Convergence estimates and acceleration of GMRES for solving linear systems

Journées Scientifiques du RT Terre et Énergies à Nouan Le Fuzelier

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Linear solvers

Find $\mathbf{x} \in \mathbb{C}^n$ such that

$$\mathbf{A}\mathbf{x} = \mathbf{b}; \quad \mathbf{A} \in \mathbb{C}^{n \times n}; \quad \mathbf{b} \in \mathbb{C}^n.$$

A can be

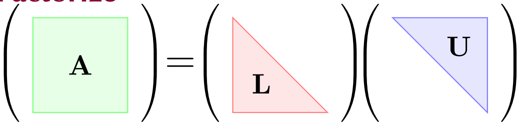
- Hermitian / non-Hermitian,
- of very high order n,
- sparse (*e.g.* finite element discretization of PDE)/ dense,
- with additional info (*e.g.*, underlying PDE) / already assembled.

Scope of my work

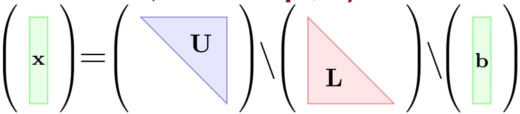
A is sparse and non-singular.

Direct solvers for **Ax** = **b**

Factorize



Then solve (in two steps, by forward and backward substitution)



Best* choice if problem is *not too large

e.g., MUMPS library co-developed by CERFACS, CNRS, ENS Lyon, INPT, Inria, Univ. Bordeaux and, since 2019, Mumps Technologies

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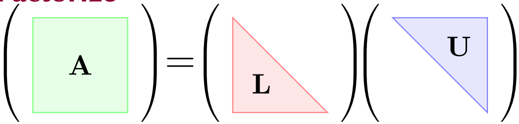

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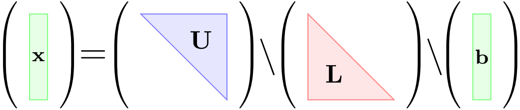

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Not too large ?

Let's say up to problem of size $n = 10^7$. **This is a very rough rule of thumb !**

Iterative solvers for $\mathbf{Ax} = \mathbf{b}$: Krylov subspace methods

- Iterative algorithm. Starts with an initial guess $\mathbf{x}_0 \in \mathbb{C}^n$.
- At iteration i:
  - $\mathbf{x}_i$ (approximate solution) characterized by:

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

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

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  - Equivalently the i-th residual $\mathbf{r}_i = \mathbf{b} - \mathbf{Ax}_i$ satisfies

$$\mathbf{r}_i = \operatorname{argmin}_{\mathbf{r} \in \mathbf{r}_0 + \mathbf{A}\mathcal{K}_i(\mathbf{A}, \mathbf{r}_0)} \{ \| \mathbf{r} \| \},$$

or

$$\| \mathbf{r}_i \| = \min_{p \in \mathbb{P}_i;\, p(0)=1} \| p(\mathbf{A}) \mathbf{r}_0 \|,$$

where $\mathbb{P}_i$ is the set of all polynomials of degree at most i.

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    where $\mathbb{P}_i$ is the set of all polynomials of degree at most i.
- For an order n matrix, the solution is found in at most n iterations (by Cayley–Hamilton theorem).

TOP 500 as of June 2024 (https://top500.org/)

	Name and Location	Total Cores	Rmax [PFlop/s]	Rpeak [PFlop/s]	Nmax	HPCG [PFlop/s]
1	Frontier Oak Ridge National Lab. (USA)	8,699,904	1,206	1,715	24,330,240	14
2	Aurora Argonne National Lab. (USA)	9,264,128	1,012	1,980	28,773,888	6
3	Eagle Microsoft Azure (USA)	2,073,600	561	847	11,796,480	
4	Supercomputer Fugaku RIKEN (Japan)	7,630,848	442	537	21,288,960	16
5	LUMI EuroHPC/CSC (Finland)	2,752,704	380	532	13,685,760	5
...						
17	CEA-HE CEA (France)	389,232	57	112	5,806,080	
...						
20	Adastra GENCI-CINES (France)	319,072	46	62	4,492,800	0.5

- 1 PFlop/s = 10^{15} floating point ops per second.
- 1000 PFLop/s = 1 EFlop/s (exaflop).

- **Rpeak** is theoretical.
- **Rmax** is experimental (solve dense problem by Linpack).
- **HPCG** is experimental (solve sparse problem iteratively).

TOP 500: Efficiency

TOP500 rank	**Name and Location**	$\frac{\textbf{Rmax}}{\textbf{Rpeak}}$ [%]	$\frac{\textbf{HPCG}}{\textbf{Rpeak}}$ [%]
1	Frontier Oak Ridge National Lab. (USA)	70	0.82
2	Aurora Argonne National Lab. (USA)	51	0.28
3	Eagle Microsoft Azure (USA)	66	
4	Supercomputer Fugaku RIKEN (Japan)	82	2.98
5	LUMI EuroHPC/CSC (Finland)	71	0.86
...			
17	CEA-HE CEA (France)	50	
...			
20	Adastra GENCI-CINES (France)	74	0.91

- It is hard to use a supercomputer efficiently.
- Scalable algorithms are vital as well as hardware and implementation.

Green 500 as of June 2024 (https://top500.org/lists/green500/)

Green500 rank	TOP500 rank	Name and Location	Total Cores	Rmax [PFlop/s]	Power [kW]	Energy Efficiency [GFlops/Watts]
1	189	JEDI EuroHPC/FZJ (Germany)	19,584	4.504	67.31	72.73
2	128	Isambard-AI phase 1 University of Bristol (UK)	34,272	7.42	117.08	68.83
3	55	Helios GPU Cyfronet (Poland)	89,760	19.14	316.88	66.95
4	329	Henri Flatiron Institute (USA)	8,288	2.88	44.07	65.40
...						
9	20	Adastra GENCI-CINES (France)	319,072	46.10	921.48	58.02
...						
13	1	Frontier Oak Ridge National Lab. (USA)	8,699,904	1,206.00	22,786.00	52.93
...						
42	2	Aurora Argonne National Lab. (USA)	9,264,128	1,012.00	38,698.36	26.15

Introduction to GMRES

GMRES [Saad and Schultz, 1986] for $\mathbf{Ax} = \mathbf{b}$; $\mathbf{A} \in \mathbb{C}^{n\times n}$; $\mathbf{b} \in \mathbb{C}^n$

- Iterative algorithm. Starts with an initial guess $\mathbf{x}_0 \in \mathbb{C}^n$.
- At iteration i:
  - $\mathbf{x}_i$ (approximate solution) characterized by:

$$\mathbf{x}_i = \text{argmin}_{\mathbf{x}\in\mathbf{x}_0+\mathcal{K}_i(\mathbf{A},\mathbf{r}_0)}\{\|\mathbf{b}-\mathbf{Ax}\|_2\},$$

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

  - $\mathbf{x}_i$ and $\mathbf{r}_i = \mathbf{b} - \mathbf{Ax}_i$ not computed at each iteration.
  - Instead, orthonormal basis for $\mathcal{K}_i$ computed by updating the orthonormal basis for $\mathcal{K}_{i-1}$ (Arnoldi).
  - Residual $\|\mathbf{b} - \mathbf{Ax}_i\|_2$ can be monitored. At convergence, $\mathbf{x}_i$ 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 $\mathbf{x}_i$ at iteration i

$$\|\mathbf{r}_i\| = \|\mathbf{b} - \mathbf{A}\mathbf{x}_i\| = \min_{p \in \mathbb{P}_i;\, p(0)=1} \|p(\mathbf{A})\mathbf{r}_0\| \text{ where } \mathbb{P}_i\text{: polynomials of degree at most } i. \tag{1}$$

See *e.g.*, [Meurant and Duintjer Tebbens, 2015]).

Convergence estimate by ideal GMRES for non-singular A

$$\frac{\|\mathbf{r}_i\|}{\|\mathbf{r}_0\|} \leqslant \min \left\{ \|p(\mathbf{A})\| \text{ such that } p \in \mathbb{P}_i \text{ and } p(0) = 1 \right\}. \tag{2}$$

[Greenbaum, Trefethen, SIAM Review, 1998]:

"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."

Convergence of GMRES does not depend only on the spectrum of A

If A is diagonalizable into $\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$

$$\frac{\|\mathbf{r}_i\|_2}{\|\mathbf{r}_0\|_2} \leqslant \min_{p\in\mathbb{P}_i;\, p(0)=1} \|p(\mathbf{A})\|_2 \leqslant \underbrace{\|\mathbf{X}\|_2 \, \|\mathbf{X}^{-1}\|_2}_{:=\kappa(\mathbf{X})} \min_{p\in\mathbb{P}_i;\, p(0)=1} \|p(\mathbf{\Lambda})\|_2$$

$$\leqslant \kappa(\mathbf{X}) \min_{p\in\mathbb{P}_i;\, p(0)=1} \max_{\lambda\in\sigma(\mathbf{A})} |p(\lambda)|.$$

[Eisenstat et al., (1983)] [Saad and Schultz (1986)].

If A is normal (e.g., Hermitian), $\kappa(\mathbf{X}) = 1$,

$$\frac{\|\mathbf{r}_i\|_2}{\|\mathbf{r}_0\|_2} \leqslant \min_{p\in\mathbb{P}_i;\, p(0)=1} \max_{\lambda\in\sigma(\mathbf{A})} |p(\lambda)|.$$

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BUT Prescribing all eigenvalues of a matrix does not impose any restrictions on the residual sequence of GMRES.

[Greenbaum, Pták, Strakoš (1996)]

Field of value bounds for GMRES

Recall that: $\|\mathbf{r}_i\|/\|\mathbf{r}_0\| \leqslant \min_{p\in\mathbb{P}_i;\, p(0)=1} \|p(\mathbf{A})\|_2$.

Elman estimate (Eisenstat, Elman, Schultz [1983])

$$\frac{\|\mathbf{r}_i\|}{\|\mathbf{r}_0\|} \leqslant \left[1 - \frac{d(0, FOV(\mathbf{A}))^2}{\|\mathbf{A}\|^2}\right]^{i/2}, \text{ where } FOV(\mathbf{A}) := \left\{\frac{\langle \mathbf{Au}, \mathbf{u}\rangle}{\langle \mathbf{u}, \mathbf{u}\rangle}; \mathbf{u} \in \mathbb{C}^n \setminus \{0\}\right\}.$$

Crouzeix-Palencia bound [2017]

$$\frac{\|\mathbf{r}_i\|}{\|\mathbf{r}_0\|} \leqslant (1+\sqrt{2}) \min_{p\in\mathbb{P}_i;\, p(0)=1} \max_{z\in FOV(\mathbf{A})} |p(z)|.$$

Indeed, $\|f(\mathbf{A})\| \leqslant (1+\sqrt{2}) \max_{z\in FOV(\mathbf{A})} |f(z)|$, for any rational function f.

Parenthesis: M. Crouzeix conjectured in 2004 that $\|f(\mathbf{A})\| \leqslant 2 \max_{z\in FOV(\mathbf{A})} |f(z)|$.

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Limitation: FOV bounds say nothing in $0 \in FOV(\mathbf{A})$.

Objectives

Fundamental Questions

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

Objective: Choose efficient accelerators

- **Preconditioner**,
- **Weighted norm**,
- **Deflation**,

in order to ensure fast convergence with respect to a (new?) **convergence bound**.

Scope: HPC

Ideally number of iterations independent of problem size and number of processors.

Preconditioning (by $\mathbf{H}$), Weighting (by $\mathbf{W}$) and Deflating (by $\mathbf{P}_D$)

Accelerating GMRES by preconditioning and weighting

- Choose a non-singular preconditioner $\mathbf{H} \in \mathbb{C}^{n \times n}$ and solve

$$\mathbf{HAx} = \mathbf{Hb} \text{ or } (\mathbf{AHu} = \mathbf{b} \text{ with } \mathbf{x} = \mathbf{Hu}).$$

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- Choose a hpd weight matrix $\mathbf{W} \in \mathbb{K}^{n\times n}$, that induces $\langle \cdot, \cdot \rangle_{\mathbf{W}}$ and $\| \cdot \|_{\mathbf{W}}$ and

$$\text{replace all } \langle \cdot, \cdot \rangle_2 \text{ in GMRES by } \langle \cdot, \cdot \rangle_{\mathbf{W}}.$$

[Cai (1989)] [Cai and Widlund (1992)] [Essai's thesis w/ Brezinski (1998)]

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  [Cai (1989)] [Cai and Widlund (1992)] [Essai's thesis w/ Brezinski (1998)]

- Characterization of the residuals $\mathbf{r}_i = \mathbf{b} - \mathbf{Ax}_i$:

$$\|\mathbf{Hr}_i\|_{\mathbf{W}} = \min_{p \in \mathbb{P}_i;\, p(0)=1} \|\mathbf{H}p(\mathbf{AH})\mathbf{r}_0\|_{\mathbf{W}}, \text{ or } \|\mathbf{r}_i\|_{\mathbf{W}} = \min_{p \in \mathbb{P}_i;\, p(0)=1} \|p(\mathbf{AH})\mathbf{r}_0\|_{\mathbf{W}}.$$

  where $\mathbb{P}_i$ is the set of polynomials of degree at most i.

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

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

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

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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 $\mathbf{Y} = \mathbf{AZ} = \mathbf{AHY}$.

Convergence of Weighted Preconditioned and Deflated GMRES (1/2)

By definition:

$$\begin{aligned}\|\mathbf{r}_1\|_{\mathbf{W}}^2 &= \min\left\{\|\mathbf{r}_0 - \alpha_0 \mathbf{P}_D \mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2;\ \alpha_0 \in \mathbb{C}\right\} \\ &= \|\mathbf{r}_0 - \underbrace{\alpha_0 \mathbf{P}_D \mathbf{A}\mathbf{H}\mathbf{r}_0}_{\mathbf{W}\text{-orthogonal projection}}\|_{\mathbf{W}}^2 \text{ with } \alpha_0 = \frac{\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0, \mathbf{r}_0\rangle_{\mathbf{W}}}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2} \\ &= \|\mathbf{r}_0\|_{\mathbf{W}}^2 - \left|\frac{\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0, \mathbf{r}_0\rangle_{\mathbf{W}}}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2}\right|^2 \|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2 .\end{aligned}$$

Finally, get a worst case GMRES bound,

$$\frac{\|\mathbf{r}_1\|_{\mathbf{W}}^2}{\|\mathbf{r}_0\|_{\mathbf{W}}^2} = 1 - \frac{|\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0, \mathbf{r}_0\rangle_{\mathbf{W}}|^2}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2 \|\mathbf{r}_0\|_{\mathbf{W}}^2} \leqslant 1 - \underbrace{\inf_{\mathbf{y}\in \operatorname{range}(\mathbf{P}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y}, \mathbf{y}\rangle_{\mathbf{W}}|^2}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y}\|_{\mathbf{W}}^2 \|\mathbf{y}\|_{\mathbf{W}}^2}}_{:=\theta(\mathbf{A},\mathbf{H},\mathbf{W},\mathbf{Y},\mathbf{Z})} .$$

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Valid also for **restarted** GMRES and **truncated** GCR (including Minimal Residual).

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By definition:

$$\|\mathbf{r}_1\|_{\mathbf{W}}^2 = \min\left\{\|\mathbf{r}_0 - \alpha_0 \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2;\ \alpha_0 \in \mathbb{C}\right\}$$

$$= \|\mathbf{r}_0 - \underbrace{\alpha_0 \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0}_{\mathbf{W}\text{-orthogonal projection}}\|_{\mathbf{W}}^2 \text{ with } \alpha_0 = \frac{\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0, \mathbf{r}_0\rangle_{\mathbf{W}}}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2}$$

$$= \|\mathbf{r}_0\|_{\mathbf{W}}^2 - \left|\frac{\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0, \mathbf{r}_0\rangle_{\mathbf{W}}}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2}\right|^2 \|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{r}_0\|_{\mathbf{W}}^2 .$$

Finally, get a worst case GMRES bound,

$$\frac{\|\mathbf{r}_i\|_{\mathbf{W}}^2}{\|\mathbf{r}_{i-1}\|_{\mathbf{W}}^2} \leqslant 1 - \underbrace{\inf_{\mathbf{y}\in\text{range}(\mathbf{P}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y}, \mathbf{y}\rangle_{\mathbf{W}}|^2}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y}\|_{\mathbf{W}}^2\|\mathbf{y}\|_{\mathbf{W}}^2}}_{:=\theta(\mathbf{A},\mathbf{H},\mathbf{W},\mathbf{Y},\mathbf{Z})} .$$

Valid also for **restarted** GMRES and **truncated** GCR (including Minimal Residual).

Convergence of Weighted Preconditioned and Deflated GMRES (2/2)

Convergence Bound

$$\frac{\|\mathbf{r}_i\|_{\mathbf{W}}^2}{\|\mathbf{r}_{i-1}\|_{\mathbf{W}}^2} \leqslant 1 - \underbrace{\inf_{\mathbf{y}\in\text{range}(\mathbf{P}_D)\setminus\{\mathbf{0}\}} \left[\frac{|\langle \mathbf{P}_D\mathbf{AHy}, \mathbf{y}\rangle_{\mathbf{W}}|}{\|\mathbf{P}_D\mathbf{AHy}\|_{\mathbf{W}}\|\mathbf{y}\|_{\mathbf{W}}}\right]^2}_{=\theta(\mathbf{A},\mathbf{H},\mathbf{W},\mathbf{Y},\mathbf{Z})}.$$

- If $\mathbf{P}_D = \mathbf{I}$, the terms can be grouped to prove *Elman's estimate*:

$$\left[\frac{|\langle \mathbf{AHy}, \mathbf{y}\rangle_{\mathbf{W}}|}{\|\mathbf{y}\|_{\mathbf{W}}^2} \times \frac{\|\mathbf{y}\|_{\mathbf{W}}}{\|\mathbf{AHy}\|_{\mathbf{W}}}\right]^2 \geqslant \left[\frac{d(0, W_{\mathbf{W}}(\mathbf{AH}))}{\|\mathbf{AH}\|_{\mathbf{W}}}\right]^2,$$

where

$$W_{\mathbf{W}}(\mathbf{AH}) := \left\{\frac{\langle \mathbf{AHu}, \mathbf{u}\rangle_{\mathbf{W}}}{\langle \mathbf{u}, \mathbf{u}\rangle_{\mathbf{W}}}; \mathbf{u} \in \mathbb{C}^n\right\}.$$

[Eisenstat, Elman, and Schultz (1983)] [Elman's PhD thesis (1982)]

Case A pd, H hpd, $\mathbf{W} = \mathbf{H}$ and $\mathbf{Y} = \mathbf{HAZ}$

Setting

Notation: Hermitian + Skew-Hermitian splitting of A

$$A = \mathbf{M} + \mathbf{N}; \text{ with } \underbrace{\mathbf{M} = \frac{\mathbf{A} + \mathbf{A}^*}{2}}_{\text{Hermitian}} \text{ and } \underbrace{\mathbf{N} = \frac{\mathbf{A} - \mathbf{A}^*}{2}}_{\text{Skew-Hermitian}}.$$

Assumptions

- **A** (the problem matrix) is positive definite *i.e.*, **M** is (Hermitian) positive definite.
- **H** (the preconditioner) is Hermitian positive definite.
- $\mathbf{W} = \mathbf{H}$ (weight matrix).

See also [Chan, Chow, Saad, and Yeung, 1999]

- $\mathbf{Y} = \mathbf{HAZ} \Rightarrow \mathbf{P}_D = \mathbf{I} - \mathbf{AZ}(\mathbf{Z}^*\mathbf{A}^*\mathbf{HAZ})^{-1}\mathbf{Z}^*\mathbf{A}^*\mathbf{H}$ is **H**-orthogonal.

Convergence under A pd, H hpd, W = H and Y = HAZ

$$\theta(\mathbf{A},\mathbf{H},\mathbf{H},\mathbf{HAZ},\mathbf{Z}) = \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{P}_D)\setminus\{\mathbf{0}\}} \frac{\langle \mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y},\mathbf{H}\mathbf{y}\rangle^2}{\|\mathbf{P}_D\mathbf{A}\mathbf{H}\mathbf{y}\|_{\mathbf{H}}^2\|\mathbf{y}\|_{\mathbf{H}}^2} \text{(by definition)}$$

$$\geqslant \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{P}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}\mathbf{H}\mathbf{y},\mathbf{H}\mathbf{y}\rangle|^2}{\|\mathbf{A}\mathbf{H}\mathbf{y}\|_{\mathbf{H}}\langle\mathbf{H}\mathbf{y},\mathbf{y}\rangle} \text{(by } \mathbf{H} \text{ hpd; } \mathbf{P}_D\ \mathbf{H}\text{-orthogonal)}$$

$$\geqslant \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y},\mathbf{y}\rangle|}{\langle\mathbf{y},\mathbf{H}\mathbf{y}\rangle} \times \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{HP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}\mathbf{y},\mathbf{y}\rangle|}{\langle\mathbf{H}^{-1}\mathbf{y},\mathbf{y}\rangle}$$

(generalizes [Starke, 1997])

$$\geqslant \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y},\mathbf{y}\rangle|}{\langle\mathbf{y},\mathbf{M}^{-1}\mathbf{y}\rangle} \times \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{\langle \mathbf{M}^{-1}\mathbf{y},\mathbf{y}\rangle}{\langle\mathbf{y},\mathbf{H}\mathbf{y}\rangle} \times \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{HP}_D)\setminus\{\mathbf{0}\}} \frac{\langle \mathbf{M}\mathbf{y},\mathbf{y}\rangle}{\langle\mathbf{H}^{-1}\mathbf{y},\mathbf{y}\rangle}$$

$$\geqslant \inf_{\mathbf{y}\in\mathrm{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y},\mathbf{y}\rangle|}{\langle\mathbf{y},\mathbf{M}^{-1}\mathbf{y}\rangle} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}, \text{ where } \mathbf{M} = 1/2(\mathbf{A}+\mathbf{A}^*).$$

Theorem 1/2: A bound that is true even without deflation

We still assume that $\mathbf{A}$ pd, $\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H}$ and $\mathbf{Y} = \mathbf{HAZ}$. Recall that

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \inf_{\mathbf{y}\in \text{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y}, \mathbf{y}\rangle|}{\langle \mathbf{y}, \mathbf{M}^{-1}\mathbf{y}\rangle} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}.$$

Theorem

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \inf_{\mathbf{y}\neq\mathbf{0}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y}, \mathbf{y}\rangle|}{\langle \mathbf{y}, \mathbf{M}^{-1}\mathbf{y}\rangle} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})} = 1 - \frac{1}{1+\rho(\mathbf{M}^{-1}\mathbf{N})^2} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}$$

where $\mathbf{M} = 1/2(\mathbf{A}+\mathbf{A}^*)$ and $\mathbf{N} = 1/2(\mathbf{A}-\mathbf{A}^*)$ by [Johnson (1973, 1975)].

- If $\mathbf{H}$ is a scalable preconditioner for $\mathbf{M}$, then $\mathbf{H}$ is a scalable preconditioner for $\mathbf{A}$.
- The bound depends on how well the Hermitian part is preconditioned and a measure of non-Hermitianness ($\rho(\mathbf{M}^{-1}\mathbf{N})$).
- Connections to [Elman, 1982].

Spectral Deflation

Theorem 2/2: A bound with a new spectral deflation space

We still assume that $\mathbf{A}$ pd, $\mathbf{H}$ hpd, $\mathbf{W} = \mathbf{H}$ and $\mathbf{Y} = \mathbf{HAZ}$. Recall that

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \inf_{\mathbf{y}\in \mathrm{range}(\mathbf{AHP}_D)\setminus\{\mathbf{0}\}} \frac{|\langle \mathbf{A}^{-1}\mathbf{y}, \mathbf{y}\rangle|}{\langle \mathbf{y}, \mathbf{M}^{-1}\mathbf{y}\rangle} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}.$$

Definition of a new spectral deflation space

Still denoting $\mathbf{M} = 1/2(\mathbf{A} + \mathbf{A}^*)$ and $\mathbf{N} = 1/2(\mathbf{A} - \mathbf{A}^*)$,

- Solve $\mathbf{N}\mathbf{z}^{(j)} = \lambda_j \mathbf{M}\mathbf{z}^{(j)}$. Properties: $\lambda_j \in i\mathbb{R}$ and $\mathbf{z}^{(j)}$ are pairwise $\mathbf{M}$-orthogonal.
- For some chosen τ, set $\mathrm{span}(\mathbf{Z}) := \mathrm{span}\{\mathbf{z}^{(j)}; |\lambda_j| > \tau\}$.
- Then

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \frac{1}{(1+\tau^2)} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}.$$

Idea of the proof

$$\mathbf{A}^{-1} = (\mathbf{M} + \mathbf{N})^{-1} = (\mathbf{I} + \mathbf{M}^{-1}\mathbf{N})^{-1}\mathbf{M}^{-1}$$

Numerical results

Advection Diffusion Reaction

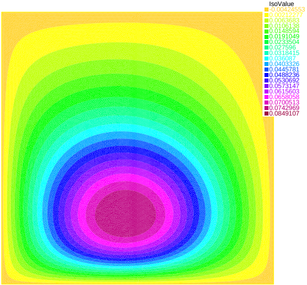
Strong Formulation

$$\begin{cases} c_0 u + \operatorname{div}(\mathbf{a} u) - \operatorname{div}(\nu \nabla u) &= f, \text{ in } \Omega = [0,1]^2, \\ u &= 0; \text{ on } \partial\Omega. \end{cases}$$

In our numerics

- $f(x,y) = \exp(-10((x-0.5)^2 + (y-0.1)^2))$,
- $\mathbf{a} = 2\pi[-(y-0.1), x-0.5]$.

Solution for $\nu = c_0 = 1$



Variational Formulation

Find $\mathbf{u} \in H^1_0(\Omega)$ such that:

$$\underbrace{\int_\Omega \left(\left(c_0 + \frac{1}{2} \operatorname{div} \mathbf{a} \right) uv + \nu \nabla u \cdot \nabla v \right)}_{\text{symmetric part}} + \underbrace{\int_\Omega \left(\frac{1}{2} \mathbf{a} \cdot \nabla u v - \frac{1}{2} \mathbf{a} \cdot \nabla v u \right)}_{\text{skew-symmetric part}} = \int_\Omega f v, \quad \forall\, v \in H^1_0(\Omega).$$

Advection-Diffusion-Reaction : What to expect without deflation ?

Lagrange Finite Element discretization of

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

Recall that

$$\frac{\|\mathbf{r}_i\|_{\mathbf{H}}}{\|\mathbf{r}_0\|_{\mathbf{H}}} \leqslant \left[1 - \frac{1}{\kappa(\mathbf{HM})(1 + \rho(\mathbf{M}^{-1}\mathbf{N})^2)}\right]^{i/2}$$

If H is DD + GenEO:

$\kappa(\mathbf{HM})$ independent of

- discretization step h
- and number of subdomains.

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

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

Convergence should not depend on h or number of subdomains

Scalability without deflation

- Freefem++ with ffddm developed by Tournier, Hecht, Jolivet, Nataf.
- Weighted GMRES with (DD + GenEO) preconditioner of $\mathbf{M}$.

```
-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

Dependency on h and strength of non-symmetry without deflation

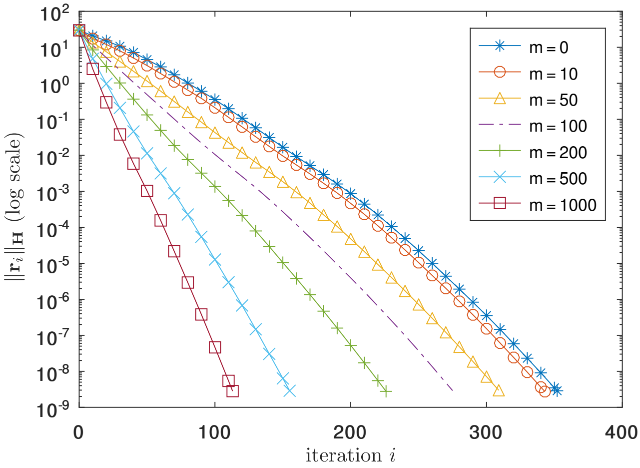
- Freefem++ with ffddm developed by Tournier, Hecht, Jolivet, Nataf.
- Weighted GMRES with (DD + GenEO) preconditioner of $\mathbf{M}$.
  - Partition into 8 subdomains computed by Metis,
  - Stopping criterion: $\|\mathbf{H}\mathbf{r}_i\| < 10^{-6}$.
- $\int_\Omega ((c_0 + \frac{1}{2}\,\mathrm{div}\,\mathbf{a})uv + \nu \nabla u \cdot \nabla v) + \int_\Omega (\frac{1}{2}\mathbf{a} \cdot \nabla uv - \frac{1}{2}\mathbf{a} \cdot \nabla vu) = \int_\Omega fv.$
  - $\mathbf{a} = 2\pi[-(y - 0.1), x - 0.5]$

Iteration count when h and strength of non-symmetry vary

	$1/h$	1000	500	200	100
	global number of dofs	1 002 001	251 001	40 401	10 201
$c_0 = \nu = 0.1$	iteration count	40	42	43	41
$c_0 = \nu = 1$	iteration count	18	19	20	21
$c_0 = \nu = 10$	iteration count	16	17	17	20

Convergence with spectral deflation when $c_0 = \nu = 0.01$

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



m	iter
0	352
10	343
50	309
100	275
200	226
500	155
1000	113

- $\kappa(\mathbf{H}_{\mathrm{DD}}\mathbf{M}) = 16.241$
- $\rho(\mathbf{M}^{-1}\mathbf{N}) = 64.6$

Spectral deflation space: solution of the Generalized eigenvalue problem

Variational Formulation discretized by $\mathbb{P}_1$ finite elements with 31502 dofs

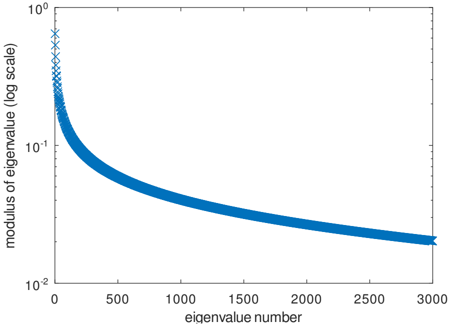
With $\mathbf{a} = 2\pi[-(y-0.1), x-0.5]$, find $\mathbf{u} \in H_0^1(\Omega)$ such that:

$$\underbrace{\int_\Omega \left(\left(c_0 + \frac{1}{2}\operatorname{div}\mathbf{a}\right) uv + \nu \nabla u \cdot \nabla v\right)}_{\mathbf{M}} + \underbrace{\int_\Omega \left(\frac{1}{2}\mathbf{a}\cdot\nabla uv - \frac{1}{2}\mathbf{a}\cdot\nabla vu\right)}_{\mathbf{N}} = \int_\Omega fv, \quad \forall\, v \in H_0^1(\Omega),$$

First 3000 (out of 31502) eigenvalues of :

$$\mathbf{N}\mathbf{z}^{(j)} = \lambda_j \mathbf{M}\mathbf{z}^{(j)}$$

in the case $c_0 = \nu = 1$.



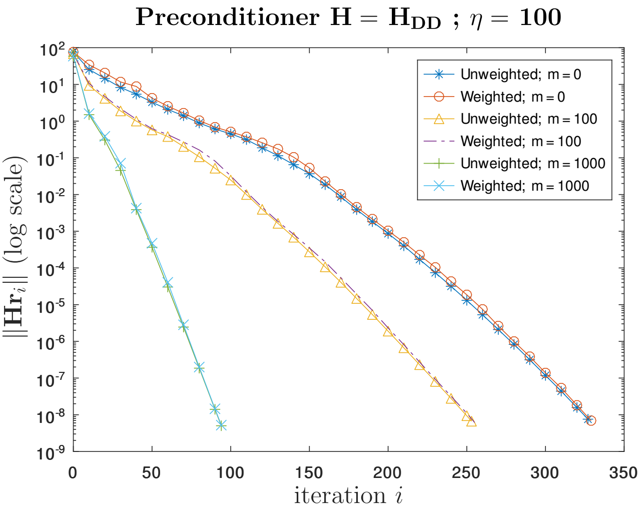
Comparison of WPD-GMRES and PD-GMRES

We compare

- Weighted GMRES
  i.e, $\mathbf{W} = \mathbf{H}$.
- (Unweighted) GMRES
  i.e, $\mathbf{W} = \mathbf{I}$.

Recall that
the residual is minimized in the **W**-norm.

Stopping criterion
$\|\mathbf{H}\mathbf{r}_i\| / \|\mathbf{H}\mathbf{r}_0\| < 10^{-10}$.



Comparison of WPD-GMRES and PD-GMRES

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  i.e, $\mathbf{W} = \mathbf{I}$.

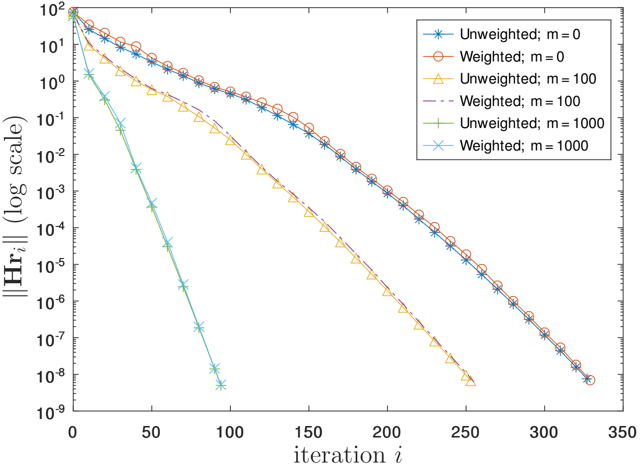
Recall that

the residual is minimized in the **W**-norm.

Stopping criterion

$\|\mathbf{H}\mathbf{r}_i\| / \|\mathbf{H}\mathbf{r}_0\| < 10^{-10}$.

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



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

Conclusion for A pd, H hpd, W = H (and Y = HAZ)

Notation: $\mathbf{M} = 1/2(\mathbf{A} + \mathbf{A}^*)$ and $\mathbf{N} = 1/2(\mathbf{A} - \mathbf{A}^*)$.

Without Deflation **[S, SISC, 2024]**

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \frac{1}{1 + \rho(\mathbf{M}^{-1}\mathbf{N})^2} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}$$

- Scalable preconditioner for Hermitian part ⇒ Scalable preconditioner for **A**.
- h independence possible for convection-diffusion.

Deflate $\mathbf{z}^{(j)}$ associated to $|\lambda_j| > \tau$ in $\mathbf{N}\mathbf{z}^{(j)} = \lambda_j \mathbf{M}\mathbf{z}^{(j)}$ [S, Szyld, To appear in SIMAX, 2024]

$$\frac{\|\mathbf{r}_{i+1}\|_{\mathbf{H}}^2}{\|\mathbf{r}_i\|_{\mathbf{H}}^2} \leqslant 1 - \frac{1}{(1 + \tau^2)} \times \frac{\lambda_{\min}(\mathbf{HM})}{\lambda_{\max}(\mathbf{HM})}.$$