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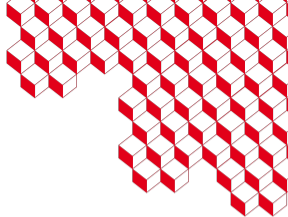
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Toward an AMG method for the indefinite Helmholtz equation

18th Copper Mountain Conference on Iterative Methods - 04/16/24

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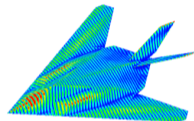
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- IV. Alternative coarse correction for indefinite problems
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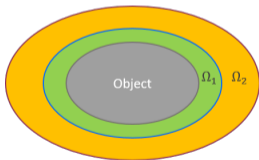
I.1 - Context

- Computation of the **Radar Cross Section** of **3D objects** covered by multiple layers of materials
- Requires **highly accurate** solution of **harmonic Maxwell's equations** in an unbounded domain
- Objects may be electrically **large** + Materials may have **large** permittivity/permeability

⇒ Requires to solve **large** and **sparse** linear systems of equations $Ax = b$



The current **domain decomposition method** is difficult to scale :



- Increase in the **number** of sub-domains

⇒ Convergence is **slower**

- Increase in the **size** of the sub-domains

⇒ Increase in computational **complexity**

We need to investigate an alternative method : **multigrid methods**.

I.2 - Fundamentals on AMG

Multigrid benefits from both **direct** and **iterative** methods :

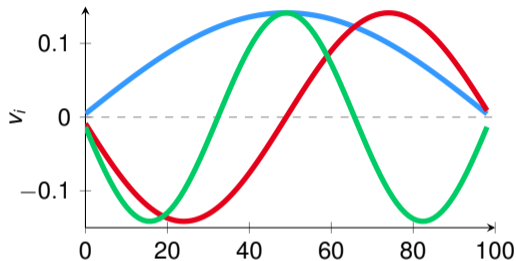
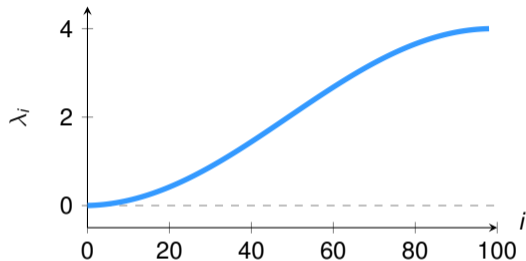
- ν iterations of a **smoother** M damp the **large eigenvectors**.
- The remaining **small eigenvectors** are projected onto a **coarse space** defined by P .

Accordingly, the two-grid error propagation matrix is

$$E_{TG} := \underbrace{(I - M^{-1}A)^\nu}_{\text{Smoother}} \cdot \underbrace{\left(I - P \left(P^T A P \right)^{-1} P^T A \right)}_{\text{Coarse Correction}} \cdot \underbrace{(I - M^{-1}A)^\nu}_{\text{Smoother}}$$

I.3 - Multigrid applied to Laplace

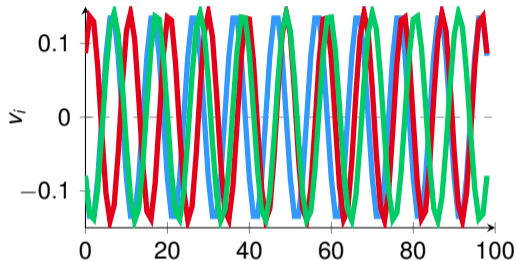
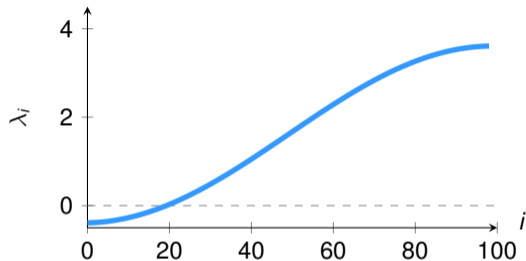
$$\text{(Laplace Problem)} \Leftrightarrow \begin{cases} -\Delta u = f \text{ on } \Omega = [0, 1] \\ u|_{\partial\Omega} = 0 \end{cases}$$



- Eigenvalues are **positives** \rightarrow Usual smoothers are perfectly appropriate
- The Near Kernel Space is **smooth** \rightarrow Convenient assumption for building interpolation
- The matrix A is **s.p.d.** $\Rightarrow \mathbf{x}_{\text{opt}} = P(P^T A P)^{-1} P^T A \mathbf{x} = \arg \min_{\tilde{\mathbf{x}} \in \text{Range}(P)} \|\mathbf{x} - \tilde{\mathbf{x}}\|_A$

I.3 - Multigrid applied to Helmholtz

(Helmholtz Problem) $\Leftrightarrow \begin{cases} -\Delta u - k^2 u = f \text{ on } \Omega = [0, 1] \\ u|_{\partial\Omega} = 0 \end{cases}$



- Eigenvalues are both **positives** and **negatives** → Necessary to find an adapted smoother
- The Near Kernel Space is **oscillatory** → Interpolation rules are difficult to design
- The matrix A is **not s.p.d.** $\Rightarrow \mathbf{x}_{\text{opt}} = P(P^T A P)^{-1} P^T A \mathbf{x} \neq \arg \min_{\tilde{\mathbf{x}} \in \text{Range}(P)} \|\mathbf{x} - \tilde{\mathbf{x}}\|_A$ not a norm

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II. Smoother for both positive and negative eigenvalues

In the indefinite case, large eigenvalues can be either **positive** or **negative**

→ *Chebyshev Polynomial Smoother* built on *normal equations* will be considered

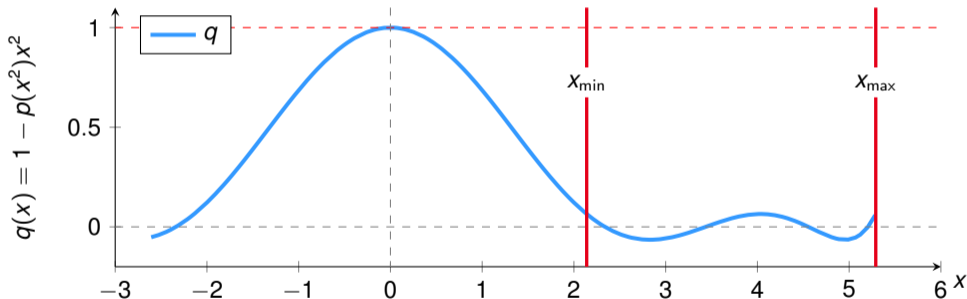


Figure 1: Spectrum of $q(A^2) := I - p(A^2)A^2$

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 - III.2 - Construction of interpolation rules for oscillatory problems
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- V. Conclusion

III.1 - Theory for SPD matrices

Let A and M be SPD matrices. The theory¹ provides the definition of the ideal interpolation operator

$$P_* := \left(I - S \left(S^T A S \right)^{-1} S^T A \right) R^T,$$

based on orthogonal coarse / fine variables selection operators R / S^T ($RS = 0$). In particular,

$$\mu_M(P_*, \mathbf{e}) = \min_P \max_{\mathbf{e} \neq 0} \mu_M(P, \mathbf{e}), \text{ with } \mu_M(P, \mathbf{e}) = \frac{\|(I - PR)\mathbf{e}\|_M^2}{\|\mathbf{e}\|_A^2}.$$

The optimal theory² provides the optimal interpolation operator $P_\#$ such that

$$\text{Range}(P_\#) = \text{span}(\{\mathbf{w}_1, \dots, \mathbf{w}_{n_c}\}), \text{ with } A\mathbf{w}_i = \sigma_i M\mathbf{w}_i \text{ and } \sigma_i \leq \sigma_{i+1}.$$

Ideal and optimal theories can coincide for a particular choice of $R_\#$ and $S_\#$ so that

$$P_\# = P_* = \left(I - S_\# \left(S_\#^T A S_\# \right)^{-1} S_\#^T A \right) R_\#^T \quad (1)$$

¹ On Generalizing the AMG Framework - Robert D. Falgout and Panayot S. Vassilevski (2003)

² Optimal Interpolation and Compatible Relaxation in Classical Algebraic Multigrid - Brannick et al. (2018)

III.2 - Interpolation rules for oscillatory problems

1 Define T_κ the set of κ test vectors such that

$$T_\kappa := \left[\begin{array}{c|c} q_m(A)\mathbf{p}_1 & \cdots & q_m(A)\mathbf{p}_\kappa \\ \hline & & \end{array} \right], \text{ with } \mathbf{p}_i := \text{random vector } (n)$$

III.3 - Interpolation rules for oscillatory problems

1 Define T_κ the set of κ test vectors such that

$$T_\kappa := \left[\begin{array}{c|ccc} q_m(A)\mathbf{p}_1 & & & \\ \hline & \cdots & & \\ & & q_m(A)\mathbf{p}_\kappa & \\ \hline & & & \end{array} \right], \text{ with } \mathbf{p}_i := \text{random vector } (n)$$

2 Let coarse and non-coarse variables selection operators respectively be

$$\hat{R}^T = [R_f \ I_c]^T, \quad \hat{S} = [I_f \ -R_f^T]^T, \quad RS = 0$$

where each row sparse row of r_i is defined as follows

$$\forall i \in \mathcal{F}, \quad \mathbf{r}_i = \arg \min_{\mathbf{r}} \sum_{j=1}^{\kappa} (T_{i,j} - \mathbf{r} \cdot T_{C_{i,j}})^2 \quad (\mathbf{r}_i \text{ row of } R_f)$$

III.3 - Interpolation rules for oscillatory problems

- 1 Define T_κ the set of κ test vectors such that

$$T_\kappa := \left[\begin{array}{c|ccc} q_m(A)\mathbf{p}_1 & & & \\ \hline & \cdots & & \\ \hline q_m(A)\mathbf{p}_\kappa & & & \\ \hline & & & \end{array} \right], \text{ with } \mathbf{p}_i := \text{random vector } (n)$$

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- 3 Approximate the ideal interpolation operator column-wise by

$$\hat{P}_{:,i} := (I - SX_i^T(X_iS^T A^T ASX_i^T)^{-1} X_iS^T A^T A)\hat{R}_{:,i}^T.$$

where X_i corresponds to a non-zero pattern constraint matrix for the i^{th} column of \hat{P} .

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- V. Conclusion

IV.1 - The problem of the classical coarse correction

We illustrate the problem of the coarse correction with a shifted 2D Laplacian problem :

$$(L_n - \alpha I_n)\mathbf{x} = \mathbf{b}, \text{ with } n = 100$$

We plot three curves which correspond to

- \mathbf{v}_1 - The smallest eigenvector of the matrix $(L_n - \alpha I_n)$
- $P(P^T P)^{-1} P^T \mathbf{v}_1$ - The L^2 -projection of \mathbf{v}_1 onto $\text{Range}(P)$
- $P(P^T A P)^{-1} A \mathbf{v}_1$ - The coarse correction applied to \mathbf{v}_1



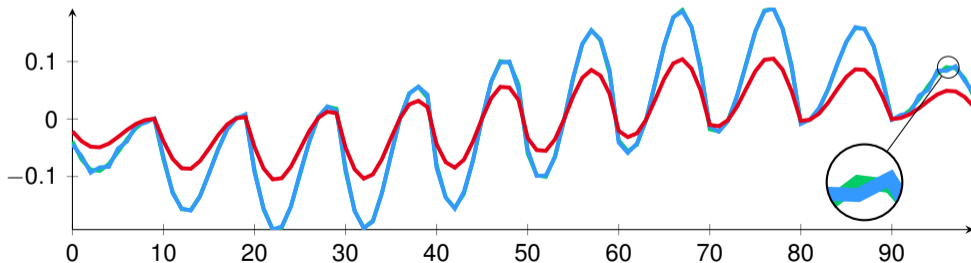
IV.1 - The problem of the classical coarse correction

We illustrate the problem of the coarse correction with a shifted 2D Laplacian problem :

$$(L_n - 0.625^2 I_n) \mathbf{x} = \mathbf{b}, \text{ with } n = 100$$

We plot three curves which correspond to

- \mathbf{v}_1 - The smallest eigenvector of the matrix $(L_n - 0.625^2 I_n)$
- $P(P^T P)^{-1} P^T \mathbf{v}_1$ - The L^2 -projection of \mathbf{v}_1 onto $\text{Range}(P)$
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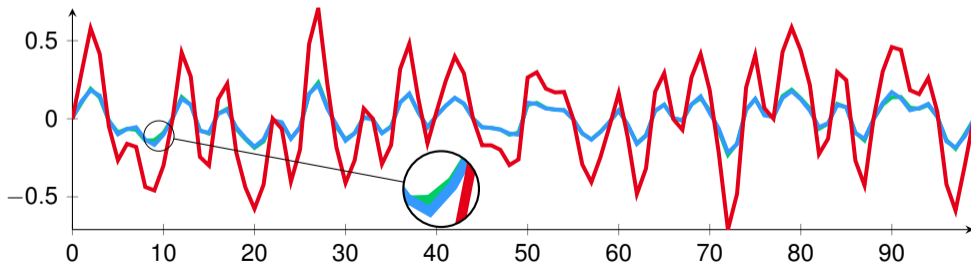
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$$(L_n - 1.435^2 I_n) \mathbf{x} = \mathbf{b}, \text{ with } n = 100$$

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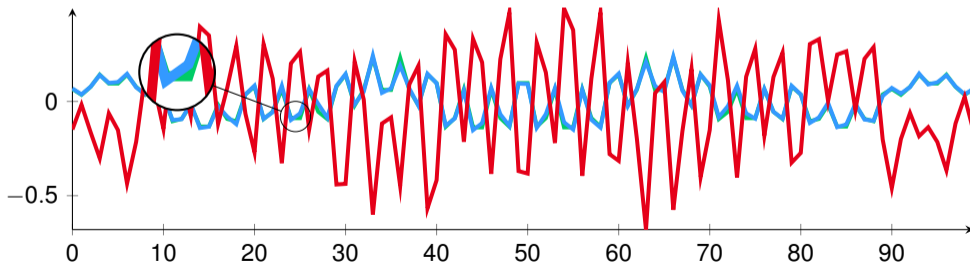
IV.1 - The problem of the classical coarse correction

We illustrate the problem of the coarse correction with a simple model problem :

$$(L_n - 1.710^2 I_n) \mathbf{x} = \mathbf{b}, \text{ with } n = 100$$

We plot three curves which correspond to

- \mathbf{v}_1 - The smallest eigenvector of the matrix $(L_n - 1.710^2 I_n)$
- $P (P^T P)^{-1} P^T \mathbf{v}_1$ - The L^2 -projection of \mathbf{v}_1 onto $\text{Range}(P)$
- $P (P^T A P)^{-1} A \mathbf{v}_1$ - The coarse correction applied to \mathbf{v}_1



IV.1 - The problem of the classical coarse correction

Let P be a $n \times 1$ interpolation operator whose range approximates a small eigenvector \mathbf{v}_1 as follows

$$\text{Range}(P) = \left\{ \mathbf{v}_1 + \sum_{j>1} \epsilon_j \mathbf{v}_j \right\}.$$

IV.1 - The problem of the classical coarse correction

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$$\text{Range}(P) = \left\{ \mathbf{v}_1 + \sum_{j>1} \epsilon_j \mathbf{v}_j \right\}.$$

Define \mathbf{p}_1 the “eigenvector pollution” of \mathbf{v}_1 such that

$$\mathbf{p}_1 := \mathbf{v}_1 - P(P^T P)^{-1} P^T \mathbf{v}_1 = - \sum_{j>1} \epsilon_j \mathbf{v}_j.$$

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This eigenvector pollution produces an “eigenvalue pollution” δ_1 so the damping factor of \mathbf{v}_1 is

$$\mathbf{v}_1^T E \mathbf{v}_1 = 1 - \frac{\lambda_1}{\lambda_1 + \delta_1} \text{ with } \delta_1 := \sum_{j>1} \epsilon_j^2 \lambda_j \geq 0.$$

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A s.p.d : $\delta_1 \geq 0 \Rightarrow 0 < \mathbf{v}_1^T E \mathbf{v}_1 < 1$ The coarse correction never amplifies the error

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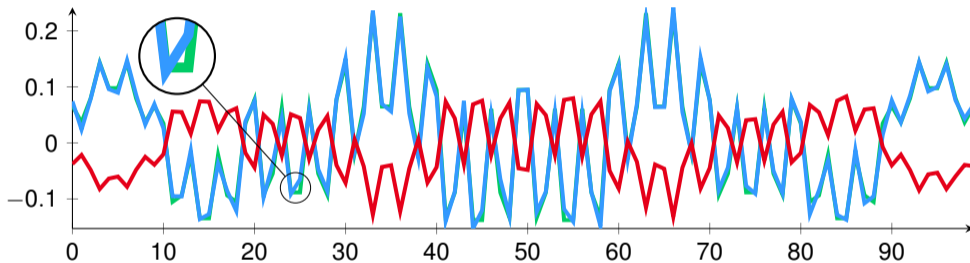
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$$\mathbf{v}_1^T E \mathbf{v}_1 = 1 - \frac{\lambda_1}{\lambda_1 + \delta_1} \text{ with } \delta_1 := \sum_{j>1} \epsilon_j^2 \lambda_j.$$

A indefinite : $-1 < \mathbf{v}_1^T E \mathbf{v}_1 < 1 \Rightarrow \delta_1 \geq -\frac{1}{2} \lambda_1 \Rightarrow$ **The coarse correction may amplify the error**

IV.2 - Alternative coarse correction

The shape of the **coarse correction vector** is correct when p_i is small, only the direction is wrong



Hence, coarse correction vectors still provide information on the near-kernel space!



IV.2 - Alternative coarse correction

For each multigrid cycle m :

- 1 Create the coarse correction subspace

$$W_m = \left[P(P^T A P)^{-1} P^T A r^{(0)}, \dots, P(P^T A P)^{-1} P^T A r^{(m)} \right]$$

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$$W_m = \left[P(P^T A P)^{-1} P^T A r^{(0)}, \dots, P(P^T A P)^{-1} P^T A r^{(m)} \right]$$

- 2 Construct the operators involved in the below generalized Arnoldi relation

$$A W_m = Z_m H_m,$$

where $\text{Range}(Z_m) = \text{span}\{A w_1, \dots, A w_m\}$ and H_m is an $m \times m$ Hessenberg matrix.

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- 3 Approximate the solution in the coarse correction subspace in a proper-norm

$$x_* = \arg \min_{\tilde{x} \in \text{Range}(W_m)} \|b - A \tilde{x}\|_2 = W_m H_m^{-1} Z_m^T b$$

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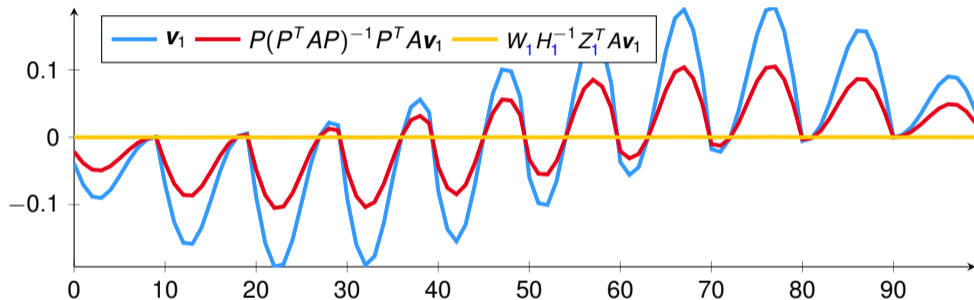
$$x_* = \arg \min_{\tilde{x} \in \text{Range}(W_m)} \|\mathbf{b} - A \tilde{x}\|_2 = W_m H_m^{-1} Z_m^T \mathbf{b}$$

Downside of euclidean minimization : Eigenvalues are squared

$$\Rightarrow \mathbf{v}_1^T E_{W_m} \mathbf{v}_1 = 1 - \frac{\lambda_1^2}{\lambda_1^2 + \delta_1} \text{ with } \delta_1 := \sum_{j>1} \epsilon_j^2 \lambda_j^2.$$

IV.2 - Alternative coarse correction

Approximation of the smallest eigenvector v_1 after 1 cycle - $(L_n - 0.625^2 I_n)$



$$\text{Range}(W_1) = \text{span} \left(\left\{ P(P^T A P)^{-1} P^T A v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

For each multigrid cycle m :

- 1 Create the coarse correction subspace

$$W_m = \left[P(P^T A P)^{-1} P^T A \mathbf{r}^{(0)}, \dots, P(P^T A P)^{-1} P^T A \mathbf{r}^{(m)} \right]$$

- 2 Construct the operators involved in the below generalized Arnoldi relation

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where $\text{Range}(Z_m) = \text{span}\{A \mathbf{w}_1, \dots, A \mathbf{w}_m\}$ and H_m is an $m \times m$ Hessenberg matrix.

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IV.2 - Alternative coarse correction

For each multigrid cycle m :

- 1 Create the **smoothed** coarse correction subspace

$$W_m = \left[q(A)^\nu P(P^T A P)^{-1} P^T A r^{(0)}, \dots, q(A)^\nu P(P^T A P)^{-1} P^T A r^{(m)} \right]$$

- 2 Construct the operators involved in the below generalized Arnoldi relation

$$A W_m = Z_m H_m,$$

where $\text{Range}(Z_m) = \text{span}\{A \mathbf{w}_1, \dots, A \mathbf{w}_m\}$ and H_m is an $m \times m$ Hessenberg matrix.

- 3 Approximate the solution in the **smoothed** coarse correction subspace in a proper-norm

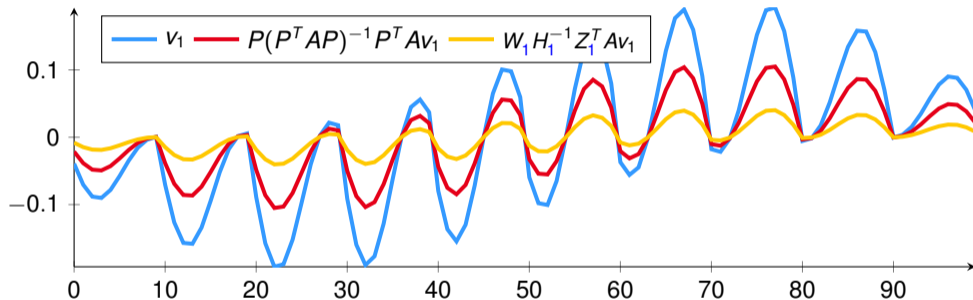
$$x_* = \arg \min_{\tilde{x} \in \text{Range}(W_m)} \|\mathbf{b} - A \tilde{x}\|_2 = W_m H_m^{-1} Z_m^T \mathbf{b}$$

Downside of euclidean minimization : Eigenvalues are squared

$$\Rightarrow \mathbf{v}_1^T E_{W_m} \mathbf{v}_1 = 1 - \frac{\lambda_1^2}{\lambda_1^2 + \delta_1} \text{ with } \delta_1 := \sum_{j>1} \left(\frac{q(\lambda_j^2)}{q(\lambda_1^2)} \right)^\nu \epsilon_j^2 \lambda_j^2.$$

IV.2 - Alternative coarse correction

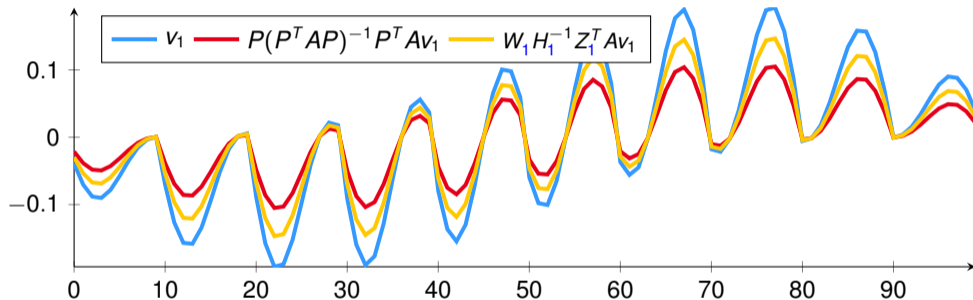
Approximation of the smallest eigenvector v_1 after 1 cycle - $(L_n - 0.625^2 I_n)$



$$\text{Range}(W_1) = \text{span} \left(\left\{ q(A) P(P^T A P)^{-1} P^T A v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

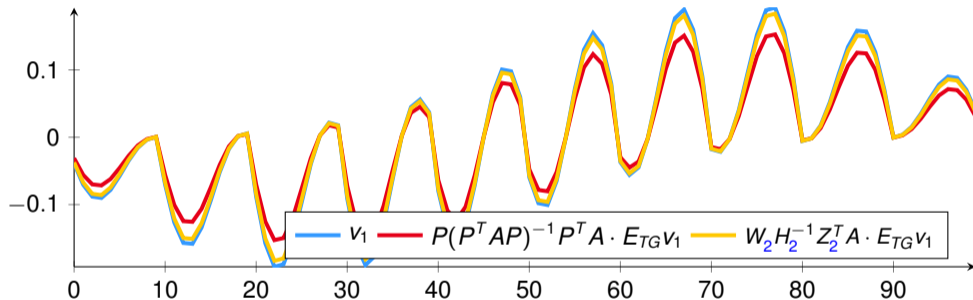
Approximation of the smallest eigenvector v_1 after 1 cycle - $(L_n - 0.625^2 I_n)$



$$\text{Range}(W_1) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

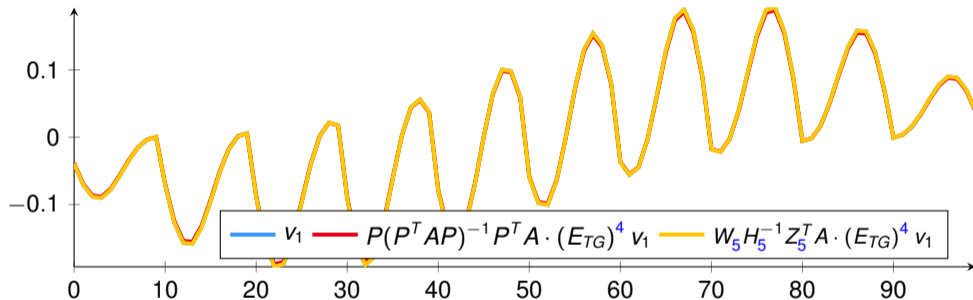
Approximation of the smallest eigenvector v_1 after 2 cycles - $(L_n - 0.625^2 I_n)$



$$\text{Range}(W_2) = \text{span} \left(\left\{ q(A)^2 P(P^T AP)^{-1} P^T A v_1, q(A)^2 P(P^T AP)^{-1} P^T A \cdot E_{TG} v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

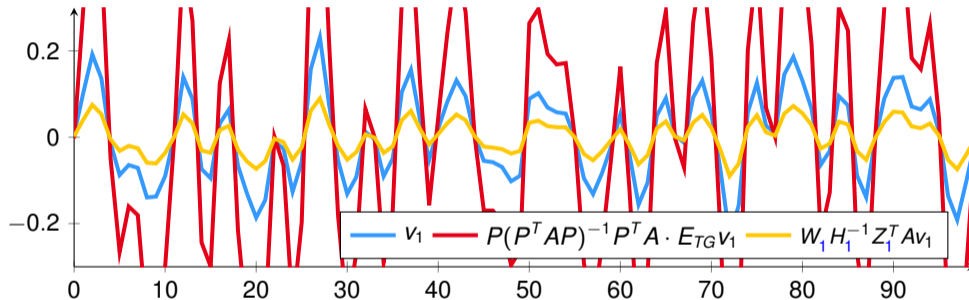
Approximation of the smallest eigenvector v_1 after 5 cycles - $(L_n - 0.625^2 I_n)$



$$\text{Range}(W_5) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1, \dots, q(A)^2 P(P^T A P)^{-1} P^T A \cdot (E_{TG})^4 v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

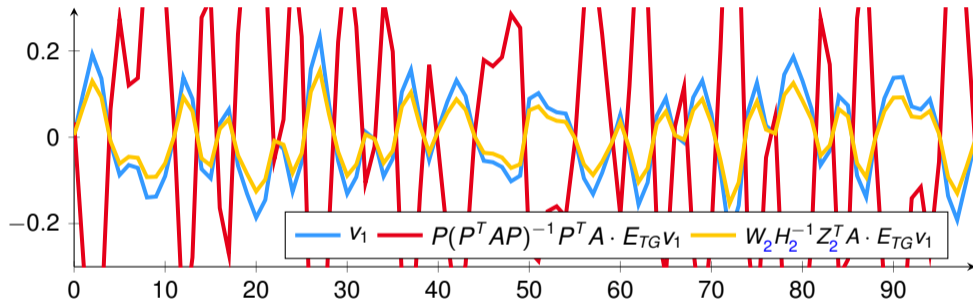
Approximation of the smallest eigenvector v_1 after 1 cycle - $(L_n - 1.435^2 I_n)$



$$\text{Range}(W_1) = \text{span} \left(\left\{ q(A)^2 P(P^T AP)^{-1} P^T A v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

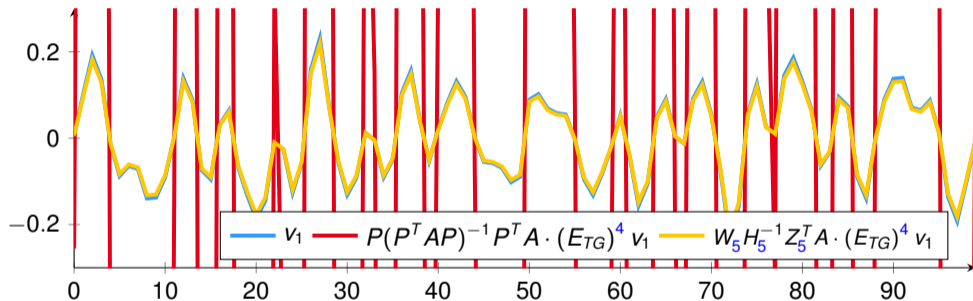
Approximation of the smallest eigenvector v_1 after 2 cycles - $(L_n - 1.435^2 I_n)$



$$\text{Range}(W_2) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1, q(A)^2 P(P^T A P)^{-1} P^T A \cdot E_{TG} v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

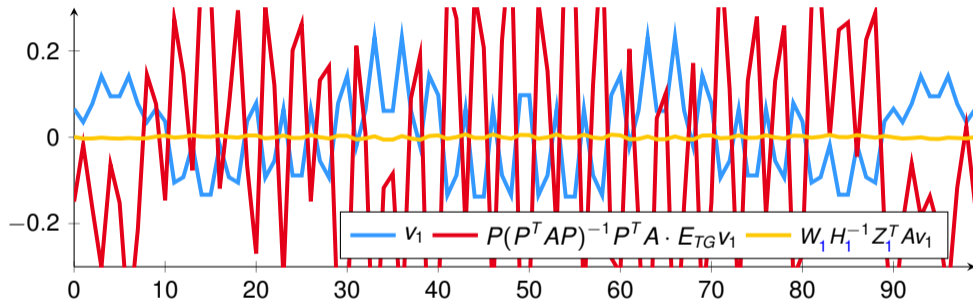
Approximation of the smallest eigenvector v_1 after 5 cycles - $(L_n - 1.435^2 I_n)$



$$\text{Range}(W_5) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1, \dots, q(A)^2 P(P^T A P)^{-1} P^T A \cdot (E_{TG})^4 v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

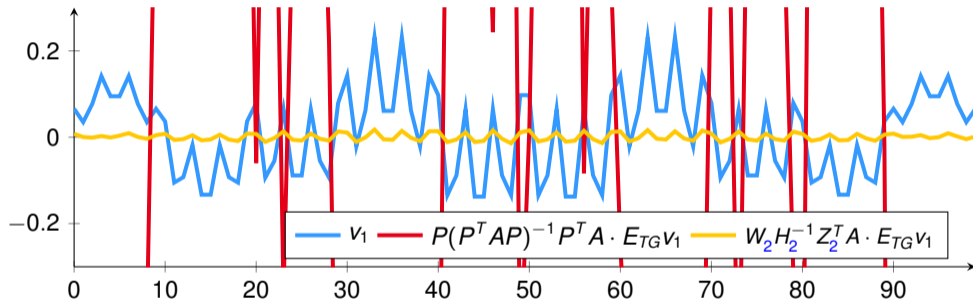
Approximation of the smallest eigenvector v_1 after 1 cycle - $(L_n - 1.713^2 I_n)$



$$\text{Range}(W_1) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

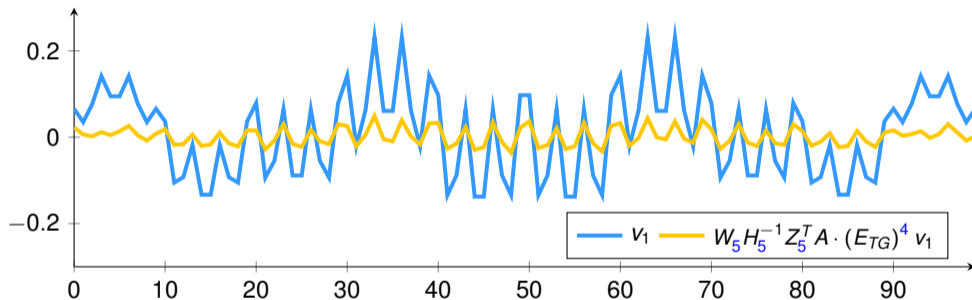
Approximation of the smallest eigenvector v_1 after 2 cycles - $(L_n - 1.713^2 I_n)$



$$\text{Range}(W_2) = \text{span} \left(\left\{ q(A)^2 P(P^T AP)^{-1} P^T A v_1, q(A)^2 P(P^T AP)^{-1} P^T A \cdot E_{TG} v_1 \right\} \right)$$

IV.2 - Alternative coarse correction

Approximation of the smallest eigenvector v_1 after 5 cycles - $(L_n - 1.713^2 I_n)$



$$\text{Range}(W_5) = \text{span} \left(\left\{ q(A)^2 P(P^T A P)^{-1} P^T A v_1, \dots, q(A)^2 P(P^T A P)^{-1} P^T A \cdot (E_{TG})^4 v_1 \right\} \right)$$

Table of contents

- I. Introduction and context on multigrid methods
- II. Smoother for both positive and negative eigenvalues
- III. Interpolation rules for oscillatory near-kernel space
- IV. Alternative coarse correction for indefinite problems
- V. Conclusion

V. Conclusion

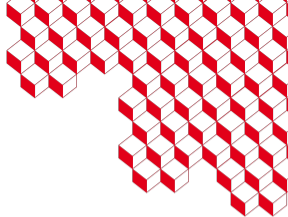
With no assumption on the underlying geometry, we designed :

- 1 A smoother for indefinite problems that damps the desired proportion of eigenvalues.
- 2 Interpolation rules that propagates the oscillatory smallest eigenvectors.
- 3 An alternative coarse correction based on Krylov outer iterations.

Topics of further research :

- 1 Enable Chebyshev nodes for disjoint intervals to avoid normal equations.
- 2 The sparsity of the interpolation operator has to be improved drastically.
- 3 Reduce the number of SpMv.

A paper is in progress...



Thanks! Any questions?

Appendix - Numerical Experiment

2D Helmholtz problem with absorbing boundary conditions, discretized with 10 points / wavelength (i.e., $kh = 0.625$).

- Number of smoothing steps $\nu := 2$.
- Number of test vectors $\kappa := 30$.
- Max number of interpolation points in the LSM set-up phase is 4.
- Multigrid stops when the relative residual norm becomes lower than 10^{-6} .

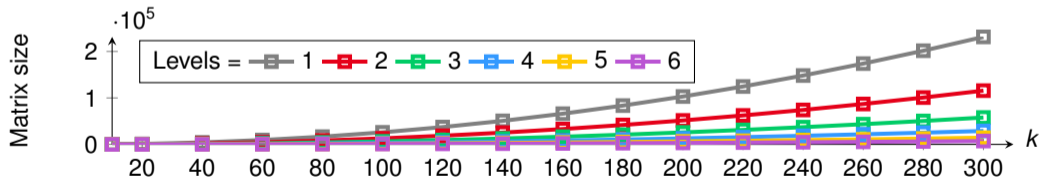


Figure 2: Number of iterations following the wavenumber k

Appendix - Numerical Experiment

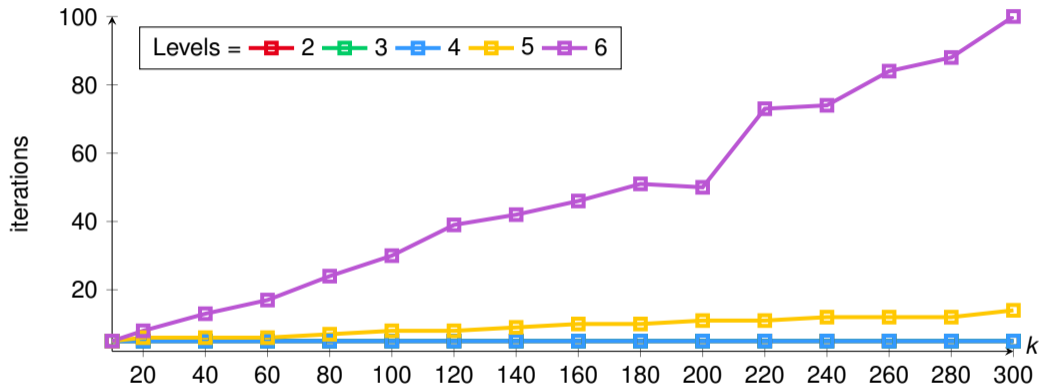


Figure 3: Number of iterations following the wavenumber k

Appendix - Numerical Experiment

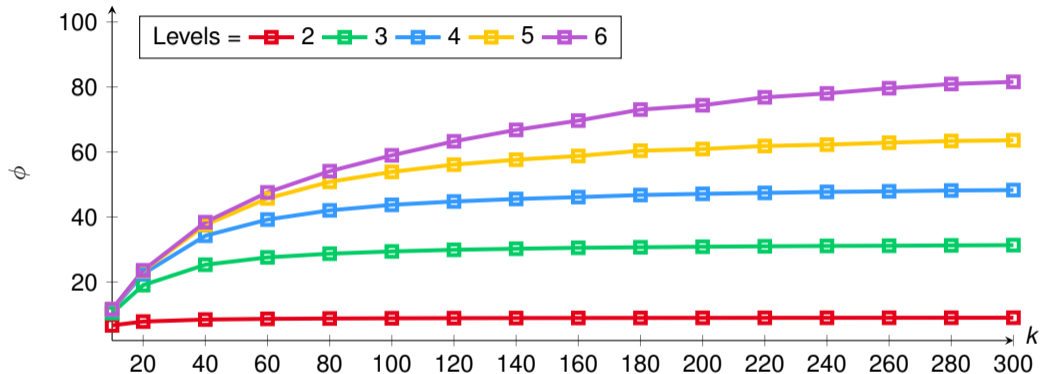


Figure 4: Operators complexity following the wavenumber k - $\phi := \frac{\sum_l \text{nnz}(A_l)}{\text{nnz}(A_0)}$