

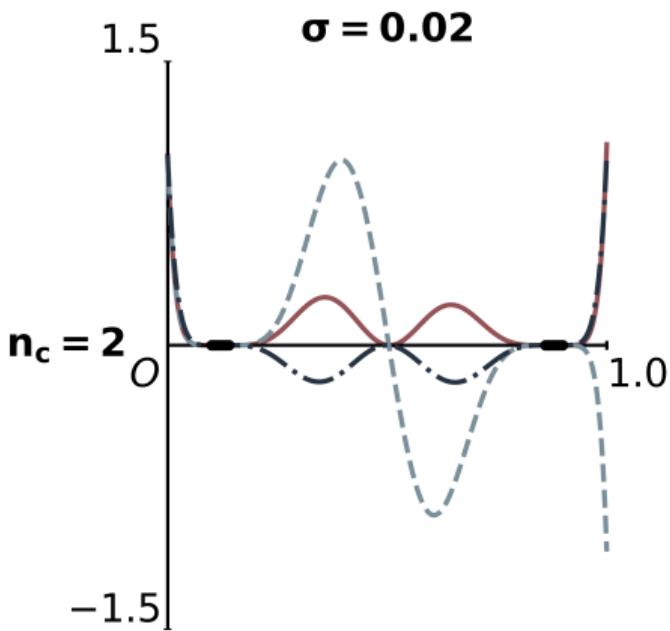
# Sharpened CG Iteration Bound for Schwarz-preconditioned High-contrast Heterogeneous Scalar Elliptic PDEs

Going Beyond Condition Number

P. Soliman<sup>1</sup>

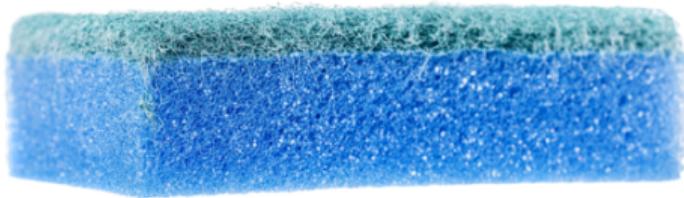
EEMCS-DIAM Numerical Analysis MSc.  
Thesis Presentation, April, 2025

<sup>1</sup> Delft University of Technology



# Opening

## Darcy Problem



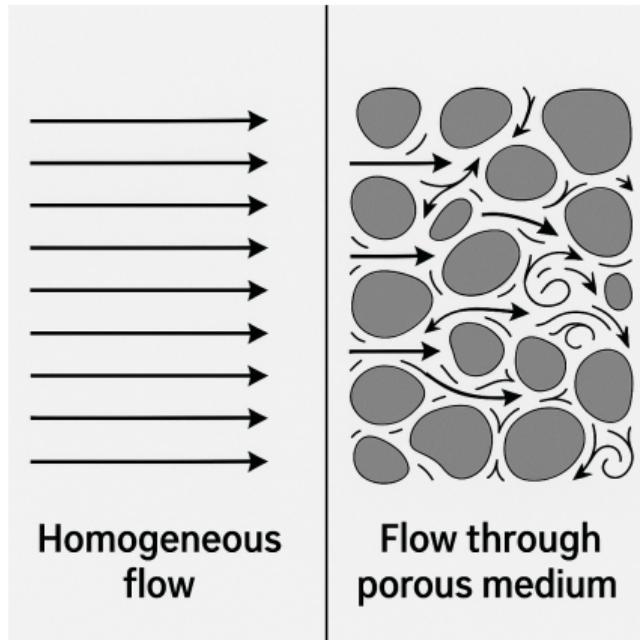
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- Simpler case; high-contrast diffusion problem for  $u, u_D \in H^1(\Omega)$ ,  $f \in L^2(\Omega)$  and  $\mathcal{C} \in L^\infty(\Omega)$

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

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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

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### Algorithm Conjugate Gradient Method<sup>1</sup>

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

**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**

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<sup>1</sup>Y. Saad. *Iterative Methods for Sparse Linear Systems*. Second. Society for Industrial and Applied Mathematics, 2003. doi: 10.1137/1.9780898718003. eprint:  
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# Background & Literature

Conjugate gradient method: residual polynomial

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

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

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- Approximate solution can be expressed as

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

# Background & Literature

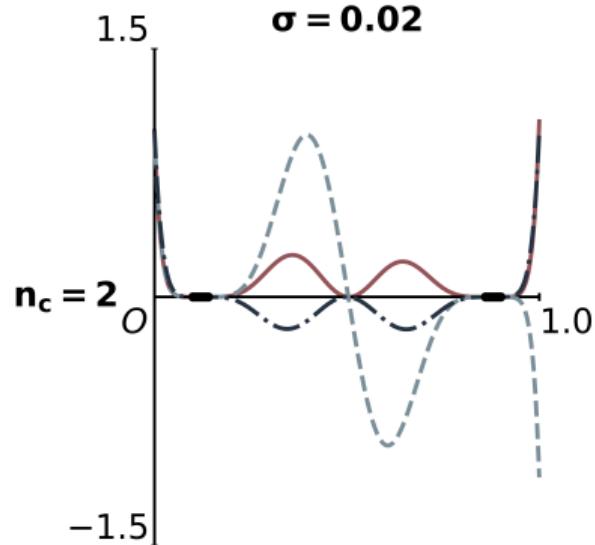
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**Figure:** Residual polynomial  $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

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- Minimize residual polynomial on eigenvalues of  $A$

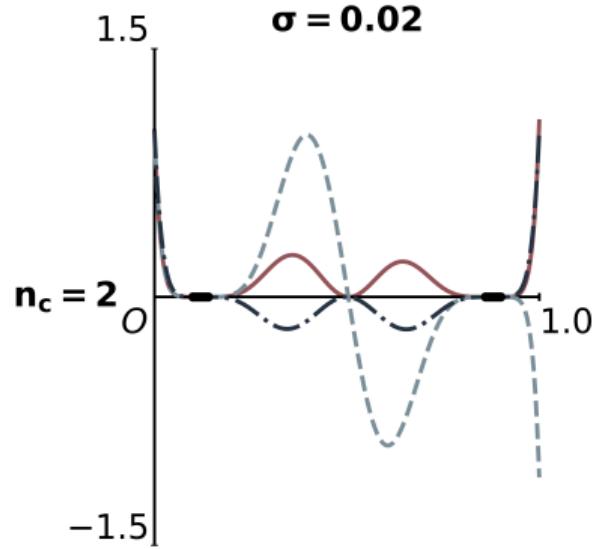


Figure: Residual polynomial  $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

# Background & Literature

## Conjugate gradient method: convergence

- Classical (condition number) convergence bound:

### Theorem

*The error of the  $m^{\text{th}}$  iterate of the CG algorithm is bounded by*

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

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

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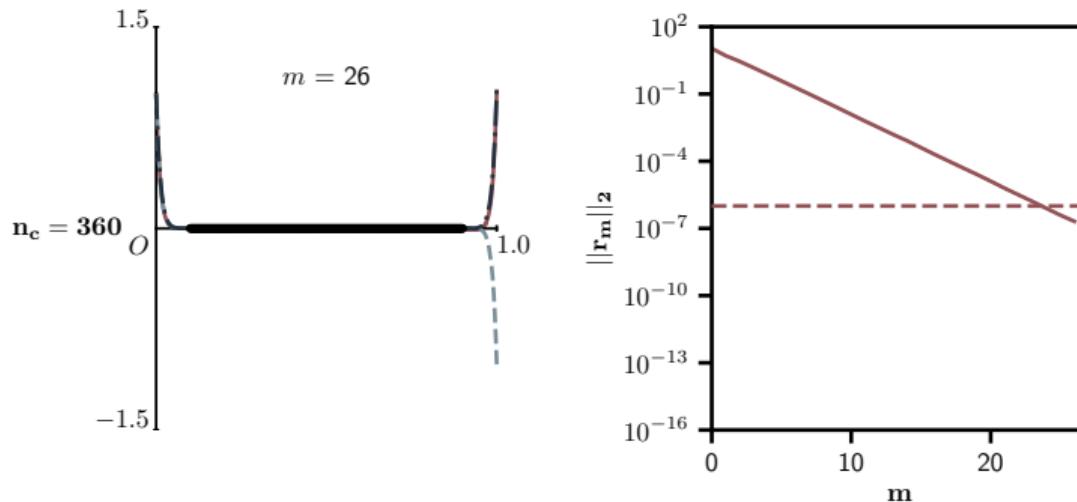
- Only sharp for **uniform** eigenvalue distributions!

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

# 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:

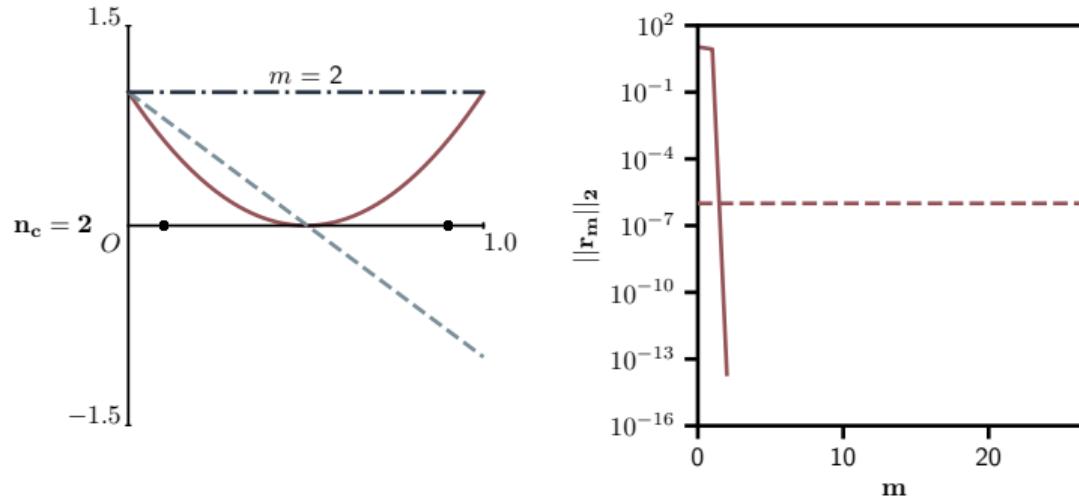


**Figure:** CG convergence for uniform spectrum.

# Background & Literature

Conjugate gradient method: spectral distribution

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



**Figure:** CG convergence for spectrum with two distinct eigenvalues.

# Background & Literature

## Conjugate gradient method: non-uniform spectra

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

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

For  $i = 1, \dots, N$

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<sup>2</sup>Z. 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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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  $\lambda_1$ .

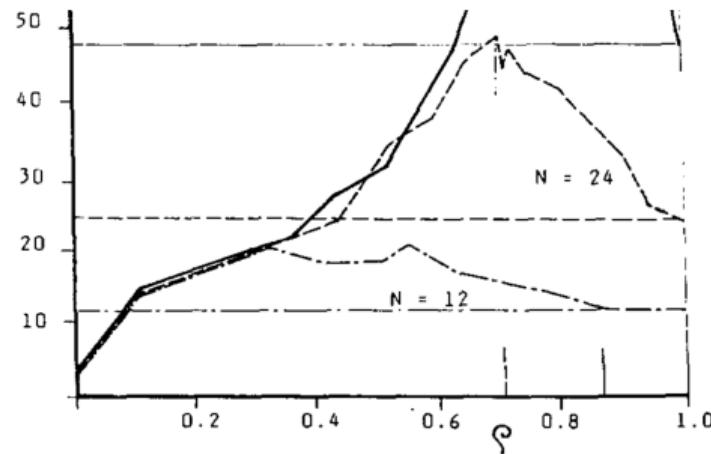


Figure: CG iterations versus  $\rho$

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## Conjugate gradient method: non-uniform spectra

- Let  $0 < a < b < c < d < 1$  and consider<sup>3</sup>

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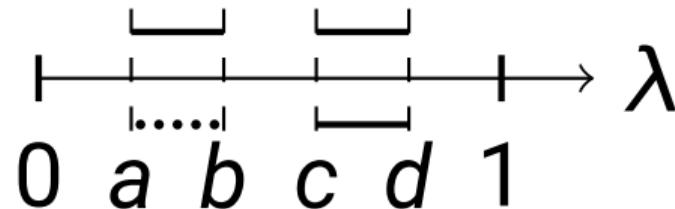
## Conjugate gradient method: non-uniform spectra

- Let  $0 < a < b < c < d < 1$  and consider<sup>3</sup>

- Two disjoint clusters

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

- Cluster with tail



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

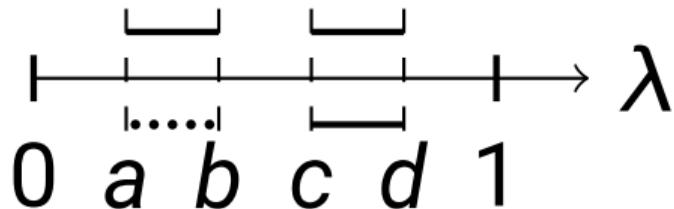
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# Background & Literature

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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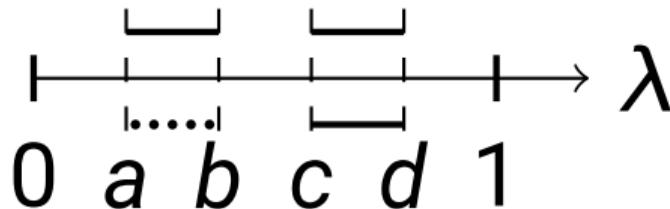
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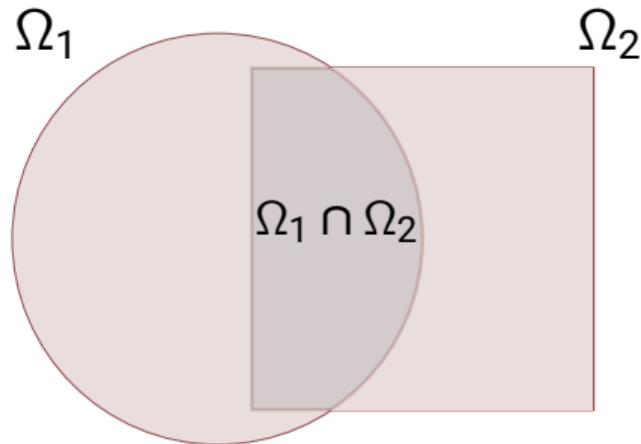
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# Background & Literature

## Schwarz preconditioners

- Derived from the Alternating Schwarz method<sup>4</sup>



**Figure:** Domain decomposition with overlapping subdomains.

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<sup>4</sup>V. 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

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- Convergence rate depends on the overlap  $\delta$  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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## Schwarz preconditioners

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- Convergence rate depends on the overlap  $\delta$  and the wave number of eigenmodes  $k$
- As a preconditioner

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

$\Omega_1$		
	$\Omega_2$	$\Omega_3$
$\Omega_4$	$\Omega_5$	$\Omega_6$
$\Omega_7$	$\Omega_8$	$\Omega_9$

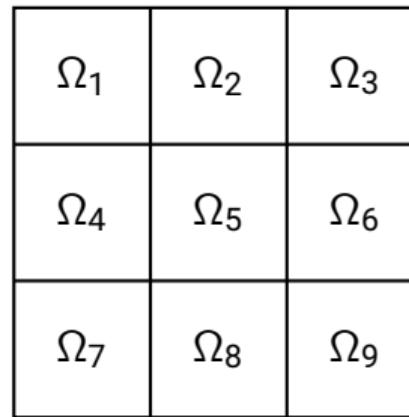
**Figure:** Domain decomposition with  $N_{\text{sub}}$  subdomains.

<sup>4</sup>V. 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 method<sup>4</sup>
- Convergence rate depends on the overlap  $\delta$  and the wave number of eigenmodes  $k$
- As a preconditioner  
$$M_{\text{ASM}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$$
- Need a coarse space  $R_0$  to counter slowly converging modes



**Figure:** Domain decomposition with  $N_{\text{sub}}$  subdomains.

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# Background & Literature

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### 2-level Additive Schwarz Preconditioner

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

<sup>4</sup>V. 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 expensive<sup>5</sup>

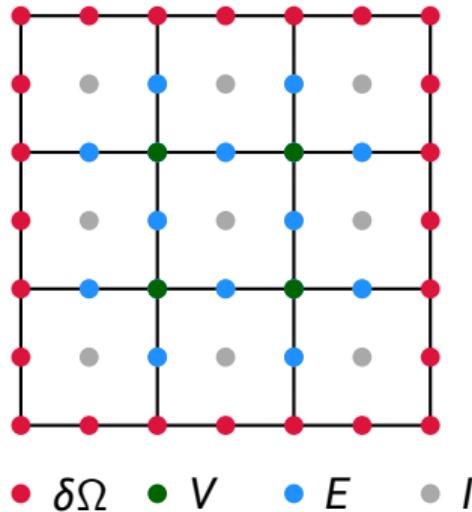
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<sup>5</sup>Heinlein (2018)

# Background & Literature

## Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive<sup>5</sup>
- Generalized framework: GDSW<sup>6</sup>, RGDSW<sup>7</sup>



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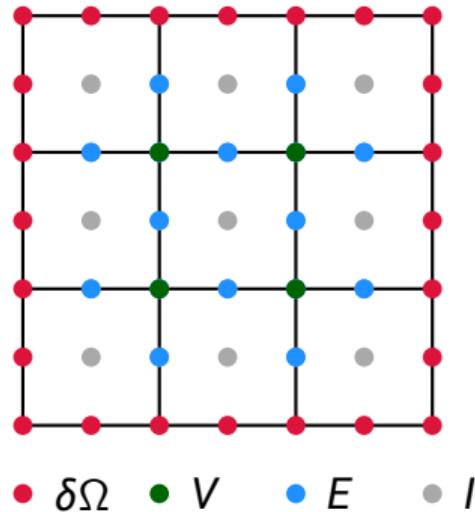
<sup>6</sup>Dohrmann, Klawonn, and Widlund (2008)

<sup>7</sup>Dohrmann and Widlund (2017)

# Background & Literature

## Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive<sup>5</sup>
- Generalized framework: GDSW<sup>6</sup>, RGDSW<sup>7</sup>
- Hybrid: AMS<sup>8</sup>



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<sup>5</sup>Heinlein (2018)

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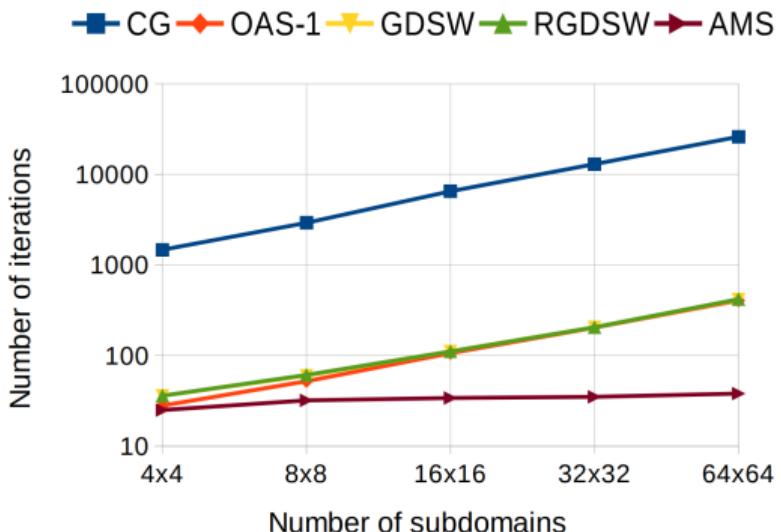
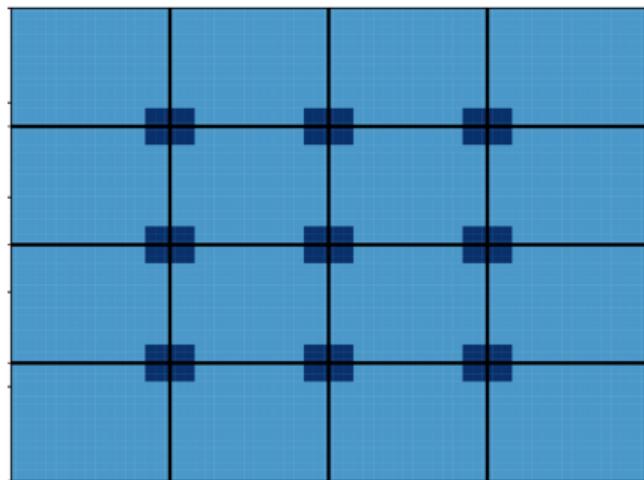
<sup>7</sup>Dohrmann and Widlund (2017)

<sup>8</sup>Alves, Heinlein, and Hajibeygi (2024)

# Background & Literature

## Tailored Coarse Spaces for High-Contrast Problems

Figures obtained from <sup>5</sup>

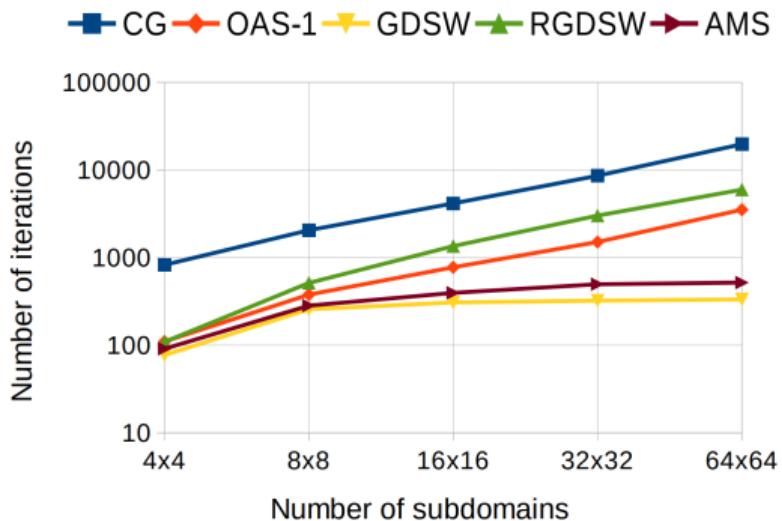
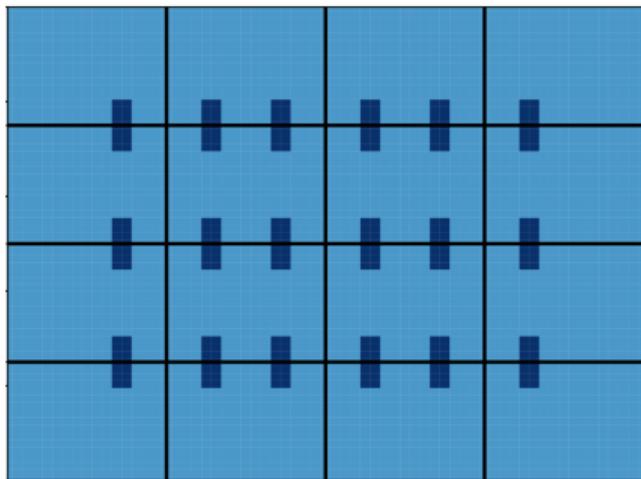


<sup>5</sup> F. A. C. S. Alves, A. Heinlein, and H. Hajibeygi. *A computational study of algebraic coarse spaces for two-level overlapping additive Schwarz preconditioners*. 2024. arXiv: 2408.08187 [math.NA]

# Background & Literature

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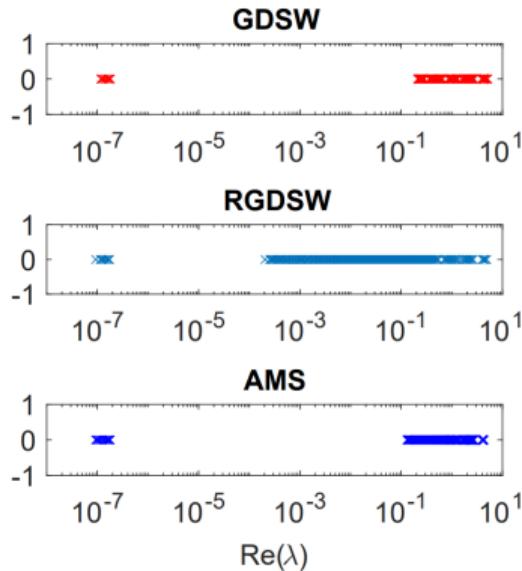
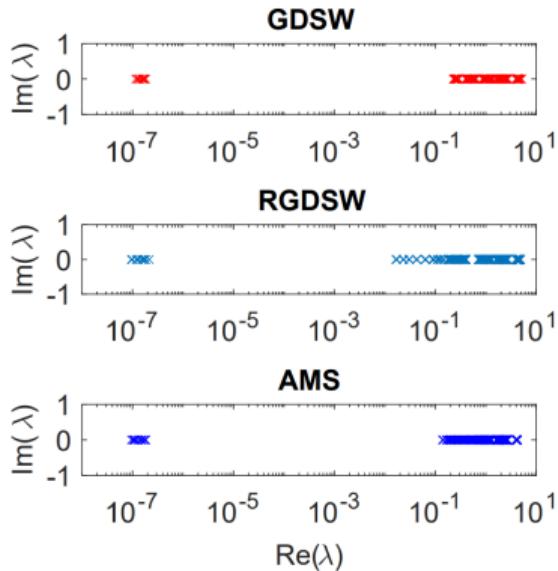


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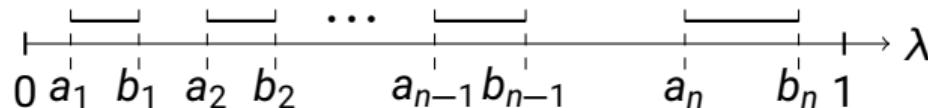
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# Structure

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

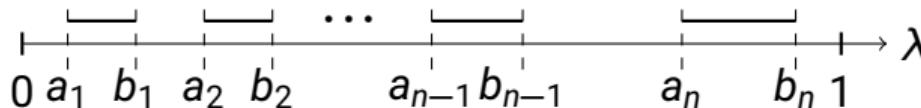
# Preliminary Results

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

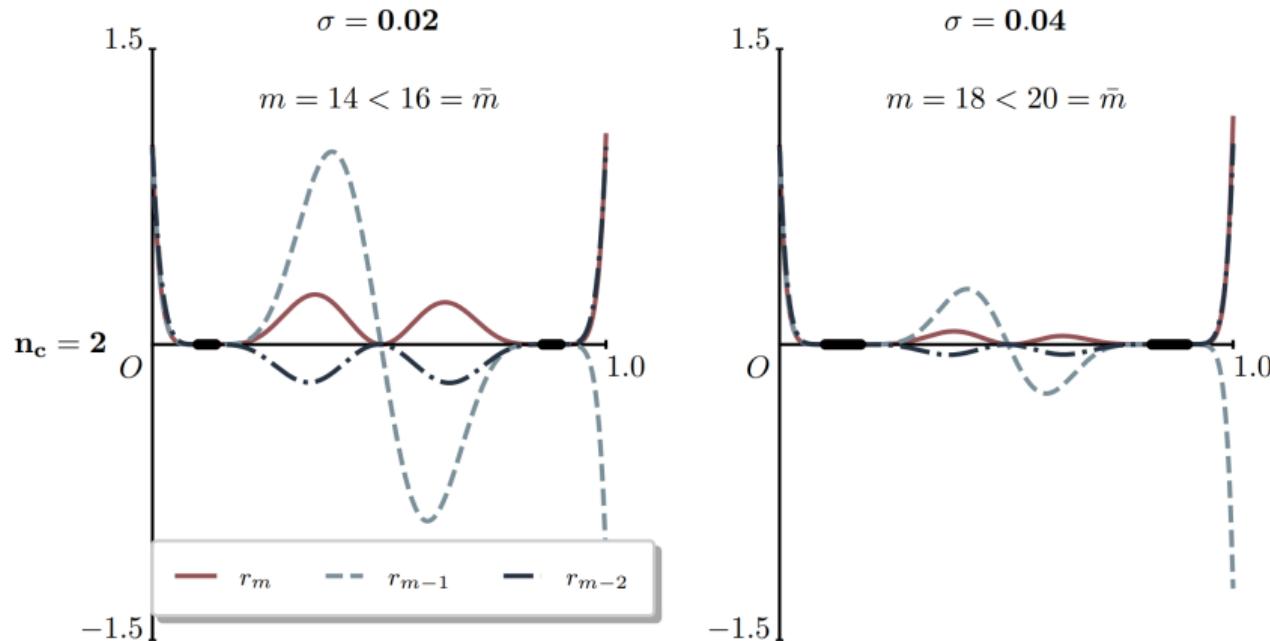
$$p_i \leq \left\lceil \log_{f_i} \frac{\epsilon}{2} + \sum_{j=1}^{i-1} p_j \log_{f_i} \frac{\zeta_2^{(j)}}{\zeta_1^{(i,j)}} \right\rceil \quad \text{and} \quad f_i = \frac{\sqrt{K_i} - 1}{\sqrt{K_i} + 1}.$$

Sharpened bound given by

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

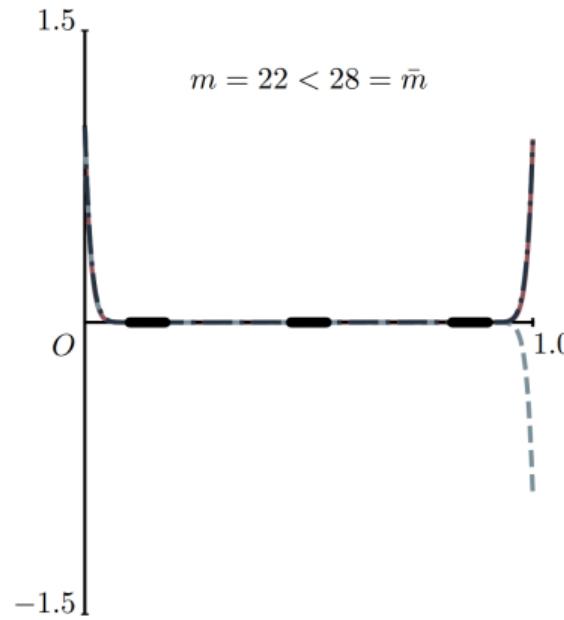
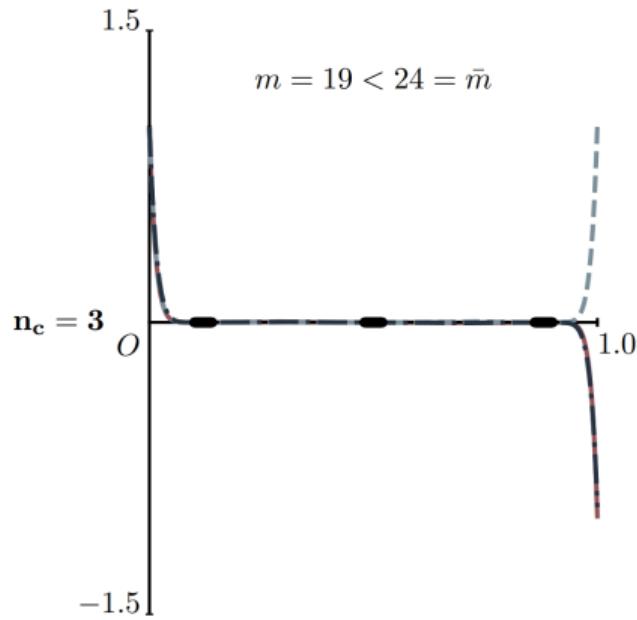
# Preliminary Results

## Generalization to multiple clusters



# Preliminary Results

## Generalization to multiple clusters



# Preliminary Results

Demo

# Structure

- Research Questions
- Background & Literature
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- Outlook

## 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?