}$ two full rank matrices.
- Let $\mathbf{P}_D = \mathbf{I} - \mathbf{AZ}(\mathbf{Y}^*\mathbf{AZ})^{-1}\mathbf{Y}^*$ (Projection if $\mathbf{Y}^*\mathbf{AZ}$ is non-singular)
- Solve in two steps

$$\mathbf{Ax} = \mathbf{b} \Leftrightarrow \quad \underbrace{\mathbf{P}_D\mathbf{Ax} = \mathbf{P}_D\mathbf{b}}_{\text{GMRES}} \quad \text{and} \quad \underbrace{(\mathbf{I} - \mathbf{P}_D)\mathbf{Ax} = (\mathbf{I} - \mathbf{P}_D)\mathbf{b}}_{\text{Direct solve}}$$

- $\mathbf{P}_D$ is efficient if m is not too large and $\mathbf{P}_D\mathbf{Ax} = \mathbf{P}_D\mathbf{b}$ is easier to solve by GMRES.

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- Solve in two steps

$$\mathbf{A}\mathbf{x} = \mathbf{b} \Leftrightarrow \underbrace{\mathbf{P}_{\mathrm{D}}\mathbf{A}\mathbf{x} = \mathbf{P}_{\mathrm{D}}\mathbf{b}}_{\text{preconditioned } \mathbf{W}\text{- GMRES}} \quad \text{and} \quad \underbrace{(\mathbf{I} - \mathbf{P}_{\mathrm{D}})\mathbf{A}\mathbf{x} = (\mathbf{I} - \mathbf{P}_{\mathrm{D}})\mathbf{b}}_{\text{Direct solve}}$$

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Requirements:

- $\mathbf{Y}^*\mathbf{AZ}$ is non-singular for the projection operators to be well defined,
- $\mathbf{Y}^*\mathbf{H}^{-1}\mathbf{Z}$ is non-singular so that GMRES iterations well defined. [Brown and Walker, 1997]

Remark: Both OK if $\mathbf{Y} = \mathbf{AZ} = \mathbf{AHY}$ $\rightarrow$ Not what we do.

Improve the $\rho(\mathbf{M}^{-1}\mathbf{N})$, or $\rho(\mathbf{HN})$, part of the bound

Convergence has been bounded with respect to

- either $[1, \kappa(\mathbf{HM})] + \mathrm{i}[-\rho(\mathbf{M}^{-1}\mathbf{N})\kappa(\mathbf{HM}), \rho(\mathbf{M}^{-1}\mathbf{N})\kappa(\mathbf{HM})]$,
- or $[\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + \mathrm{i}[-\rho(\mathbf{HN}), \rho(\mathbf{HN})]$,

(where again, $\mathbf{M} = 1/2(\mathbf{A} + \mathbf{A}^*)$, $\mathbf{N} = 1/2(\mathbf{A} + \mathbf{A}^*)$, $\mathbf{H}$:hpd preconditioner.)

This is the plan

- Choose $\mathbf{H}$ such that the spectrum of $(\mathbf{HM})$ is nice,
- Deflate away the vectors that make $\rho(\mathbf{M}^{-1}\mathbf{N})$ or $\rho(\mathbf{HN})$ large.

Crouzeix-Palencia analysis of deflated GMRES under our assumptions

The deflated problem is: $\mathbf{P}_\mathrm{D}\mathbf{A}\mathbf{x} = \mathbf{P}_\mathrm{D}\mathbf{b}$; $\quad \mathbf{P}_\mathrm{D} = \mathbf{I} - \mathbf{A}\mathbf{Z}(\mathbf{Y}^*\mathbf{A}\mathbf{Z})^{-1}\mathbf{Y}^*$
which we precondition on the right by $\mathbf{H}$ and solve by $\mathbf{H}$-weighted GMRES.

$$\frac{\|\mathbf{r}_\mathrm{k}\|_\mathbf{H}}{\|\mathbf{r}_0\|_\mathbf{H}} \leqslant (1+\sqrt{2}) \min_{q \in \mathbb{P}_\mathrm{k};\, q(0)=1} \max_{z \in \Omega} |q(z)|,$$

where

$$\Omega = \mathrm{FOV}^\mathbf{H}\left(\mathbf{P}_\mathrm{D}\mathbf{A}\mathbf{H}_{|\,\mathrm{range}(\mathbf{P}_\mathrm{D})}\right)$$
$$\subset \underbrace{\left\{\frac{\langle \mathbf{H}\mathbf{M}\mathbf{H}\mathbf{x}, \mathbf{x}\rangle}{\langle \mathbf{H}\mathbf{x}, \mathbf{x}\rangle}; \mathbf{x} \in \mathrm{range}(\mathbf{P}_\mathrm{D})\right\}}_{\subset[\lambda_{\min}(\mathbf{HM}),\lambda_{\max}(\mathbf{HM})]} + \underbrace{\left\{\frac{\langle \mathbf{H}\mathbf{N}\mathbf{H}\mathbf{x}, \mathbf{x}\rangle}{\langle \mathbf{H}\mathbf{x}, \mathbf{x}\rangle}; \mathbf{x} \in \mathrm{range}(\mathbf{P}_\mathrm{D})\right\}}_{\subset i\mathbb{R}}.$$

by applying the theorem in the Hilbert space $(\mathrm{range}(\mathbf{P}_\mathrm{D}), \langle,\rangle_\mathbf{W}, \|\|_\mathbf{W})$
and with the technical assumption that $\mathbf{Y} = \mathbf{H}\mathbf{A}\mathbf{Z}$.

Spectral Deflation space

- There exists a basis $(\mathbf{y}_1, \dots, \mathbf{y}_n)$ of $\mathbb{C}^n$ such that

$$\mathbf{H}^{-1}\mathbf{y}_k = \lambda_k \mathbf{N}\mathbf{y}_k; \ \langle \mathbf{y}_k, \mathbf{y}_l \rangle_{\mathbf{H}^{-1}} = \delta_{kl},$$

  because $\mathbf{H}^{-1}$ is hpd, $\mathbf{N}$ is skew-Hermitian.

- Set $\mathbf{Y}$ (in $\mathbf{P}_D = \mathbf{I} - \mathbf{AZ}(\mathbf{Y}^*\mathbf{AZ})^{-1}\mathbf{Y}^*$) s.t. $\operatorname{range}(\mathbf{Y}) = \operatorname{span}\{\mathbf{y}_k; |\lambda_k| > \tau\}$. Then,

$$\operatorname{range}(\mathbf{P}_D) = \ker(\mathbf{Y}^*) = \operatorname{span}\left\{\mathbf{H}^{-1}\mathbf{y}_k; |\lambda_k| \leqslant \tau\right\}.$$

- Finally,

$$\begin{aligned}\operatorname{FOV}^{\mathbf{H}}\left(\mathbf{P}_D\mathbf{AH}_{|\operatorname{range}(\mathbf{P}_D)}\right) &\subset [\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + \left\{\frac{\langle \mathbf{HNHx}, \mathbf{x}\rangle}{\langle \mathbf{Hx}, \mathbf{x}\rangle}; \mathbf{x} \in \operatorname{range}(\mathbf{P}_D)\right\} \\ &\subset [\lambda_{\min}(\mathbf{HM}), \lambda_{\max}(\mathbf{HM})] + i[-\tau, \tau].\end{aligned}$$

$\rightarrow$ Convergence bound that depends only on spectrum of $\mathbf{HM}$ and τ.

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Numerics

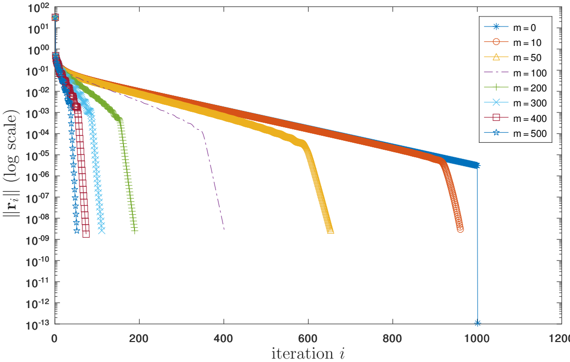
Scaled Jordan block unpreconditioned – Deflation of eigenvectors of $\mathbf{HM}$

$$\mathbf{A} = \begin{pmatrix} 1 & 0.99 & & & \\ & 1 & 0.99 & & \\ & & \ddots & \ddots & \\ & & & 1 & 0.99 \\ & & & & 1 \end{pmatrix}$$

$\mathbf{A} \in \mathbb{R}^{1000 \times 1000}$; $\mathbf{A}$ pd

Observations

- $\kappa(\mathbf{M}) = 199.$
- Deflating 50 eigenvectors decreases iteration count by 348.
- Deflating 100 eigenvectors decreases iteration count by 600.



m	0	10	50	100	200	300	400	500
iter	1000	959	652	400	188	110	73	51

m is the number of deflated vectors.

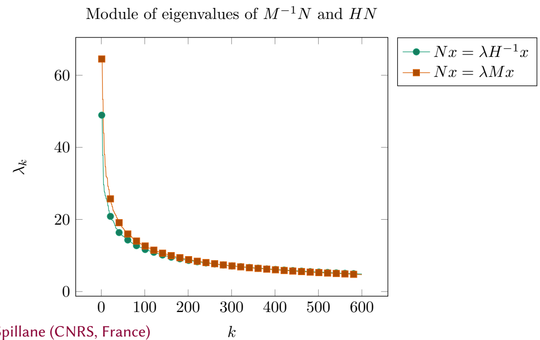
Back to Advection-Diffusion-Reaction preconditioned by DD

Domain decomposition preconditioner H (hpd) for M

$$\kappa(\mathbf{HM}) = 14.3.$$

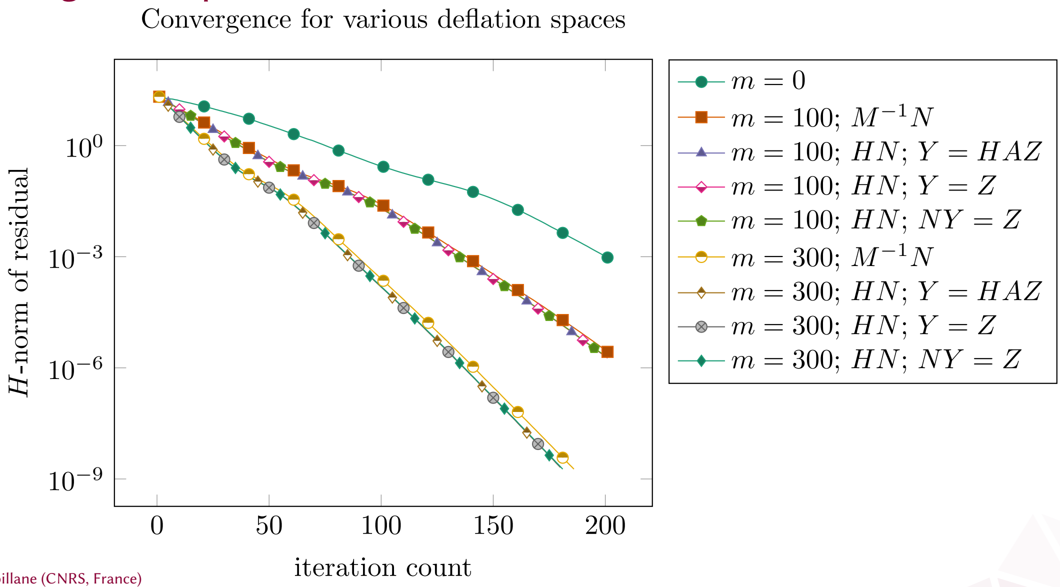
Lagrange Finite Element discretization of

$$\underbrace{\int_\Omega ((\mathrm{c}_0 + \frac{1}{2}\operatorname{div}\mathbf{a})\mathrm{uv} + \nu\nabla\mathrm{u}\cdot\nabla\mathrm{v})}_{\text{"}\mathbf{M}\text{"}} + \underbrace{\int_\Omega (\frac{1}{2}\mathbf{a}\cdot\nabla\mathrm{uv} - \frac{1}{2}\mathbf{a}\cdot\nabla\mathrm{vu})}_{\text{"}\mathbf{N}\text{"}} = \int_\Omega \mathrm{fv}.$$



Gevp	$\mathbf{Nx} = \lambda\mathbf{Mx}$	$\mathbf{Nx} = \lambda\mathbf{H}^{-1}\mathbf{x}$
$\rho = \lvert\lambda_1\rvert$	64.5	48.9
$\lvert\lambda_{101}\rvert$	12.7	11.7
$\lvert\lambda_{301}\rvert$	7.11	7.10
$\lvert\lambda_{600}\rvert$	4.69	4.87

Convergence improves with deflation



A puzzle: Comparison of W-GMRES and GMRES

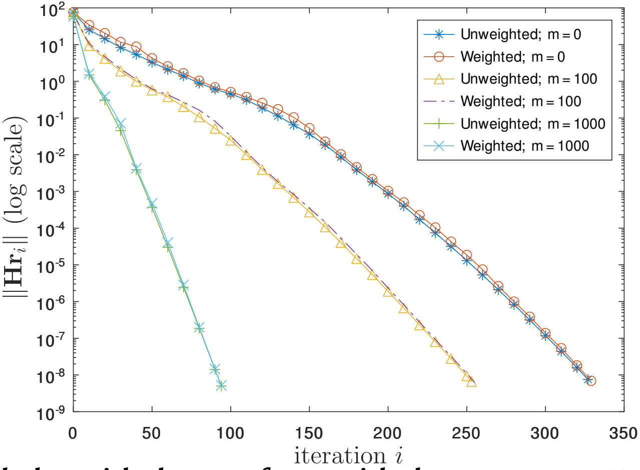
We compare

- Weighted GMRES
  i.e, $\mathbf{W} = \mathbf{H}$, with right preconditioning.
  Minimize: $\|\mathbf{r}_\mathrm{i}\|_\mathbf{W}$.
- (Unweighted) GMRES
  i.e, $\mathbf{W} = \mathbf{I}$, with left preconditioning.
  Minimize: $\|\mathbf{H}\mathbf{r}_\mathrm{i}\|$.

Stopping criterion

$\|\mathbf{H}\mathbf{r}_\mathrm{i}\|/\|\mathbf{H}\mathbf{r}_0\| < 10^{-10}$.

Preconditioner $\mathbf{H} = \mathbf{H}_{\mathrm{DD}}$; $\eta = 100$



$\rightarrow$ **the weight helps with the proof, not with the convergence.**

Prescribe simultaneous convergence curves

Any non-increasing curves are simultaneously possible

Joint work with Pierre Matalon (École polytechnique) inspired by [Greenbaum, Pták and Strakoš, 1996]

Theorem 1: Weighted and unweighted

Consider two prescribed convergence curves:

- $\mathtt{r}_0 > \mathtt{r}_1 > \mathtt{r}_2 > \ldots$ for $\mathbf{I}$-GMRES,
- $\mathtt{r}'_0 > \mathtt{r}'_1 > \mathtt{r}'_2 > \ldots$ for $\mathbf{W}$-GMRES.

There exists a system $\mathbf{Ax} = \mathbf{b}$ and a hpd weight matrix $\mathbf{W}$ such that both convergence curves are realized. Additionally, the eigenvalues of $\mathbf{A}$ can be prescribed.

Theorem 2: Left and right preconditioning.

Consider two prescribed convergence curves:

- $\mathtt{r}_0 > \mathtt{r}_1 > \mathtt{r}_2 > \ldots$ for right preconditioned GMRES,
- $\mathtt{r}'_0 > \mathtt{r}'_1 > \mathtt{r}'_2 > \ldots$ for left preconditioned GMRES.

There exists a system $\mathbf{Ax} = \mathbf{b}$ and a preconditioner $\mathbf{H}$ such that both convergence curves are realized. Additionally, the eigenvalues of $\mathbf{AH}$ can be prescribed.

Pierre Matalon is speaking about this result (and more) on Thursday at 14:40 in CT01.

Conclusion

For pd $\mathbf{A}$, proposed a pair of accelerators $(\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H})$ [S, SISC, 2024]

- Polynomial convergence bound that depends only on
  - either, $\lambda_{\min}(\mathbf{HM})$, $\lambda_{\max}(\mathbf{HM})$ and $\rho(\mathbf{NH})$,
  - or, $\kappa(\mathbf{HM})$ and $\rho(\mathbf{M}^{-1}\mathbf{N})$.
- Achieve scalability if $\mathbf{HM}$ "scales".
- Achieve h-independence for Advection-Diffusion-Reaction.

Added spectral deflation of high-frequency eigenvectors of $\mathbf{HN}$ (or $\mathbf{M}^{-1}\mathbf{N}$) [S, Szyld, SIMAX, 2024] [S, Szyld, Preprint, 2025]

- Replaces $\rho(\mathbf{NH})$ or $\rho(\mathbf{M}^{-1}\mathbf{N})$ in the bound by the frequency threshold τ.
- Reduces the iteration count as predicted.

In an effort to compare convergence of GMRES and W-GMRES [Matalon, S, Preprint, 2025]

- Simultaneous prescription of two convergence curves.

Thank you for you attention.

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(ANR is the French national research agency)

I will be looking for a postdoc in 2026.
Get in touch if you enjoy Krylov subpace methods and Domain Decomposition.

You may also enjoy the talks by:
E. Fressart, P. Matalon, E. Parolin, T. Raynaud, R. Scheichl.