

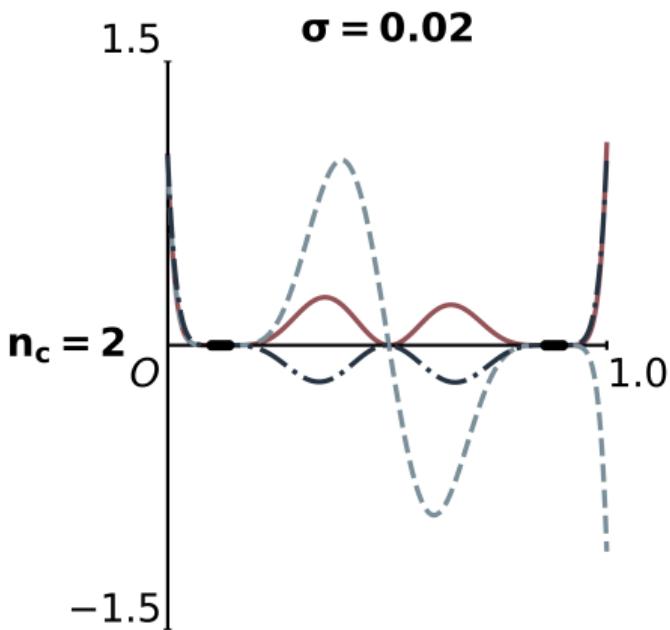
Sharpened CG Iteration Bound for Schwarz-preconditioned High-contrast Heterogeneous Scalar Elliptic PDEs

Going Beyond Condition Number

P. Soliman¹

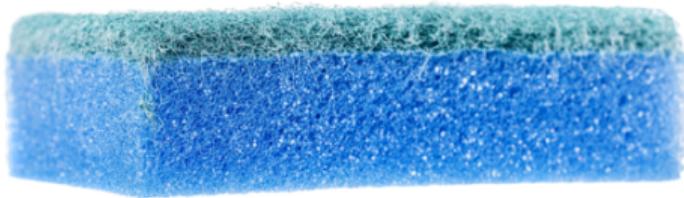
EEMCS-DIAM Numerical Analysis MSc.
Thesis Presentation, April, 2025

¹ Delft University of Technology



Opening

Darcy Problem



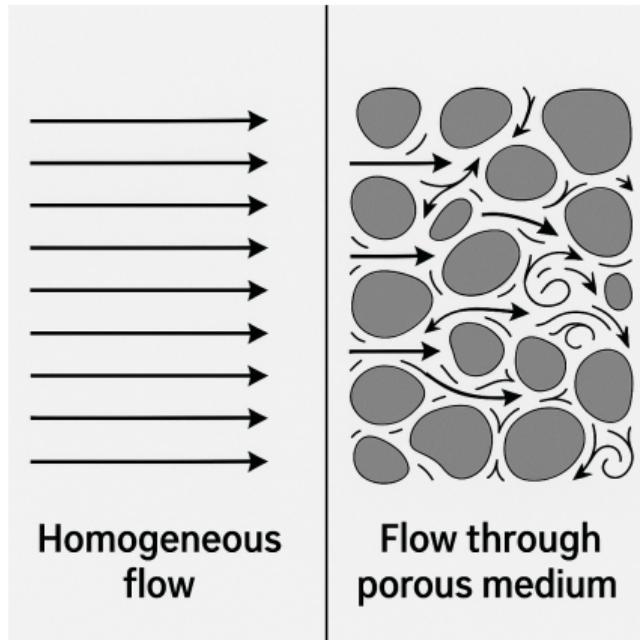
Opening

Darcy Problem



Opening

Darcy Problem



Opening

Darcy Problem

- Simpler case; high-contrast diffusion problem for $u, u_D \in H^1(\Omega)$, $f \in L^2(\Omega)$ and $\mathcal{C} \in L^\infty(\Omega)$

$$\begin{aligned}-\nabla \cdot (\mathcal{C} \nabla u) &= f && \text{in } \Omega \\ u &= u_D && \text{on } \partial\Omega\end{aligned}$$

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- Find $u \in V = \{u \in H^1(\Omega) | u_{\delta\Omega} = u_D\}$

$$a(u, w) = \int_{\Omega} \mathcal{C} \nabla u \cdot \nabla w \, dx = \int_{\Omega} f w \, dx = (f, w) \quad \text{for all } w \in H_0^1(\Omega).$$

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- Introduce some computational mesh \mathcal{T}_h with DOFs \mathcal{N}
- Discretize $V_h \subset V$ and $V_{h,0} = V_h \cap H_0^1(\Omega) = \text{span}\{\phi_k\}_{k \in \mathcal{N}}$

$$A\mathbf{u} = \mathbf{b} \quad A_{ij} = a(\phi_j, \phi_i)_{L^2} \quad b_i = (f, \phi_i) \quad \forall i, j \in \mathcal{N}$$

Structure

- Research Questions
- Background & Literature
- Preliminary Results
- Outlook

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Research Questions

Main Research Question

How can we refine the CG iteration bound for Schwarz-preconditioned high-contrast heterogeneous elliptic problems beyond the classical condition number-based bound?

Research Questions

Subsidiary Research Questions

- Q1** What other spectral characteristics like the condition number can we consider?
- Q2** How to estimate the characteristics from **Q1**?
- Q3** Given a toy eigenspectrum, how can we sharpen the CG iteration bound?
- Q4** How does the sharpened bound from **Q3** compare to the classical CG bound?
- Q5** How does the performance described in **Q4** depend on the characteristics found in **Q1**?
- Q6** Can the sharpened bound from **Q3** distinguish between preconditioners?

Structure

- Research Questions
- **Background & Literature**
- Preliminary Results
- Outlook

Background & Literature

Conjugate gradient method

Algorithm Conjugate Gradient Method¹

$$\mathbf{r}_0 = \mathbf{b} - A\mathbf{u}_0, \mathbf{p}_0 = \mathbf{r}_0, \beta_0 = 0$$

for $j = 0, 1, 2, \dots, m$ **do**

$$\alpha_j = (\mathbf{r}_j, \mathbf{r}_j) / (A\mathbf{p}_j, \mathbf{p}_j)$$

$$\mathbf{u}_{j+1} = \mathbf{u}_j + \alpha_j \mathbf{p}_j$$

$$\mathbf{r}_{j+1} = \mathbf{r}_j - \alpha_j A\mathbf{p}_j$$

$$\beta_j = (\mathbf{r}_{j+1}, \mathbf{r}_{j+1}) / (\mathbf{r}_j, \mathbf{r}_j)$$

$$\mathbf{p}_{j+1} = \mathbf{r}_{j+1} + \beta_j \mathbf{p}_j$$

end for

¹Y. Saad. *Iterative Methods for Sparse Linear Systems*. Second. Society for Industrial and Applied Mathematics, 2003. doi: 10.1137/1.9780898718003. eprint:
<https://pubs.siam.org/doi/book/10.1137/1.9780898718003>

Background & Literature

Conjugate gradient method: residual polynomial

- Iterative, projection method onto a Krylov subspace $\mathcal{K}_m(A_0, \mathbf{r}_0)$ given by

$$\text{span}\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \dots, A^{m-1}\mathbf{r}_0\}$$

Background & Literature

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- Approximate solution can be expressed as

$$\mathbf{u}_m = \mathbf{u}_0 + \sum_{i=0}^{m-1} c_i A^i \mathbf{r}_0 = \mathbf{u}_0 + q_{m-1}(A) \mathbf{r}_0$$

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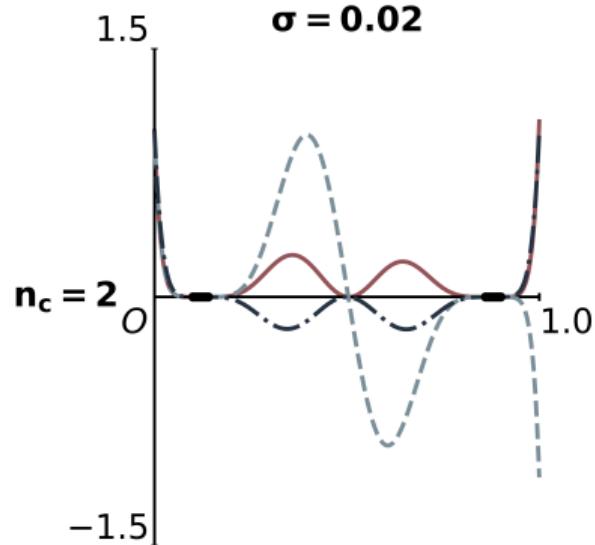


Figure: Residual polynomial $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

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- Minimize residual polynomial on eigenvalues of A

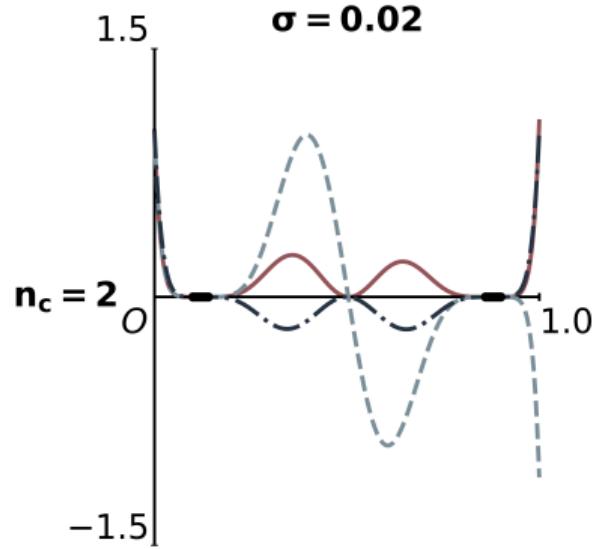


Figure: Residual polynomial $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

Background & Literature

Conjugate gradient method: convergence

- Classical (condition number) convergence bound:

Theorem

The error of the m^{th} iterate of the CG algorithm is bounded by

$$\|\mathbf{e}_m\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m \|\mathbf{e}_0\|_A,$$

where $\kappa = \lambda_{\max}/\lambda_{\min}$ is the condition number of (symmetric matrix) A.

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where $\kappa = \lambda_{\max}/\lambda_{\min}$ is the condition number of (symmetric matrix) A .

- Only sharp for **uniform** eigenvalue distributions!

$$\|\mathbf{e}_m\|_A \leq \min_{r \in \mathcal{P}_{m-1}, r(0)=1} \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |r(\lambda)| \|\mathbf{e}_0\|_A \stackrel{\text{uniform } \sigma(A)}{=} \frac{\|\mathbf{e}_0\|}{C_m \left(\frac{\kappa+1}{\kappa-1} \right)}$$

Background & Literature

Conjugate gradient method: spectral distribution

Setting $\lambda_{\min} = 0.1$ and $\lambda_{\max} = 0.9$ gives $m_{\text{classical}} = 26$. Worst case distribution:

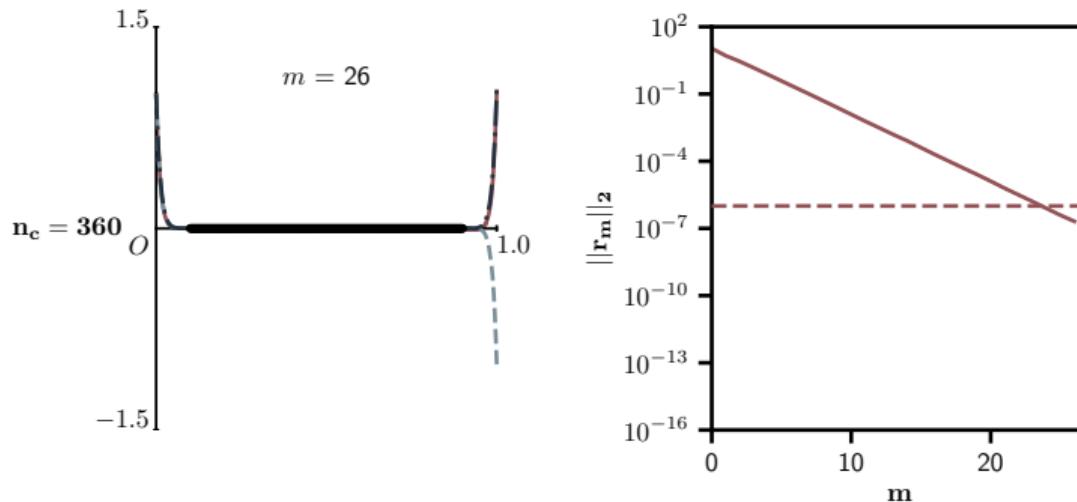


Figure: CG convergence for uniform spectrum.

Background & Literature

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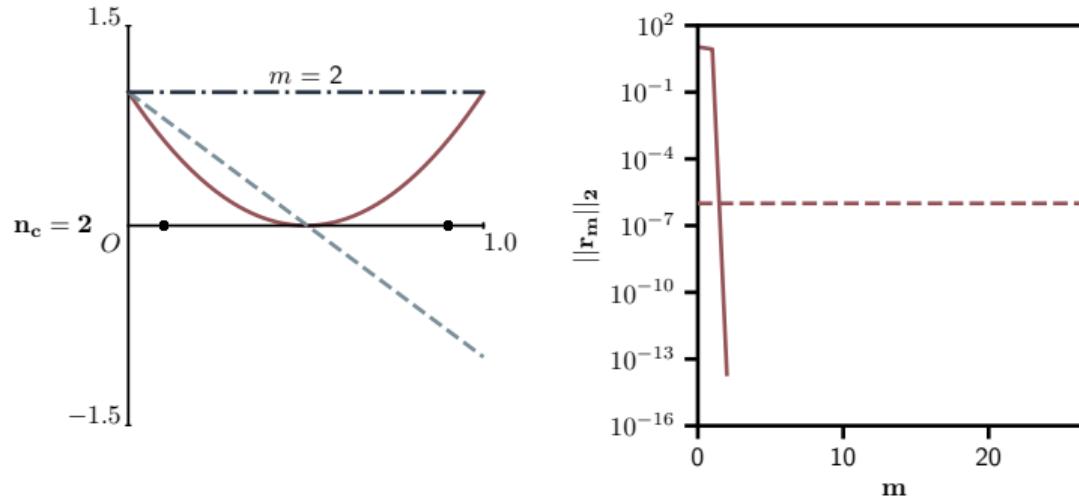


Figure: CG convergence for spectrum with two distinct eigenvalues.

Background & Literature

Conjugate gradient method: non-uniform spectra

- Clusterpoint distribution ($0 < \rho \leq 1$)²

$$\lambda_i = \lambda_1 + \frac{i-1}{N-1}(\lambda_N - \lambda_1)\rho_i^{N-i},$$

For $i = 1, \dots, N$

²Z. Strakoš. "On the real convergence rate of the conjugate gradient method". In: *Linear Algebra and its Applications* 154-156 (1991), pp. 535–549. ISSN: 0024-3795. doi: [https://doi.org/10.1016/0024-3795\(91\)90393-B](https://doi.org/10.1016/0024-3795(91)90393-B)

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- $\rho = 1$ gives uniform distribution

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$$\lambda_i = \lambda_1 + \frac{i-1}{N-1}(\lambda_N - \lambda_1)\rho^{N-i},$$

For $i = 1, \dots, N$

- $\rho = 1$ gives uniform distribution
- $\rho = 0$ gives two distinct eigenvalues
- $0 < \rho < 1$ gives a spectrum with a clusterpoint at λ_1 .

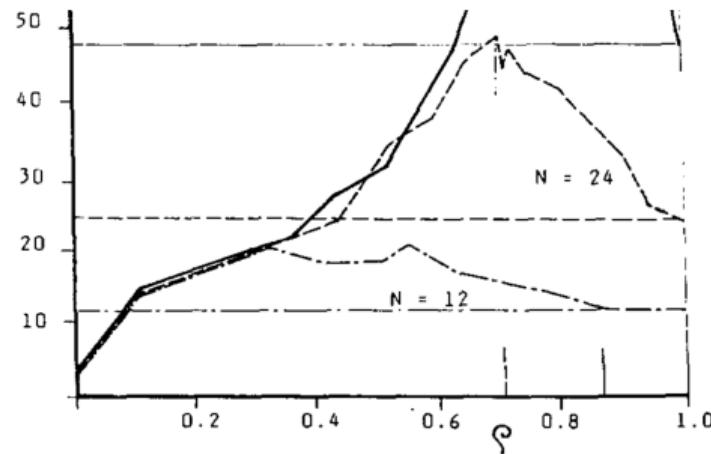


Figure: CG iterations versus ρ

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Background & Literature

Conjugate gradient method: non-uniform spectra

- Let $0 < a < b < c < d < 1$ and consider³

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Background & Literature

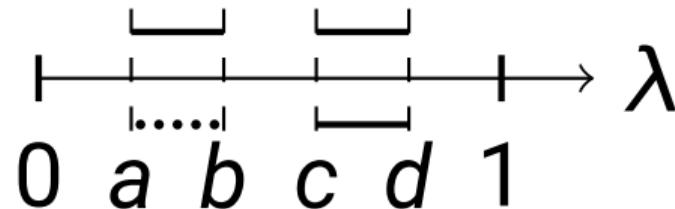
Conjugate gradient method: non-uniform spectra

- Let $0 < a < b < c < d < 1$ and consider³

- Two disjoint clusters

$$\sigma_1(A) = [a, b] \cup [c, d]$$

- Cluster with tail



$$\sigma_2(A) = [c, d] \bigcup_{\substack{i=1 \\ \lambda_i \in [a,b]}}^{N_{\text{tail}}} \lambda_i$$

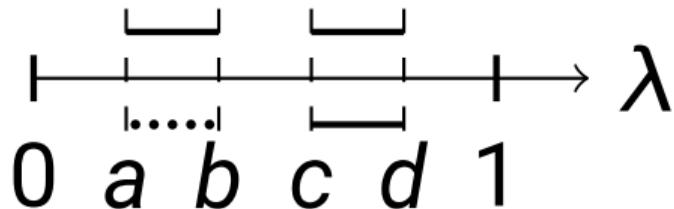
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Background & Literature

Conjugate gradient method: non-uniform spectra

- A-norm optimality of CG

$$\|\mathbf{e}_m\|_A = \min_{r \in \mathcal{P}_m, r(0)=1} \sum_{i=1}^m \frac{r(\lambda_i)^2}{\lambda_i} \rho_{0,i}^2$$



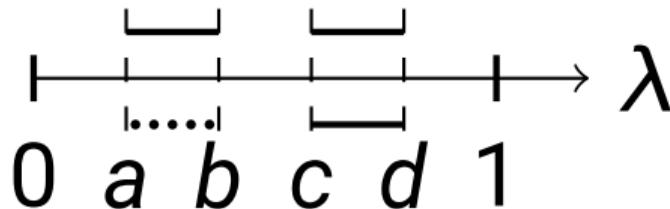
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- We look for $r_{\bar{m}} = \hat{r}_p \hat{r}_{\bar{m}-p} \in \mathcal{P}_{\bar{m}}$ ³

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Let $\epsilon = \frac{\|\mathbf{e}_m\|_A}{\|\mathbf{e}_0\|_A}$ relative error

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- We look for $r_{\bar{m}} = \hat{r}_p \hat{r}_{\bar{m}-p} \in \mathcal{P}_{\bar{m}}^3$

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$$\bar{m} = \left\lceil \frac{1}{2} \sqrt{\frac{d}{c}} \ln \frac{2}{\epsilon} + \left(1 + \frac{1}{2} \sqrt{\frac{d}{c}} \ln \frac{4d}{e} \right) p \right\rceil, \text{ where } e = \begin{cases} b, & \text{two clusters} \\ a, & \text{cluster with tail} \end{cases}$$

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Background & Literature

Schwarz preconditioners

- Derived from the Alternating Schwarz method⁴

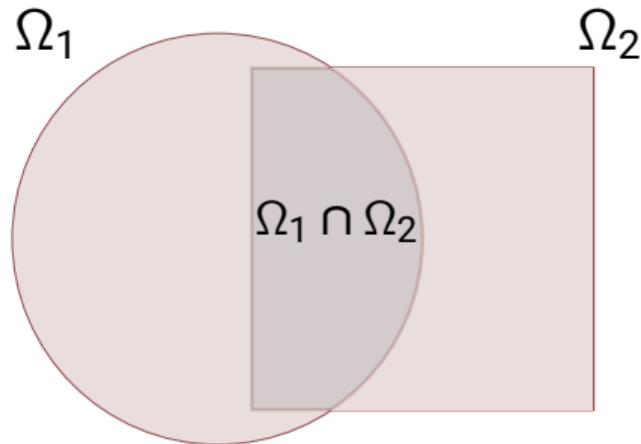


Figure: Domain decomposition with overlapping subdomains.

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⁴V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. doi: 10.1137/1.9781611974065. eprint: <https://pubs.siam.org/doi/pdf/10.1137/1.9781611974065>

Background & Literature

Schwarz preconditioners

- Derived from the Alternating Schwarz method⁴
- Convergence rate depends on the overlap δ and the wave number of eigenmodes k

2D Alternating Schwarz Example

Let $\Omega_1 = (-\infty, \delta) \times \mathbb{R}$, $\Omega_2 = (\delta, \infty) \times \mathbb{R}$

$$-(\eta - \Delta)u = f \text{ in } \mathbb{R}^2,$$

u bounded at infinity.

Then the convergence rate is given by

$$\rho_{2D}(k; \eta, \delta) = e^{-\delta \sqrt{\eta + k^2}}$$

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Background & Literature

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- As a preconditioner

$$M_{\text{OAS-1}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$$

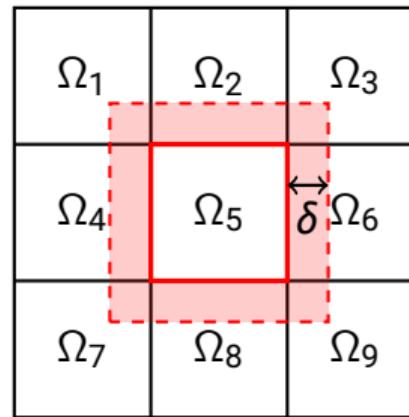


Figure: Domain decomposition with N_{sub} subdomains.

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- As a preconditioner
$$M_{\text{OAS-1}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$$
- Need a coarse space R_0 to counter slowly converging modes

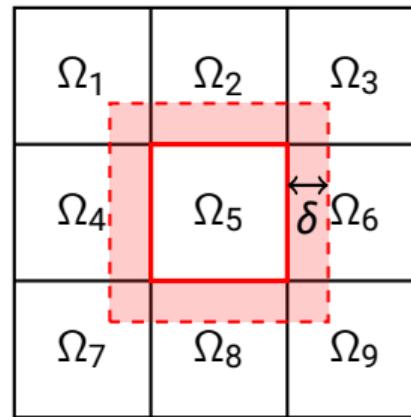


Figure: Domain decomposition with N_{sub} subdomains.

⁴V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. doi: 10.1137/1.9781611974065. eprint: <https://pubs.siam.org/doi/pdf/10.1137/1.9781611974065>

Background & Literature

Schwarz preconditioners

- Derived from the Alternating Schwarz method⁴
- Convergence rate depends on the overlap δ and the wave number of eigenmodes k
- As a preconditioner
$$M_{\text{OAS-1}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$$
- Need a coarse space R_0 to counter slowly converging modes

2-level Additive Schwarz Preconditioner

$$M_{\text{OAS-2}} = R_0^T A_0^{-1} R_0 + M_{\text{OAS-1}}$$

⁴V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. doi: 10.1137/1.9781611974065. eprint: <https://pubs.siam.org/doi/pdf/10.1137/1.9781611974065>

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

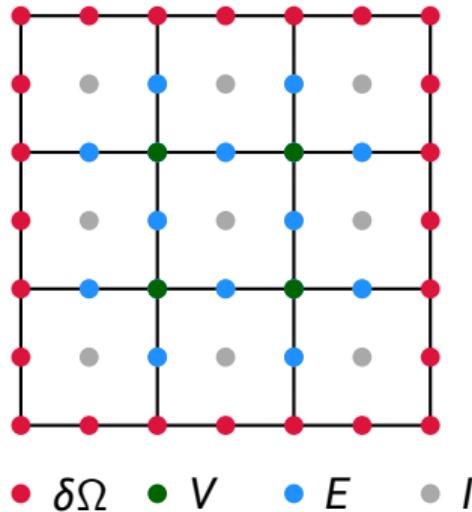
- MsFEM-based: robust for high-contrast, but computationally expensive⁵

⁵Heinlein (2018)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive⁵
- Generalized framework: GDSW⁶, RGDSW⁷



⁵Heinlein (2018)

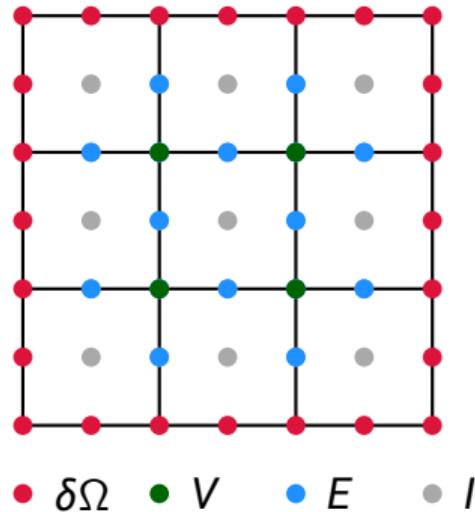
⁶Dohrmann, Klawonn, and Widlund (2008)

⁷Dohrmann and Widlund (2017)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive⁵
- Generalized framework: GDSW⁶, RGDSW⁷
- Hybrid: AMS⁸



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⁵Heinlein (2018)

⁶Dohrmann, Klawonn, and Widlund (2008)

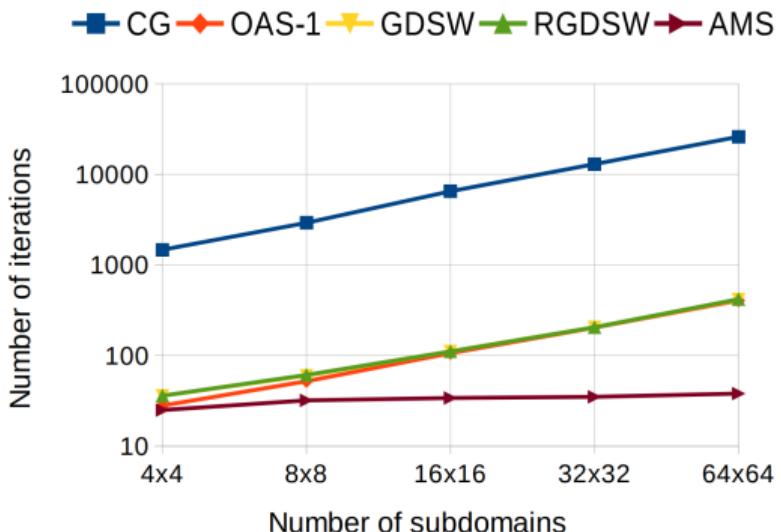
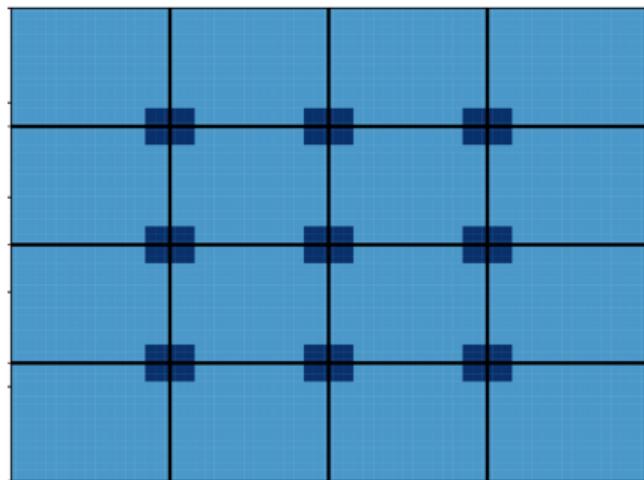
⁷Dohrmann and Widlund (2017)

⁸Alves, Heinlein, and Hajibeygi (2024)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

Figures obtained from ⁵

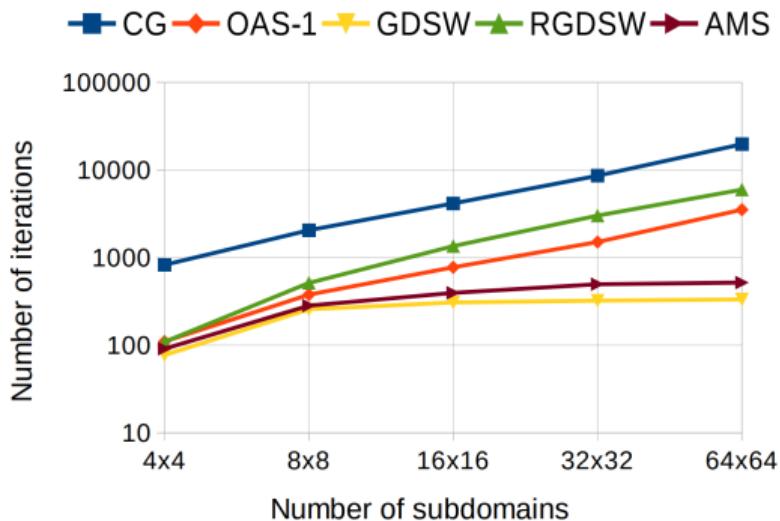
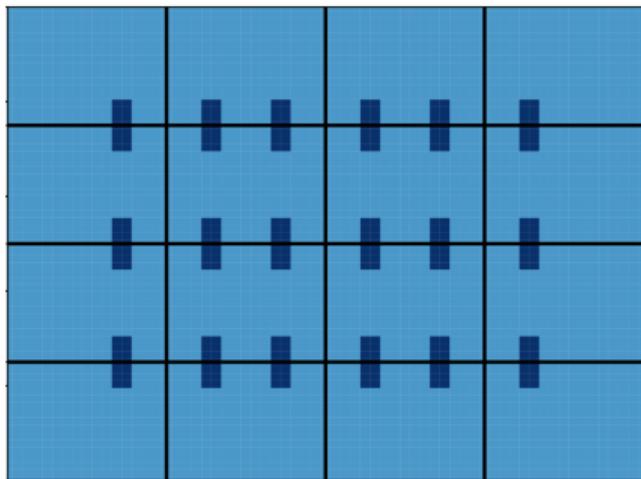


⁵ F. A. C. S. Alves, A. Heinlein, and H. Hajibeygi. *A computational study of algebraic coarse spaces for two-level overlapping additive Schwarz preconditioners*. 2024. arXiv: 2408.08187 [math.NA]

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

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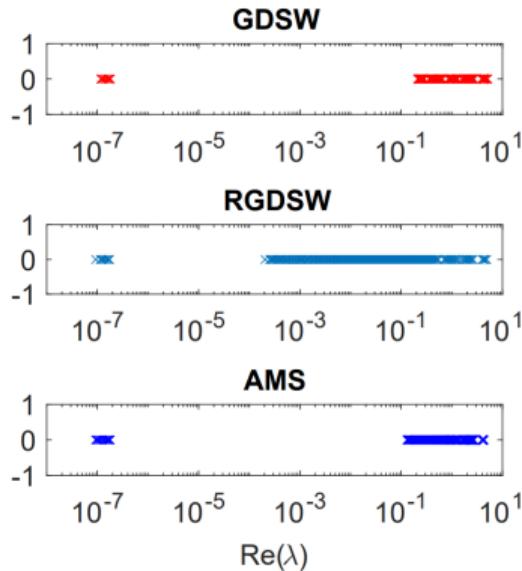
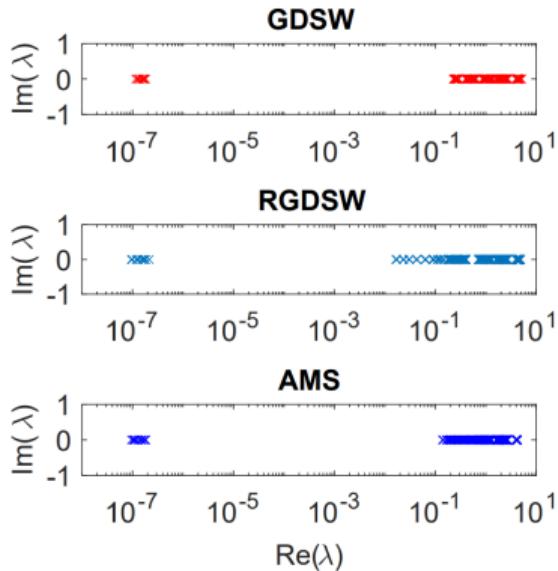


⁵ F. A. C. S. Alves, A. Heinlein, and H. Hajibeygi. *A computational study of algebraic coarse spaces for two-level overlapping additive Schwarz preconditioners*. 2024. arXiv: 2408.08187 [math.NA]

Background & Literature

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Figures obtained from ⁵



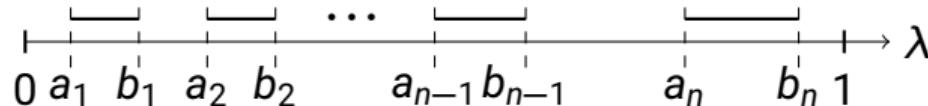
⁵ F. A. C. S. Alves, A. Heinlein, and H. Hajibeygi. *A computational study of algebraic coarse spaces for two-level overlapping additive Schwarz preconditioners*. 2024. arXiv: 2408.08187 [math.NA]

Structure

- Research Questions
- Background & Literature
- Preliminary Results
- Outlook

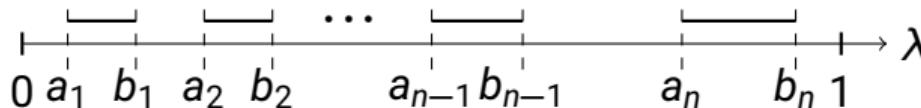
Preliminary Results

Generalization to multiple clusters



Preliminary Results

Generalization to multiple clusters



Building on the work of Axelsson we can imagine $r_{\bar{m}} = \hat{r}_{p_1} \hat{r}_{p_2} \dots \hat{r}_{p_n} \in \mathcal{P}_{\bar{m}}$ with

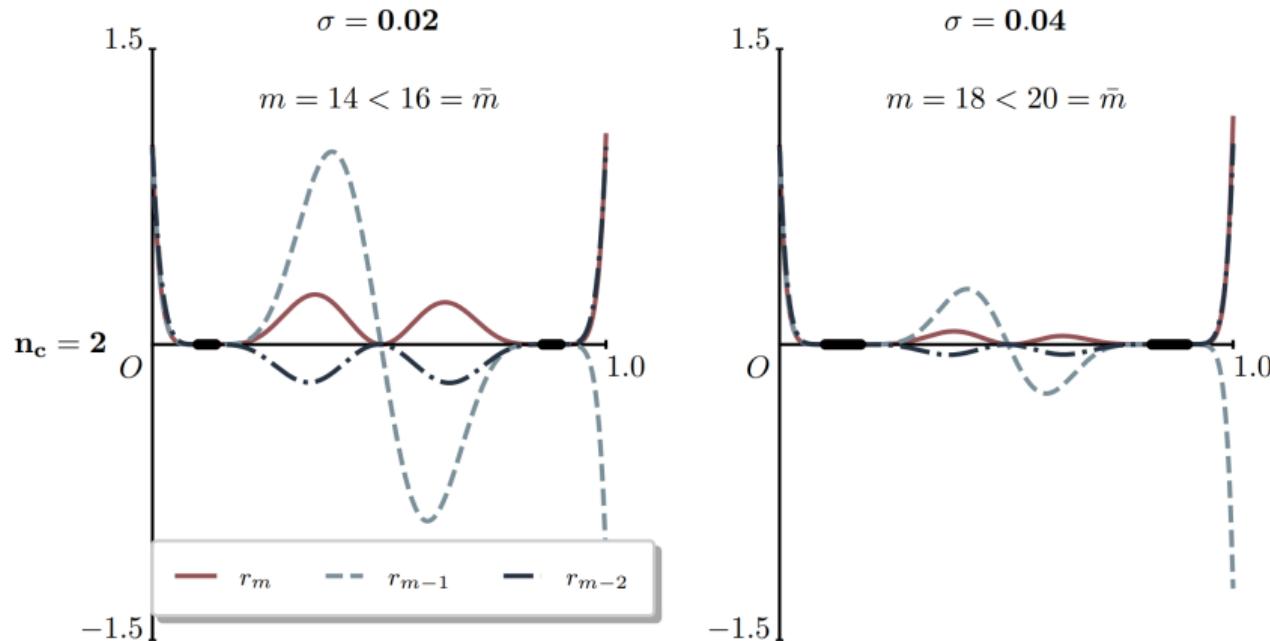
$$p_i \leq \left\lceil \log_{f_i} \frac{\epsilon}{2} + \sum_{j=1}^{i-1} p_j \log_{f_i} \frac{\zeta_2^{(j)}}{\zeta_1^{(i,j)}} \right\rceil \quad \text{and} \quad f_i = \frac{\sqrt{\kappa_i} - 1}{\sqrt{\kappa_i} + 1}.$$

Sharpened bound given by

$$\bar{m} = \sum_{i=1}^n p_i.$$

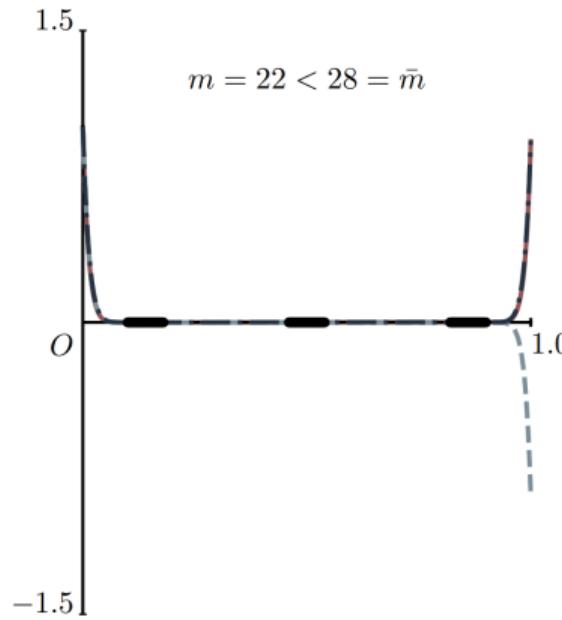
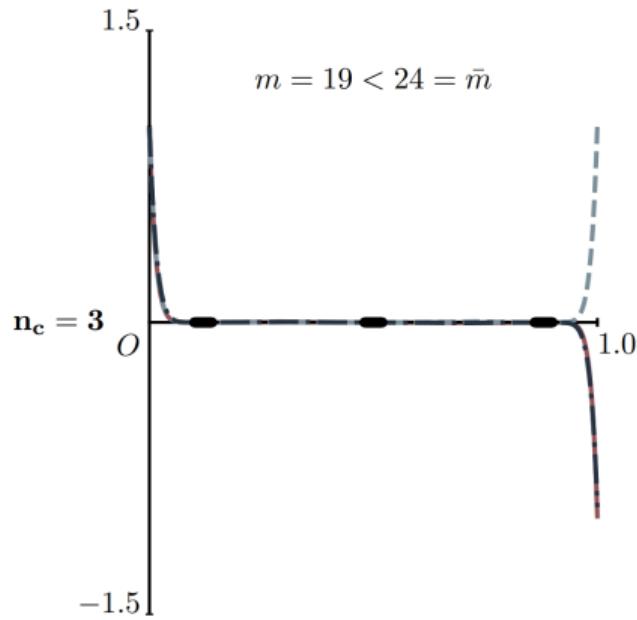
Preliminary Results

Generalization to multiple clusters



Preliminary Results

Generalization to multiple clusters



Preliminary Results

Demo

Structure

- Research Questions
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Outlook

Progress

- Q1** What other spectral characteristics like the condition number can we consider?

- Q3** Given a toy eigenspectrum, how can we sharpen the CG iteration bound?

Outlook

Progress

- Q1** What other spectral characteristics like the condition number can we consider?

- Q3** Given a toy eigenspectrum, how can we sharpen the CG iteration bound?
- Q4** How does the sharpened bound from **Q3** compare to the classical CG bound?
- Q5** How does the performance described in **Q4** depend on the characteristics found in **Q1**?
- Q6** Can the sharpened bound from **Q3** distinguish between preconditioners?

Outlook

Progress

- Q1** What other spectral characteristics like the condition number can we consider?
- Q2** How to estimate the characteristics from **Q1**?
- Q3** Given a toy eigenspectrum, how can we sharpen the CG iteration bound?
- Q4** How does the sharpened bound from **Q3** compare to the classical CG bound?
- Q5** How does the performance described in **Q4** depend on the characteristics found in **Q1**?
- Q6** Can the sharpened bound from **Q3** distinguish between preconditioners?