

Deflation-based Preconditioning for Immersed Finite Element Methods

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Content

1. Industrial mathematics
2. Immersed Finite Elements
3. Robust solvers
4. Numerical experiments
5. Conclusions
6. References

Stefan problem

Problem: moving boundary problems

Industry: Philips, wet chemical etching of IC

C. Vuik and C. Cuvelier

Numerical solution of an etching problem

J. Comp. Physics, 59, pp. 247-263, 1985

C. Vuik

An L2-error estimate for an approximation of the solution of a parabolic variational inequality

Numer. Math., 57, pp. 453-471, 1990

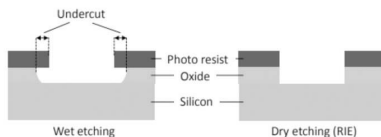


Figure: Etching

Dissolution of particles in multi-component alloys

Industry: Tata Steel Paper: A level set method for three dimensional vector Stefan problems:
Dissolution of stoichiometric particles in multi-component alloys
E. Javierre and C. Vuik and F.J. Vermolen and A. Segal
Journal of Computational Physics, 224, pp. 222-240, 2007

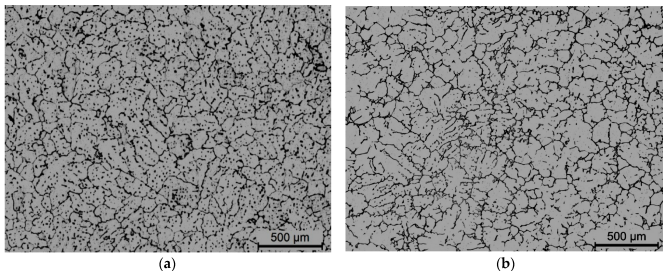


Figure: Particles

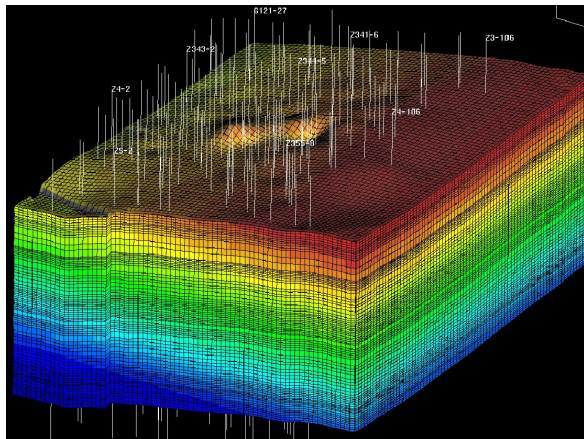
Flow in porous media

Industry: Shell

Paper: The construction of projection vectors for a Deflated ICCG method applied to problems with extreme contrasts in the coefficients

C. Vuik and A. Segal and J.A. Meijerink and G.T. Wijma

Journal of Computational Physics, 172, pp. 426–450, 2001



Figure

Wave problems

Industry: Shell: seismic, Philips: blue-ray disk, Hospitals: medical images

Papers:

A Novel Multigrid Based Preconditioner For Heterogeneous Helmholtz Problems

Y.A. Erlangga and C.W. Oosterlee and C. Vuik

SIAM J. Sci. Comput., 27, pp. 1471-1492, 2006

Scalable multi-level deflation preconditioning for highly indefinite time-harmonic waves

V. Dwarka and C. Vuik

Journal of Computational Physics, 469, 111327, 2022

Setting

Solve a large sparse linear system

$$A\mathbf{x} = \mathbf{b}$$

$A \in \mathbb{R}^{n \times n}$ is symmetric positive definite (SPD) and stems from a FEM discretization. Typical examples:

1. $A = K$ (Poisson problem, elliptic PDEs,...)
2. $A = M$ (L^2 projection, explicit time-stepping,...)
3. $A = K + \gamma M$ with $\gamma > 0$ (Implicit time-stepping)

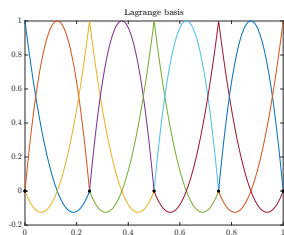
$$K_{ij} = \int_{\Omega} \nabla \varphi_i \cdot \nabla \varphi_j \quad (\text{Stiffness matrix}) \quad M_{ij} = \int_{\Omega} \varphi_i \varphi_j \quad (\text{Mass matrix})$$

for a finite element basis $\Phi = \{\varphi_1, \dots, \varphi_n\}$.

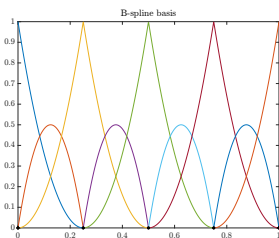
Finite element bases

The basis Φ may be:

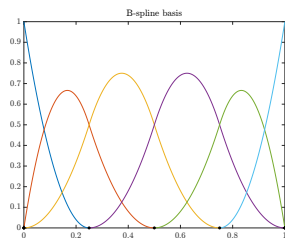
- $\Phi = \{L_1, \dots, L_n\}$, the Lagrange basis (standard FEM)
- $\Phi = \{B_1, \dots, B_n\}$, a spline basis, e.g. the B-spline basis (Isogeometric analysis). Spline spaces are C^k continuous with $0 \leq k \leq p - 1$.



(a) Lagrange basis



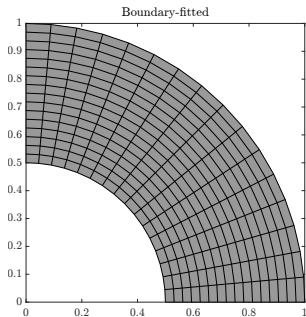
(b) C^0 B-spline basis



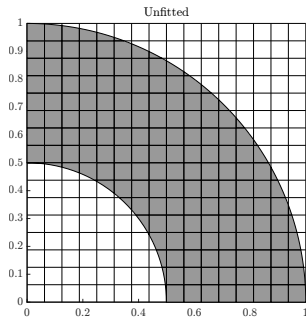
(c) C^1 B-spline basis

Boundary-fitted vs immersed finite element discretizations

How to solve a PDE on a complicated domain Ω ? How can we build a finite element mesh?



- + Imposition of boundary conditions
- + Availability of h, p -robust preconditioners
- Mesh quality
- Flexibility, complexity



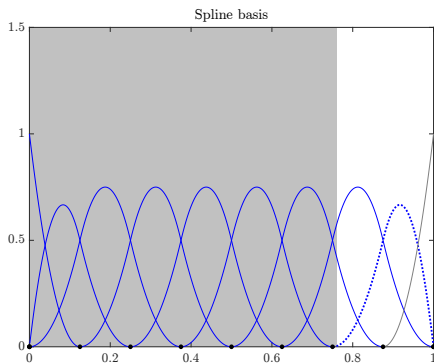
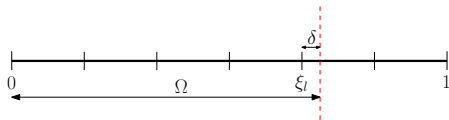
- + Flexibility
- Imposition of boundary conditions
- Integration on trimmed elements
- Stability, CFL condition
- Ill-conditioning

Source of ill-conditioning

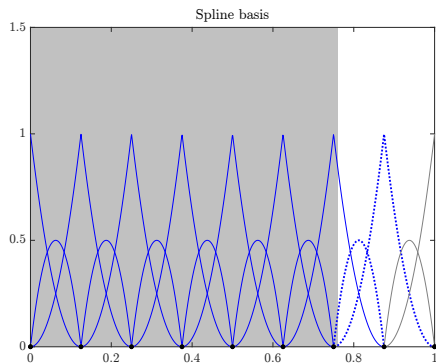
Small cut elements cause extreme ill-conditioning; i.e. there exists a function $u \in V_h$ such that

$$\|u\|_a^2 = a(u, u) \lesssim \epsilon \|u\|_2^2 \implies \lambda_{\min}(A) \lesssim \epsilon.$$

Example: consider a quadratic spline discretization on $(0, 1) \supset (0, 0.75 + \epsilon)$



(a) C^1 smoothness



(b) C^0 smoothness

Non-preconditioned case

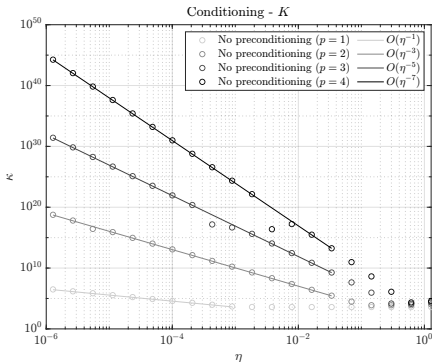
The problem is caused by basis functions whose active support $\text{supp}_\Omega(\varphi) = \text{supp}(\varphi_i) \cap \Omega$ only contains trimmed elements.

Under some shape regularity assumption, we can prove that (de Prenter et al. 2017)

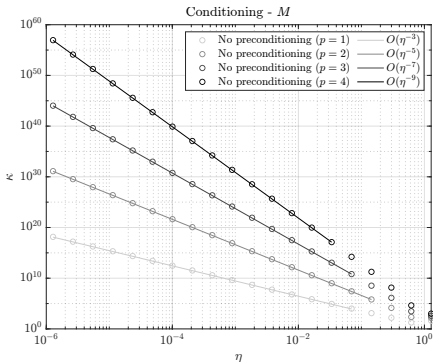
$$\kappa(K) \gtrsim \eta^{-(2p+1-2/d)}$$

$$\kappa(M) \gtrsim \eta^{-(2p+1)}$$

where $\eta = \min_{T \in \mathcal{T}_h} |T \cap \Omega|/|T|$ and $\kappa(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$ is the spectral condition number (for an SPD matrix A).



(a) $\kappa(K)$



(b) $\kappa(M)$

Overview of solutions

Multiple solutions to the ill-conditioning issue

- Fictitious domain stabilization (or α -stabilization, finite cell method) (Parvizian et al. 2007) integrates the weak form over the entire extended domain by weighting the fictitious part by a small parameter α .
 - + Improves the conditioning
 - to the detriment of accuracy...
- Polynomial extension techniques; e.g. extended B-splines (Höllig 2003; Marussig et al. 2017; Buffa et al. 2020)
 - + Solves the conditioning and stability issues
 - Quite intrusive (modifies the approximation space)
- Eigenvalue stabilization (Eisenräger et al. 2024). Local modifications to the element matrices during assembly.
 - + Solves the conditioning issue
 - Quite intrusive.
 - Parameter-dependent. Bad choices may affect the accuracy.
- Preconditioning (de Prenter et al. 2017; de Prenter et al. 2019). Chooses a different basis for the approximation space.
 - + Operates on the solver, not the approximation space.
 - Does not resolve stability issues.

Jacobi preconditioning

- In some cases, a Jacobi preconditioner is enough! Solve $\hat{A}\hat{\mathbf{x}} = \hat{\mathbf{b}}$, where

$$\hat{A} = D^{-1}AD^{-1}, \quad \hat{\mathbf{x}} = D\mathbf{x}, \quad \text{and} \quad \hat{\mathbf{b}} = D^{-1}\mathbf{b}$$

for $D = \sqrt{\text{diag}(A)}$.

- In most cases, Jacobi preconditioning helps but is insufficient... The issue stems from near linear dependencies among rescaled basis functions.

Counter-example for the Lagrange basis in 1D

Define

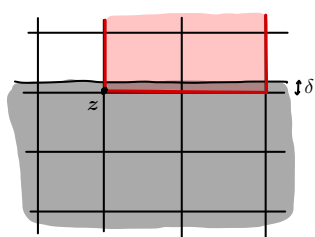
$$u(\xi) = \begin{cases} (\xi - \xi_l)^p & \text{if } \xi \in \Omega_\ell, \\ 0 & \text{otherwise.} \end{cases}$$

One can easily show that $u \in V_h$ and

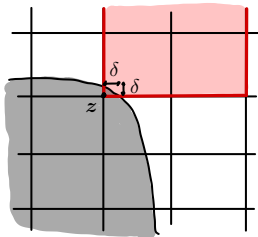
$$\lambda_{\min}(\hat{A}) = \min_{\substack{\hat{\mathbf{v}} \in \mathbb{R}^n \\ \hat{\mathbf{v}} \neq 0}} \frac{\hat{\mathbf{v}}^T \hat{A} \hat{\mathbf{v}}}{\|\hat{\mathbf{v}}\|_2^2} \leq \frac{\hat{\mathbf{u}}^T \hat{A} \hat{\mathbf{u}}}{\|\hat{\mathbf{u}}\|_2^2} = \frac{\|u\|_a^2}{\|\hat{\mathbf{u}}\|_2^2} \sim \eta^{2(p-1)} \implies \kappa(\hat{A}) \gtrsim \eta^{-2(p-1)}.$$

Extension

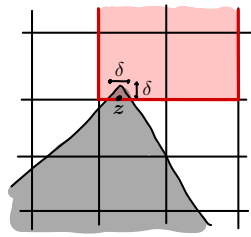
The analysis in 2D is much more complicated and depends on the basis, continuity, position of the knots or interpolation points and cut configuration. Three representative cases:



Configuration (a)



Configuration (b)



Configuration (c)

Cut configuration	Lagrange basis	B-spline basis
1D	$\gtrsim \eta^{-2(p-1)}$	~ 1
2D - (a) ("sliver cut")	$\gtrsim \eta^{-2(p-1)}$	~ 1
2D - (b) ("corner cut")	$\gtrsim \eta^{-2(p-1)}$	~ 1
2D - (c) ("middle cut")	$\begin{cases} \gtrsim \eta^{-(2p-1)} & \text{if } z_1 \notin \mathcal{B}_{\xi_{1,i}}(\delta) \\ \gtrsim \eta^{-2(p-1)} & \text{if } z_1 \in \mathcal{B}_{\xi_{1,i}}(\delta) \end{cases}$	$\begin{cases} \gtrsim \eta^{-p} & \text{if } z_1 \notin \mathcal{B}_{\xi_{l_1}}(\delta) \\ \gtrsim \eta^{-k} & \text{if } z_1 \in \mathcal{B}_{\xi_{l_1}}(\delta) \end{cases}$

State-of-the-art (I)

- de Prenter et al. 2017 proposed the Symmetric Incomplete Permuted Inverse Cholesky (SIPIC), constructed as follows:
 1. Initial Jacobi preconditioning
 2. Detect near linear dependencies by looking for the off-diagonal elements of \hat{A} of magnitude ≈ 1
 3. Locally orthogonalize the functions identified
 4. Update the preconditioner and repeat the process until all off-diagonal elements are small enough (in magnitude).
- The detection procedure of SIPIC is sometimes insufficient for detecting near linear dependencies. Counter-example: the matrix

$$\begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 \end{pmatrix}$$

is singular but does not have any off-diagonal entry close to 1 ($1/\sqrt{2} \approx 0.707$).

State-of-the-art (II)

- Two years later, [de Prenter et al. 2019](#) suggested an additive Schwarz-type preconditioner by forming the approximate inverse preconditioner

$$S = \sum_{i=1}^N P_i (P_i^T A P_i)^{-1} P_i^T,$$

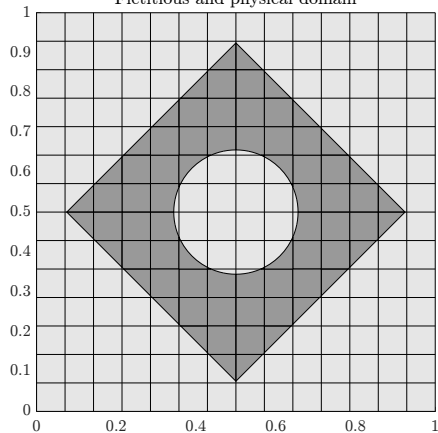
where $P_i = [e_{\mathcal{K}_i(1)}, \dots, e_{\mathcal{K}_i(m)}]$ contains the columns of the identity matrix for an index block \mathcal{K}_i selected based on the geometry.

- The quality of the preconditioner critically depends on the choice of index blocks and none of the strategies proposed in the literature are entirely robust.

Counter-example

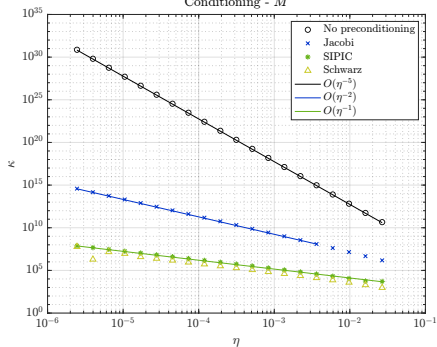
Geometry from de Prenter et al. 2017

Fictitious and physical domain



(a) Geometry

Conditioning - M



(b) Condition number

Deflation - Introduction

- The convergence of iterative methods applied to $A\mathbf{x} = \mathbf{b}$ is plagued by the small eigenvalues. (Dia21JV ; Vuik et al. 1999; Frank and Vuik 2001; Nabben and Vuik 2006)
- Define a projector

$$P = I - AZ(Z^T AZ)^{-1}Z^T$$

for a full-rank matrix $Z \in \mathbb{R}^{n \times r}$ with $r \ll n$ and solve the projected system $PA\tilde{\mathbf{x}} = P\mathbf{b}$ with e.g. Conjugate Gradients (CG).

- Recover the solution of $A\mathbf{x} = \mathbf{b}$ through the transformation

$$\mathbf{x} = Z(Z^T AZ)^{-1}Z^T \mathbf{b} + P^T \tilde{\mathbf{x}}.$$

Lemma

If A is SPD, then

1. $\ker(PA) = R(Z)$
2. PA is symmetric positive semidefinite

We define the *effective condition number* of PA

$$\kappa_{\text{eff}}(PA) = \frac{\lambda_n(PA)}{\lambda_{r+1}(PA)}.$$

Lemma

$$\kappa_{\text{eff}}(PA) \leq \kappa(A).$$

Deflation - Construction

Let $(\lambda_k, \mathbf{v}_k)$ denote the eigenpairs of A .

Lemma

If $Z = [\mathbf{v}_1, \dots, \mathbf{v}_r]$ contains the r smallest eigenvectors of A , then

$$PA\mathbf{v}_k = \begin{cases} 0 & \text{for } k = 1, \dots, r, \\ \lambda_k \mathbf{v}_k & \text{for } k = r + 1, \dots, n. \end{cases}$$

But computing eigenvectors is never practical, especially not in this setting.

How to construct Z ? Recall that $\ker(PA) = R(Z)$. We actually don't need eigenvectors. We only need a basis for the smallest eigenspace.

- Define the set of cut elements

$$\mathcal{T}_C = \{T \in \mathcal{T}_h : |T \cap \Omega| < |T|\}$$

and its complement $\mathcal{T}'_C = \mathcal{T}_h \setminus \mathcal{T}_C$, the set of uncut elements.

- Define the cut and uncut regions of the computational domain

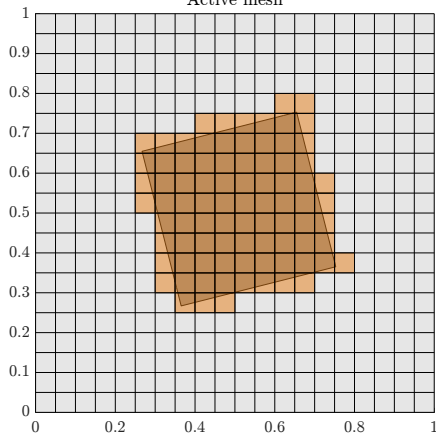
$$\Omega_C = \bigcup_{T \in \mathcal{T}_C} T \quad \text{and} \quad \Omega'_C = \bigcup_{T \in \mathcal{T}'_C} T.$$

- The set of "cut basis functions" is

$$\Phi_C = \{\varphi \in \Phi : \text{supp}_\Omega(\varphi) \subseteq \Omega_C\}.$$

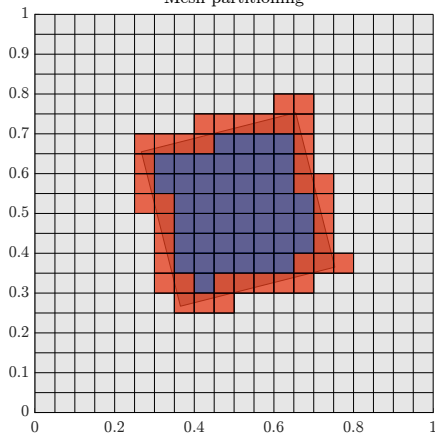
Deflation - Construction

Active mesh



(a) Fictitious domain $\widehat{\Omega}$ (light gray), physical domain Ω (dark gray) and computational domain Ω_h (orange)

Mesh partitioning



(b) Partitioning of the computational domain Ω_h in cut Ω'_C (red) and uncut Ω'_C (blue) regions

For $Z = [e_{i_1}, \dots, e_{i_r}]$ for indices i_k corresponding to functions in Φ_C .

Remarks

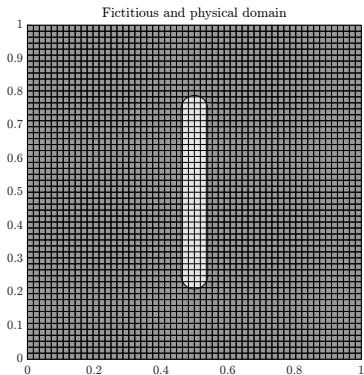
- Deflation is often combined with a standard SPD preconditioner M (e.g. incomplete Cholesky, Jacobi,...). Here we use Jacobi.
- It is sometimes possible to reduce Φ_C to only consider functions that cannot be cured by Jacobi.

Numerical experiment

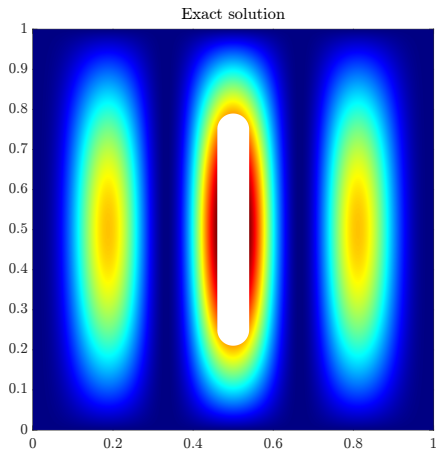
Solve the Poisson problem with the manufactured solution

$$u(x, y) = x(1 - x) \sin(3\pi x)^2 \sin(\pi y)$$

on a plate with a cut-out discretized with quadratic Lagrange polynomials. Solve a sequence of problems by slightly increasing the radius of the cut-out.

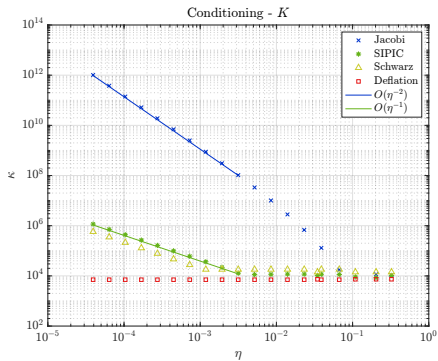


(a) Fictitious domain $\widehat{\Omega}$ (light gray) and physical domain Ω (dark gray)

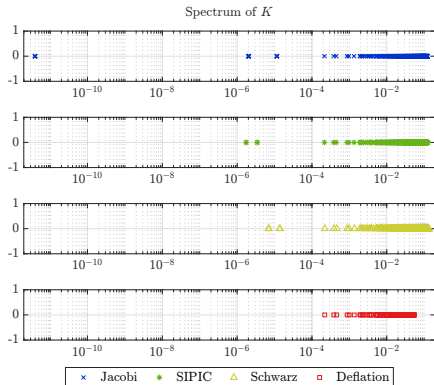


(b) Solution

Conditioning and spectrum



(a) Condition numbers for 20 logarithmically spaced values of ϵ between 10^{-4} and 10^{-2}



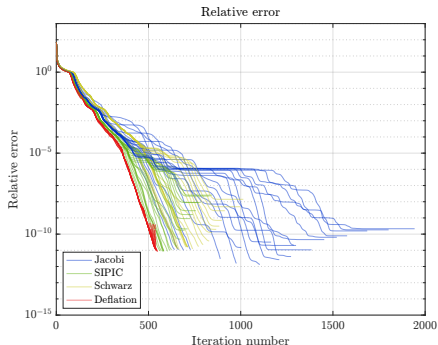
(b) First 500 eigenvalues of the preconditioned spectrum for $\epsilon = 10^{-4}$

Figure: Condition numbers and eigenvalues of the preconditioned systems

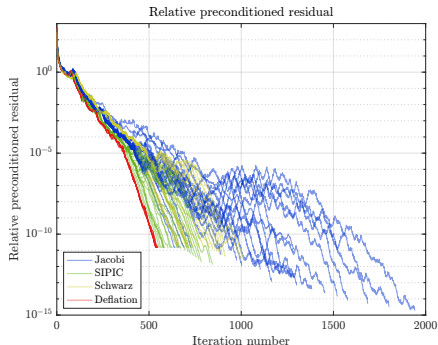
Error and preconditioned residual

$$\frac{\|\mathbf{u} - \mathbf{u}_k\|_A}{\|\mathbf{u}\|_A} = \frac{|u_h - u_{h,k}|_{H^1}}{|u_h|_{H^1}} \quad (\text{Error})$$

$$\frac{\|\mathbf{r}_k\|_{M^{-1}}}{\|\mathbf{b}\|_{M^{-1}}} \quad (\text{Preconditioned residual})$$



(a) Relative error



(b) Relative preconditioned residual

Figure: Convergence of the relative error and preconditioned residuals

Number of iterations

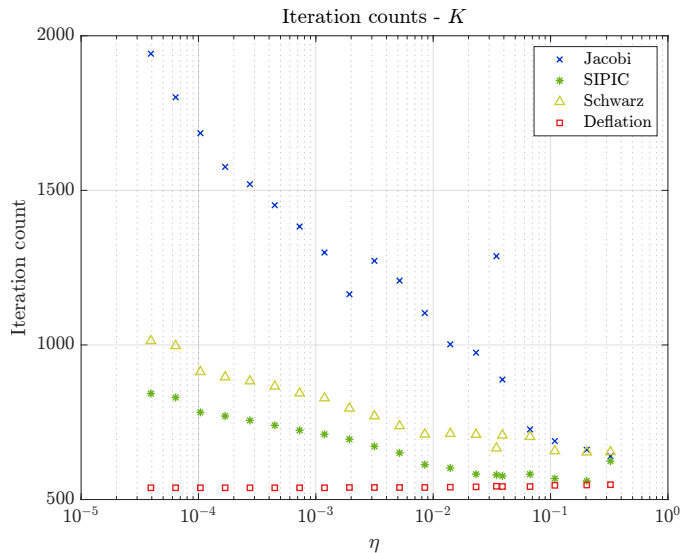


Figure: Number of iterations

Number of iterations

η	Jacobi	SIPIC	Schwarz	Deflation
3.24×10^{-1}	640	624	654	548
2.03×10^{-1}	661	560	653	547
1.09×10^{-1}	689	568	657	546
3.46×10^{-2}	1287	580	666	543
6.69×10^{-2}	727	582	703	542
3.89×10^{-2}	888	576	708	542
2.32×10^{-2}	975	582	710	541
1.40×10^{-2}	1002	602	713	540
8.48×10^{-3}	1103	613	711	539
5.17×10^{-3}	1208	651	738	539
3.16×10^{-3}	1272	672	770	539
1.93×10^{-3}	1164	695	795	539
1.18×10^{-3}	1299	711	828	538
7.30×10^{-4}	1383	724	844	538
4.50×10^{-4}	1452	740	866	538
2.70×10^{-4}	1520	756	883	538
1.70×10^{-4}	1576	770	896	538
1.00×10^{-4}	1685	782	913	538
6.00×10^{-5}	1801	830	997	538
4.00×10^{-5}	1942	843	1013	538

Table: Iteration counts

Conclusion

- + Deflation-based preconditioning perfectly resolves the ill-conditioning caused by badly cut elements.
- But must be combined with other h, p -robust preconditioners.
- Deflation remains a “global” strategy (contrary to Schwarz) and the deflation rank may become quite large for C^0 discretizations.

Paper

Yannis Voet, Matthias Moller, Pablo Antolin, Cornelis Vuik

Deflation-based preconditioning for immersed finite element methods and immersogeometric analysis

<http://arxiv.org/abs/2604.12848>

Future work: extension to indefinite and non-symmetric systems.

Thank you!

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