

Preconditioning with guaranteed bounds to every eigenvalue of the resulting matrix



Ivana Pultarová¹, Liya Gaynutdinova¹, Martin Ladecký², Jan Zeman¹

¹Faculty of Civil Engineering, CTU in Prague

²Laboratory for Simulation, University of Freiburg

Student's mathematical seminar - FJFI CVUT, March 20, 2024

Outline

- 1 Preconditioning
- 2 Paper from 2009 and new preconditioner
- 3 Applications
 - FEM-heat
 - FEM-elast
 - SGFEM
 - FDM
 - DG
- 4 Convergence
- 5 Conclusion
- 6 Question

Ingredients:

Linear algebra

Courant-Fischer min-max principle

Finite element method (FEM)

Finite difference method (FDM)

Preconditioning

Numerical solution of partial differential equations (PDEs), e.g. $\nabla \cdot a \nabla u = f$, by finite element method (FEM), finite difference method (FDM), ... leads to

$$Ax = b.$$

Matrix A

- symmetric and positive definite
- sparse
- high condition number!! (ill-conditioned problems)

Condition number $\kappa(A)$

$$\kappa(A) \approx \frac{\text{relative error of } x}{\text{relative error of } A}$$

definition

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| \quad \dots \quad \text{for 2-norm } \kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$$

Numerical methods often converge slowly for high $\kappa(A)$!!

Preconditioning

We can consider P "very similar" to A and solve

$$P^{-\frac{1}{2}} A P^{-\frac{1}{2}} y = P^{-\frac{1}{2}} b, \quad x = P^{-\frac{1}{2}} y.$$

In the conjugate gradient (CG) method ... one additional mult. $P^{-1} A x^{(k)}$

Getting P :

- diagonal scaling $P = D = \text{diag}(A) \approx A$
- incomplete Choleski decomposition $P = LL^T \approx A$
- multigrid and multilevel methods, ...
- for special settings ... more powerful special preconditioners:
e.g. rectangular D and periodic boundary conditions,
then P^{-1} easily obtained via FFT !!

Piece of history

2009 [Nielsen, Tveito, Hackbusch](#), Preconditioning by inverting the Laplacian; an analysis of the eigenvalues:

If a continuous, for all $x \in D$, $\lambda = a(x)$ there is a nontrivial u that

$$\nabla \cdot a \nabla u = \lambda \Delta u.$$

2019 [Gergelits, Nielsen, Strakoš](#), Laplacian preconditioning of elliptic PDEs: Localization of the eigenvalues of the discretized operator

All eigenvalues of $P^{-1}A$ contained in intervals of values of a on supports of FE basis functions.

$\implies$ bounds to every eigenvalue of the preconditioned matrix $P^{-1}A$!!

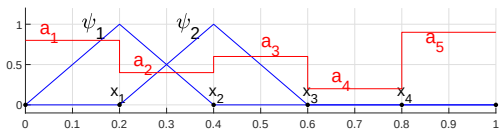
[[Gergelits, Nielsen, Strakoš](#), 2020, 2022, [Nielsen, Strakoš](#), 2024.]

Our approach is different than that of Gergelits and Strakoš:

Example. Let us solve $-(au')' = f$ on $D = (0,1)$ with $u(0) = 0$ and $u(1) = 0$ and use $-u''$ as preconditioner.

Discretization by FEM, ψ_i , $i = 1, \dots, 4$.

Let a be piecewise constant.



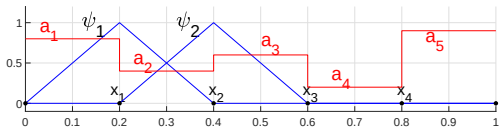
Stiffness matrix $A_{ij} = \int_D a \psi_j' \psi_i' dx$

Integrating element by element: $A = \sum_{j=1}^5 A^{(j)}$:

$$A^{(1)} = \frac{a_1}{h} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A^{(2)} = \frac{a_2}{h} \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \text{ etc.}$$

Preconditioning matrix $P = \sum_{j=1}^5 P^{(j)}$: $P^{(j)}$ the same as $A^{(j)}$ with $a_j = 1$.

Example (cont.)



$0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_4$ generalized eigenvalues of $Au = \lambda Pu$ or $P^{-1}Au = \lambda u$

$$\lambda_1 = \min_v \frac{v^T A v}{v^T P v} = \min_v \frac{\sum_{j=1}^5 v^T A^{(j)} v}{\sum_{j=1}^5 v^T P^{(j)} v} \geq \min_{j=1, \dots, 5} \frac{a_j}{1} = a_4 =: \lambda_1^L$$

$$\lambda_2 = (\text{Courant-Fischer}) = \max_{\dim V=1, v \perp V} \min_v \frac{v^T A v}{v^T P v} \geq \min_{v_3=0} \frac{v^T A v}{v^T P v} \geq \min_{j=1, \dots, 5} a_j = a_4 =: \lambda_2^L$$

$$\lambda_3 = (\text{C.-F.}) = \max_{\dim V=2, v \perp V} \min_v \frac{v^T A v}{v^T P v} \geq \min_{v_3=0, v_4=0} \frac{v^T A v}{v^T P v} \geq \min_{j=1, 2, 3, 5} a_j = a_2 =: \lambda_3^L$$

etc. ...

$\Rightarrow$ lower bounds λ_j^L to all λ 's of $P^{-1}A$.

Similarly, upper bounds λ_j^U to all λ 's of $P^{-1}A$

$$\lambda_j^U = a_3, a_3, a_1, a_5$$

$$\lambda_1, \lambda_2, \lambda_3, \lambda_4$$

$$\lambda_j^L = a_4, a_4, a_2, a_2$$

Our approach: Elliptic PDE

$$-\nabla \cdot (a \nabla u) = f, \quad x \in D,$$

with some b.c.; weak form

$$\int_D a \nabla u \cdot \nabla v \, dx = \int_D f v \, dx,$$

discretized

$$A u = b.$$

Preconditioner

$$-\nabla \cdot (a^p \nabla u), \quad x \in D,$$

with constant a^p , discretized

$$P.$$

Solve *preconditioned problem* $P^{-1} A u = P^{-1} b$ or $P^{-\frac{1}{2}} A P^{-\frac{1}{2}} y = P^{-\frac{1}{2}} b$.

We get

- bounds to *all individual eigenvalues* $0 < \lambda_1 \leq \dots \leq \lambda_N$ of $P^{-1} A$
- fast convergence !!

Useful, if:

- P efficiently solvable (e.g. by fast discrete Fourier transform)
- used multiple times for many A 's

Example of PDE in 2D

$$-\nabla \cdot (a \nabla u) = f$$

FEM (Lagrange)

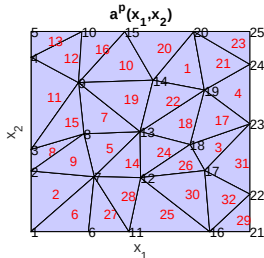
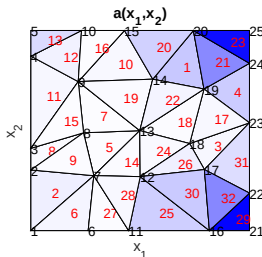
triangulation

$$D = \bigcup_{n=1}^{N_e} D_n$$

N_e elements

N DOFs

data of A and $P \rightarrow$



A and P built from **local matrices**:

$$A = \sum_{n=1}^{N_e} A^{(n)} \left(= \sum_{n=1}^{N_e} \frac{a_n}{a_n^p} P^{(n)} \right), \quad P = \sum_{n=1}^{N_e} P^{(n)},$$

$$A_{ij}^{(n)} = \int_{D_n} a \nabla \phi_j \cdot \nabla \phi_i \, dx, \quad P_{ij}^{(n)} = \int_{D_n} a^p \nabla \phi_j \cdot \nabla \phi_i \, dx.$$

Important: $A^{(n)}$ and $P^{(n)}$ have the same kernels, $n = 1, \dots, N_e$.

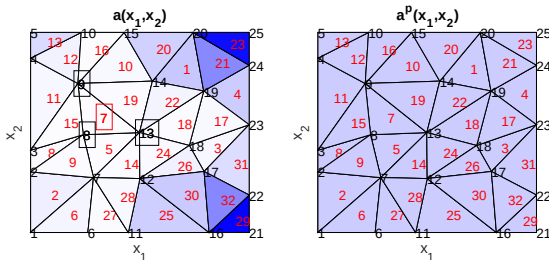
Eigenvalues $0 < \lambda_1 \leq \dots \leq \lambda_N$ of $P^{-1}A$.

Bounds $\lambda_k^L \leq \lambda_k \leq \lambda_k^U$, $k = 1, \dots, N$.

Lower bounds:

$$\boxed{\lambda_1} = \min_v \frac{v^T A v}{v^T P v} = \min_v \frac{\sum v^T A^{(n)} v}{\sum v^T P^{(n)} v} \geq \max \left\{ \lambda; v^T A^{(n)} v \geq \lambda v^T P^{(n)} v, \forall v, n \right\} =: \boxed{\lambda_1^L}$$

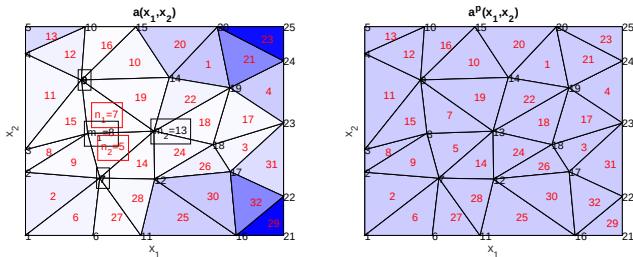
Get $n_1 = 7$ where the max is achieved and choose $m_1 = 8$ (DOF) attached to D_{n_1} .



$$\boxed{\lambda_2} = \max_{\dim V=1} \min_{v, v \perp V} \frac{v^T A v}{v^T P v} \geq \min_{v, v_{m_1}=0} \frac{\sum v^T A^{(n)} v}{\sum v^T P^{(n)} v} \geq \max \left\{ \lambda; v^T A^{(n)} v \geq \lambda v^T P^{(n)} v, \forall n, v, v_{m_1}=0 \right\} =: \boxed{\lambda_2^L}$$

Get $n_2 = 5$ where the max is achieved and choose $m_2 = 13$ (DOF) attached to D_{n_2} .

... we have λ_1^L and λ_2^L , and m_1 and m_2 DOFs excluded:



$$\boxed{\lambda_3} = \max_{\dim V=2} \min_{v, v \perp V} \frac{v^T A v}{v^T P v} \geq \min_{v \neq 0, v_{m_1}=0, v_{m_2}=0} \frac{\sum v^T A^{(n)} v}{\sum v^T P^{(n)} v} \geq \max \left\{ \lambda; v^T A^{(n)} v \geq \lambda v^T P^{(n)} v, \forall n, v, v_{m_1}=0, v_{m_2}=0 \right\} =: \boxed{\lambda_3^L}$$

Get n_3 where the max is achieved and choose m_3 (DOF) attached to D_{n_3} .

... etc.

$$\text{Finally, } \boxed{\lambda_k^L} \leq \lambda_k \leq \boxed{\lambda_k^U}, \quad k = 1, \dots, N.$$

Efficient algorithm for FEM: find minima (and maxima) of $(a^P)^{-1}a$ on supports of all basis functions, and sort the sequence, and get λ_k^L (and λ_k^U).

Theorem. Let $A^{(n)}$ and $P^{(n)}$ have the same kernels and be positive semi-definite, $n = 1, \dots, N_e$, and

$$A = \sum_{n=1}^{N_e} A^{(n)}, \quad P = \sum_{n=1}^{N_e} P^{(n)}.$$

Let for $k = 1, \dots, N$,

$$\lambda_k^L = \max \left\{ \lambda; v^T A^{(n)} v \geq \lambda v^T P^{(n)} v, n = 1, \dots, N_e, v \in \mathbb{R}^N, v_j = 0 \text{ for all } j \in T_{k-1}^L \right\} \quad (1)$$

where $T_0^L = \emptyset$ and $T_k^L = T_{k-1}^L \cup \{m_k\}$, $k = 0, 1, \dots, N-1$,

where m_k is a single (arbitrary) integer such that the maximum in (1) is achieved for $n = n_k$ and

$$m_k \in S_{n_k} \setminus T_{k-1}^L,$$

where S_n is the set of DOFs non-zero in A_n .

(Analogously for the upper bounds λ_k^U .)

Then

$$\lambda_k^L \leq \lambda_k \leq \lambda_k^U, \quad k = 1, \dots, N,$$

where λ_k are increasingly ordered eigenvalues of $P^{-1}A$.

FEM - heat equation

The second order elliptic differential equation

$$-\nabla \cdot (\mathbf{a}(\mathbf{x}) \nabla u(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x} \in D,$$

defined on $D = (0,1) \times (0,1)$ with Dirichlet and Robin b.c. and with

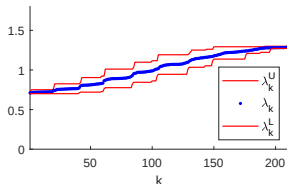
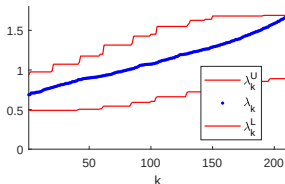
$$\mathbf{a}(\mathbf{x}) = \left(1 + 0.3 \cos\left((x_1 + x_2) \frac{\pi}{2}\right)\right) \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix},$$

preconditioned by the operator with

$$\mathbf{a}^{p1}(\mathbf{x}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{or} \quad \mathbf{a}^{p2}(\mathbf{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}.$$

$N_e = 450$, $N = 210$.

Eigenvalues of $P^{-1}A$ and their bounds for precondition. data $\mathbf{a}^{p1}$ and $\mathbf{a}^{p2}$:



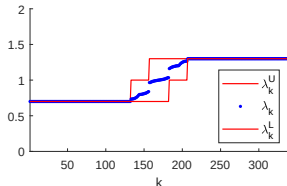
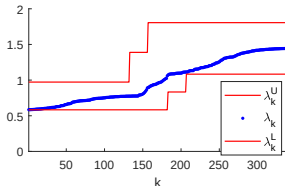
FEM - linear elasticity equation

$$\int_D \partial \mathbf{v}^T \mathbf{C} \partial \mathbf{u} \, dx = \int_D \mathbf{v}^T \mathbf{F} \, dx, \quad \partial \mathbf{v}^T = \begin{pmatrix} \frac{\partial v_1}{\partial x_1} & 0 & \frac{\partial v_1}{\partial x_2} \\ 0 & \frac{\partial v_2}{\partial x_2} & \frac{\partial v_2}{\partial x_1} \end{pmatrix}$$

$$\mathbf{C} = (1 + 0.3 \operatorname{sign}(x_1 + x_2 - 1)) \begin{pmatrix} 0.8 & 0.2 & 0 \\ 0.2 & 0.8 & 0 \\ 0 & 0 & 0.3 \end{pmatrix}.$$

Preconditioning matrix with

$$\mathbf{C}^{p1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0.5 \end{pmatrix} \quad \text{or} \quad \mathbf{C}^{p2} = \begin{pmatrix} 0.8 & 0.2 & 0 \\ 0.2 & 0.8 & 0 \\ 0 & 0 & 0.3 \end{pmatrix}$$

Eigenvalues of $P^{-1}A$ and their bounds for precondition. data $\mathbf{C}^{p1}$ and $\mathbf{C}^{p2}$:

SGFEM - stochastic (spectral) Galerkin finite element method

$$-\nabla \cdot ((a_0(x) + \xi a_1(x)) \nabla u(x, \xi)) = f(x),$$

where $x \in D = (0, 1)$, Gaussian r.v. ξ , Dirichlet b.c for all $\xi \in \Omega$,

$$a_0(x) = 4 + \text{sign}(x - 0.3), \quad a_1(x) = 0.2.$$

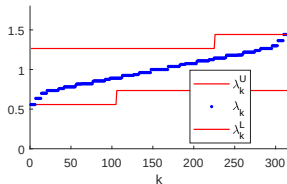
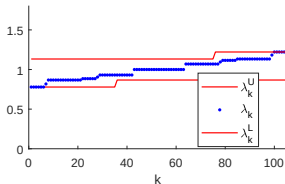
$N^{\text{fe}} = 21$, and either $N^{\text{pol}} = 5$, or $N^{\text{pol}} = 15$.

Then either $N = 105$ or $N = 315$. Then

$$A = A_{(0)} + A_{(1)}, \quad P = A_{(0)}.$$

(Condition number $\kappa \leq \lambda_N^U / \lambda_1^L$.)

Eigenvalues of $P^{-1}A$ and their bounds for $N^{\text{pol}} = 5$ and $N^{\text{pol}} = 15$:



FDM - finite difference method

Finite difference scheme in 2D

$$\frac{\partial}{\partial x_1} \left(c \frac{\partial u}{\partial x_1} \right) (x_{ij}) \approx \frac{(c_{i-1,j} + c_{ij})u_{i-1,j} - (c_{i-1,j} + 2c_{ij} + c_{i+1,j})u_{i,j} + (c_{ij} + c_{i+1,j})u_{i+1,j}}{2h_1^2}$$

$$\frac{\partial}{\partial x_2} \left(c \frac{\partial u}{\partial x_2} \right) (x_{ij}) \approx \frac{(c_{i,j-1} + c_{ij})u_{i,j-1} - (c_{i,j-1} + 2c_{ij} + c_{i,j+1})u_{i,j} + (c_{ij} + c_{i,j+1})u_{i,j+1}}{2h_2^2}$$

mixed derivatives for varying coefficients

$$\begin{aligned} & \left(\frac{\partial}{\partial x_1} \left(c \frac{\partial u}{\partial x_2} \right) + \frac{\partial}{\partial x_2} \left(c \frac{\partial u}{\partial x_1} \right) \right) (x_{ij}) \\ & \approx \frac{1}{4h_1h_2} ((u_{i-1,j-1}(c_{ij} + c_{i-1,j-1}) + u_{i+1,j+1}(c_{ij} + c_{i+1,j+1}) \\ & - u_{i-1,j+1}(c_{ij} + c_{i-1,j+1}) - u_{i+1,j-1}(c_{ij} + c_{i+1,j-1}) \\ & + u_{ij}(c_{i-1,j+1} + c_{i+1,j-1} - c_{i+1,j+1} - c_{i-1,j-1})) \end{aligned}$$

orthogonal and uniform grid

symmetric matrices A and P

matrices A and P obtained from local matrices $A^{(n)}$ and $P^{(n)}$ (2×2 nodes)

Example for **FDM**:

$$-\nabla \cdot (\mathbf{a}(\mathbf{x}) \nabla u(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x} \in D,$$

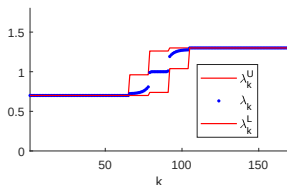
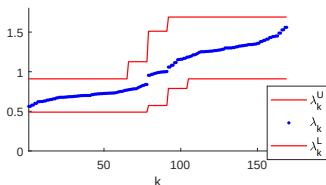
$$\mathbf{a}(\mathbf{x}) = (1 + 0.3 \operatorname{sign}(x_2 - 0.5)) \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix},$$

and two preconditioners with

$$\mathbf{a}^{p1}(\mathbf{x}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{or} \quad \mathbf{a}^{p2}(\mathbf{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}.$$

$$N_e = 196, \quad N = 169.$$

Eigenvalues of $P^{-1}A$ and their bounds for precondition. data $\mathbf{a}^{p1}$ and $\mathbf{a}^{p2}$:



DG - discontinuous Galerkin method

$$-\nabla \cdot (a(x) \nabla u(x)) + c(x) u(x) = f(x), \quad x \in D, \quad u(x) = 0, \quad x \in \partial D,$$

discretization by DG, penalty constant σ , stiffness matrix A

$$\begin{aligned} (A_k)_{ij} = & \frac{1}{3} \int_{\tau_r \cup \tau_s} a \nabla \varphi_j \cdot \nabla \varphi_i \, dx + \frac{1}{3} \int_{\tau_r \cup \tau_s} c \varphi_j \varphi_i \, dx \\ & - \int_{\varepsilon_k} \{ \{ a \nabla \varphi_i \} \} [\![\varphi_j]\!] + \{ \{ a \nabla \varphi_j \} \} [\![\varphi_i]\!] \, ds + \int_{\varepsilon_k} \sigma [\![\varphi_j]\!] [\![\varphi_i]\!] \, ds \end{aligned}$$

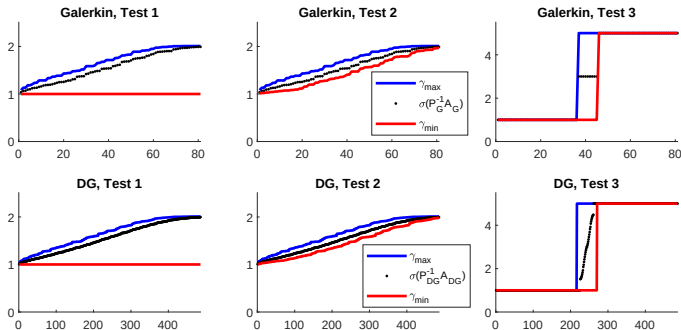
preconditioning matrix P

$$\begin{aligned} (P_k)_{ij} = & \frac{1}{3} \int_{\tau_r \cup \tau_s} a^p \nabla \varphi_j \cdot \nabla \varphi_i \, dx + \frac{1}{3} \int_{\tau_r \cup \tau_s} c^p \varphi_j \varphi_i \, dx \\ & - \int_{\varepsilon_k} \{ \{ a^p \nabla \varphi_i \} \} [\![\varphi_j]\!] + \{ \{ a^p \nabla \varphi_j \} \} [\![\varphi_i]\!] \, ds + \int_{\varepsilon_k} \sigma^p [\![\varphi_j]\!] [\![\varphi_i]\!] \, ds \end{aligned}$$

$$-\nabla \cdot (a(x) \nabla u(x)) + c(x)u(x) = f(x)$$

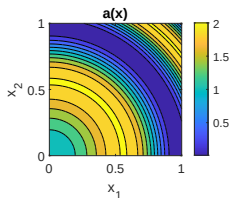
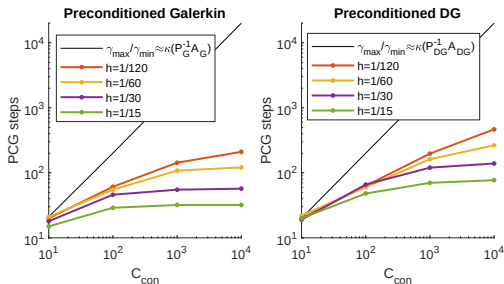
	a	a^P	c	c^P
Test 1	$(1 + \sin(x_1 x_2 \pi)) \operatorname{diag}(3, 1) + \frac{1}{10} I$	$\operatorname{diag}(3, 1)$	1	1
Test 2	$(1 + \sin(x_1 x_2 \pi)) \operatorname{diag}(3, 1) + \frac{1}{10} I$	$\operatorname{diag}(3, 1)$	0	0
Test 3	$I \ (x_1 < 0.5), \ 5I \ (x_1 \geq 0.5)$	I	0	0

Eigenvalues of $P^{-1}A$ and their bounds for precond. data a^P :



Convergence of CG for (preconditioned) DG:

growing contrast of $a(x)$... growing $\kappa(P^{-1}A)$
 ... but number of CG steps stagnates



New pre-
conditioning

Pre-
conditioning

Paper
from
2009
and new
precon-
ditioner

Applications

FEM-
heat

FEM-
elast

SGFEM

FDM

DG

Convergence

Conclusion

Question

Paper

Ladecký, Leute, Falsafi, Pultarová, Pastewka, Junge, Zeman, An optimal preconditioned FFT-accelerated finite element solver for homogenization, Applied Mathematics and Computation, 2023

Conclusion

- Very good (optimal) preconditioner if we can invert P e.g. by FFT.
- Guaranteed two-sided bounds to all eigenvalues of $P^{-1}A$.
- A and P must be built from local matrices.
- Local matrices $A^{(j)}$ and $P^{(j)}$ must share their kernels.
- Condition number upper bounds.

References

- Ladecký, Pultarová, Zeman, Guaranteed two-sided bounds on all eigenvalues of preconditioned diffusion and elasticity problems solved by the finite element method, 2020
- Pultarová, Ladecký, Two-sided guaranteed bounds to individual eigenvalues of preconditioned finite element and finite difference problems, 2022
- Ladecký, Leute, Falsafi, Pultarová, Pastewka, Junge, Zeman, An Optimal Preconditioned FFT-accelerated Finite Element Solver for Homogenization, 2023
- Gaynutdinova, Ladecký, Pultarová, Vlasák, Zeman, Preconditioned discontinuous Galerkin method and convection-diffusion-reaction problems with guaranteed bounds to resulting spectra, 2024

Martin's question

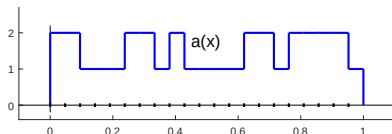
Let $D = (0, 1) = \cup_{j=1}^N I_j$, A and P obtained by FEM with piecewise linear basis functions:

$$Au \approx -(au')' \quad \text{and} \quad Pu \approx -u'',$$

and

$$a(x) = \begin{cases} 1 & x \in \cup_{j \in J} I_j \\ 2 & x \in D \setminus \cup_{j \in J} I_j \end{cases} \quad \begin{matrix} |J| = N_1 \\ N - |J| = N_2 \end{matrix}$$

and periodic b.c.



Question:

How many **1's**, **2's** and **other numbers** are in the spectrum of $P^{-1}A$?

More questions:

- More levels of "steps"
- 2D problems
- non-symmetric problems

...