Applying GMRES to the Helmholtz equation with strong trapping: how does the number of iterations depend on the frequency?

Jeffrey Galkowski [1] Pierre Marchand [2] Alastair Spence [2] Euan Spence [2]

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[1]University College London

[2]University of Bath

Considered problem

Scattering problem

- Solving Helmholtz equation $-\Delta u - k^2 u = 0$ in $\mathbb{R}^d \setminus \overline{\Omega}$, where Ω is an obstacle containing an open cavity, with particular attention to elliptic cavity.
- Plane wave $u^I(\mathsf{x}) = e^{ik\mathsf{d}\cdot\mathsf{x}}$ with $\mathsf{d} = [\cos(\theta), \sin(\theta), 0]$.

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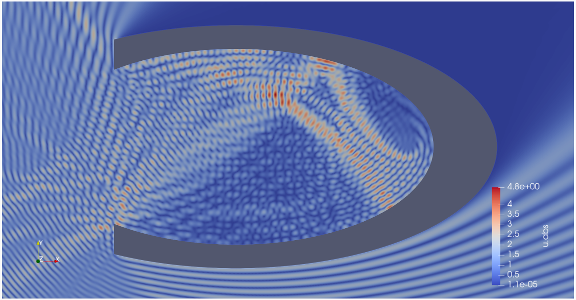

Figure 1: Absolute value of total field for $k = 122.473337808880$ and $\theta = \pi/4$

Fundamental solution

$$G_k(\mathsf{x}) := \frac{i}{4} H_0^{(1)}(k\|\mathsf{x}\|) \quad \text{for } \mathsf{x} \in \mathbb{R}^2 \setminus \{0\}, \quad \text{and} \quad \frac{e^{ik\|\mathsf{x}\|}}{4\pi\|\mathsf{x}\|} \quad \text{for } \mathsf{x} \in \mathbb{R}^3 \setminus \{0\},$$

Integral representation theorem

$$\int_{\partial\Omega} \mathsf{n}(\mathsf{y}) \cdot \nabla_{\mathsf{y}} G(\mathsf{x}-\mathsf{y}) u^s(\mathsf{y})\, \mathrm{d}\sigma(\mathsf{y}) - \int_{\partial\Omega} G(\mathsf{x}-\mathsf{y}) \frac{\partial u^s}{\partial \mathsf{n}}(\mathsf{y})\, \mathrm{d}\sigma(\mathsf{y}) = \begin{cases} u^s \text{ in } \mathbb{R}^d \setminus \overline{\Omega} \\ 0 \text{ in } \Omega \end{cases}$$

Boundary Integral Equations

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$$\mathcal{D}_k(u) - \mathcal{S}_k\left(\frac{\partial u}{\partial \mathbf{n}}\right) + u^I = u, \text{ in } \mathbb{R}^d \setminus \overline{\Omega}$$

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Dirichlet problem (sound-soft problem) $\gamma(u) = 0$

$$\gamma \circ \mathcal{S}_k\left(\frac{\partial u}{\partial \mathbf{n}}\right) = \gamma(u^I), \quad \text{and} \quad \frac{\partial}{\partial \mathbf{n}} \circ \mathcal{S}_k\left(\frac{\partial u}{\partial \mathbf{n}}\right) + \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial u^i}{\partial \mathbf{n}}$$

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$$S_k\left(\frac{\partial u}{\partial \mathbf{n}}\right) = \gamma(u^I), \quad \text{and} \quad \left(\frac{I}{2} + D_k'\right)\left(\frac{\partial u}{\partial \mathbf{n}}\right) = \frac{\partial u^i}{\partial \mathbf{n}}$$

Direct formulations

- Dirichlet problem (sound-soft problem):

$$A'_{k,\eta} := \frac{1}{2}I_{\mathrm{d}} + D'_k - i\eta S_k, \quad A'_{k,\eta} : L_2 \to L_2$$

$$A'_{k,\eta}\frac{\partial u}{\partial n} = \frac{\partial u^I}{\partial n} - i\eta\gamma u^I$$

- Neumann problem (sound-hard problem)

$$B_{k,\eta} := H_k + i\eta\left(\frac{1}{2}I_{\mathrm{d}} - D_k\right), \quad B_{k,\eta} : H_1 \to L_2$$

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Both are well-posed if $\Re(\eta) \neq 0$, we can use regularization for $B_{k,\eta}$

Quasimodes

Definition

v_α is said to be a quasimode if

$$-\Delta v_\alpha - k_\alpha^2 v_\alpha = O(L(k_\alpha)^{-1})$$

with Dirichlet boundary condition and the Sommerfeld radiation condition, where $\|v_\alpha\|_{L_2} = 1$ and $L(k_\alpha)$ "large".

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From Betcke, Chandler-Wilde, Graham, Langdon, and Lindner 2010

- $\|(A'_{k_\alpha,k_\alpha})^{-1}\|_{L_2\to L_2} \gtrsim L(k_\alpha)$
- if $\mathbb{R}^d \setminus \overline{\Omega}$ contains the ellipse $E := \{(x_1, x_2) \,:\, (x_1/a_1)^2 + (x_2/a_2)^2 < 1\}$, and $\partial\Omega$ coincides with the boundary of E in the neighborhoods of the points $(0, \pm a_2)$, then

  $L(t) = e^{\beta t}$ and k_α is related to eigenvalues of the Laplacian

Idea behind constructing quasimodes

Step 1 Build eigenfunctions of the Laplacian in E: using Matthieu functions, there exists

$$-\Delta u_{m,n} = k_{m,n}^2 u_{m,n}, \quad \text{in } E$$

Step 2 These eigenfunctions are exponentially localizing along the minor axis

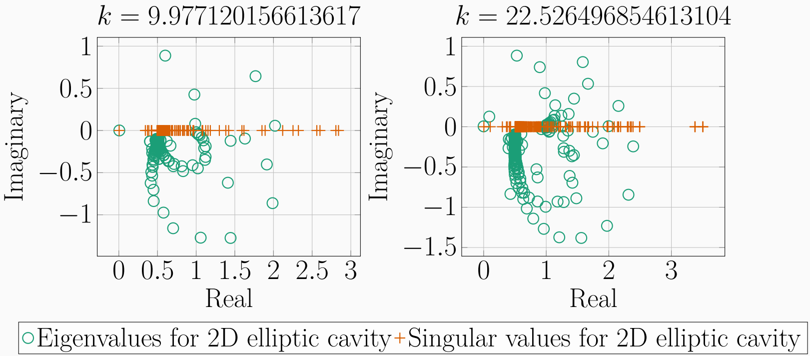
Step 3 Build quasimodes with particular extension and modification of these eigenfunctions to show $L(t) = e^{\beta t}$

Step 4 Using Weyl's law, the density of quasimodes is related to the density of eigenvalues for the Laplacian. It is $O(k^{d-1})$ in an interval.

Eigenvalues and singular values of $A'_{k,k}$

Discretization: P1 element, 10 points by wavelength

$$\mathsf{A}'_{k,k}\mathsf{v} = \lambda \mathsf{M}\mathsf{v}$$



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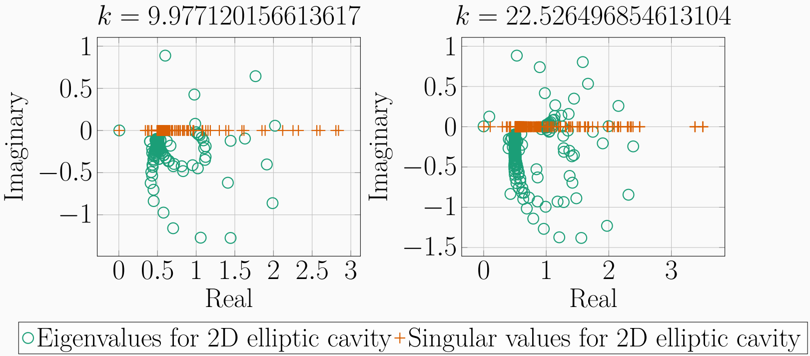
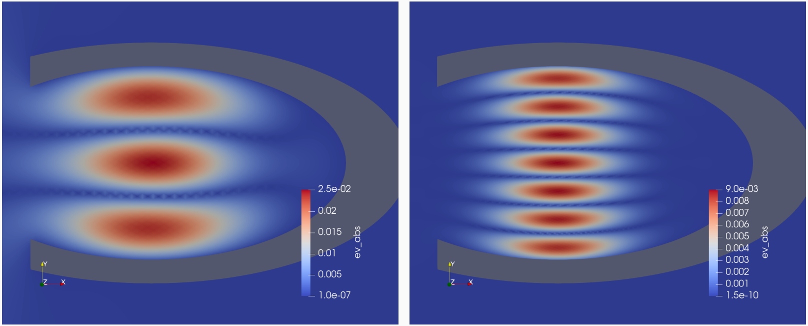


(Quasimode implies small eigenvalue) is difficult to prove!

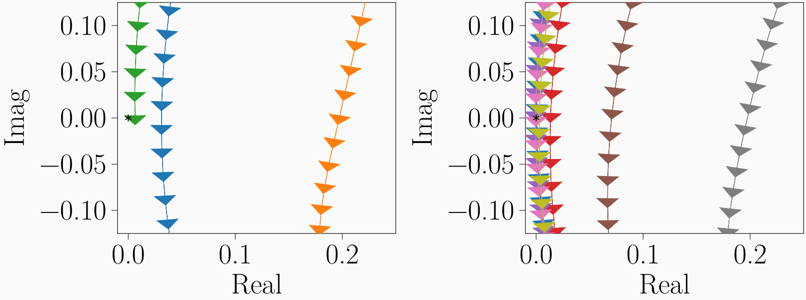
(see preprint Galkowski, Marchand, and E. A. Spence 2021 for PDE)

Eigenfunctions and bouncing ball modes



(a) $k = 9.977120156613617$ (b) $k = 22.526496854613104$

Figure 2: Eigenfunction associated with the smallest eigenvalue



(a) $k \in (5, 10)$

(b) $k \in (20, 25)$

Figure 3: Flow of eigenvalues for A'_k

How does GMRes depend on the frequency?

- $A'_{k,\eta}$ and $B_{k,\eta}$ are **non-normal**, so **GMRes** is often used to solve the associated linear system.

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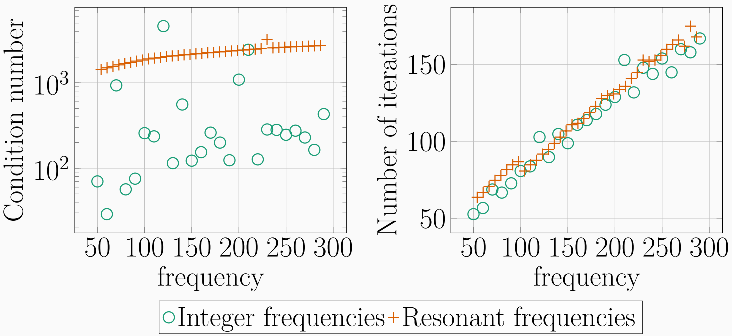

Figure 4: Scattering problem for an elliptic cavity with a plane wave of incident angle $\theta = 4\pi/10$ and $\mathsf{M}^{-1}\mathsf{A}'_{k,k}$

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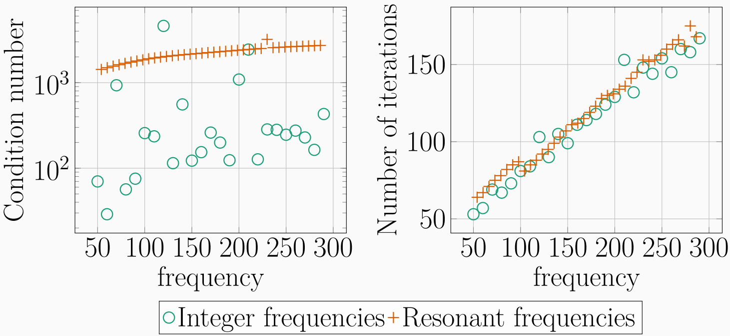

Figure 4: Scattering problem for an elliptic cavity with a plane wave of incident angle $\theta = 4\pi/10$ and $\mathsf{M}^{-1}\mathsf{A}'_{k,k}$

- **Goal:** get a better understanding of the k-dependency.

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GMRes convergence

Definition

Let $\mathsf{A} \in \mathbb{C}^{n\times n}$ non-singular, $\mathsf{b} \in \mathbb{C}^n$. We define

- initial guess: x_0
- initial residual: $\mathsf{r}_0 := \mathsf{b} - \mathsf{A}\mathsf{x}_0$
- Krylov space: $\mathcal{K}_m := \mathrm{Span}\left\{\mathsf{r}_0, \mathsf{A}\mathsf{r}_0, \ldots, \mathsf{A}^{m-1}\mathsf{r}_0\right\}$,

By definition,

$$\|\mathsf{r}_m\|_2 = \min_{x_m \in \mathsf{x}_0 + \mathcal{K}_m,} \|\mathsf{b} - \mathsf{A}\mathsf{x}_m\|_2 = \min_{\substack{p_m \in \mathbb{P}_m, \\ p_m(0)=1}} \|p_m(\mathsf{A})\mathsf{r}_0\|_2.$$

It is difficult to take into account r_0 in the analysis (very little literature and few results). Usually, one uses

$$\frac{\|\mathsf{r}_m\|_2}{\|\mathsf{r}_0\|_2} \leq \min_{\substack{p_m \in \mathbb{P}_m, \\ p_m(0)=1}} \|p_m(\mathsf{A})\|, \quad \text{(but not sharp)}$$

GMRes bounds: eigenvalues

Suppose $\mathsf{A} = \mathsf{V}\mathsf{D}\mathsf{V}^{-}1$

$$\min_{\substack{p_m \in \mathbb{P}_m, \\ p_m(0)=1}} \|p_m(\mathsf{A})\| \leq \kappa(\mathsf{V}) \min_{\substack{p_m \in \mathbb{P}_m, \\ p_m(0)=1}} \|p_m(\mathsf{D})\| \leq \kappa(\mathsf{V}) \min_{\substack{p_m \in \mathbb{P}_m, \\ p_m(0)=1}} \max_{\lambda \in \Lambda(\mathsf{A})} |p_m(\lambda)|$$

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Spectrum is not enough to describe GMRes convergence

GMRes bounds: numerical range

(Crouzeix and Palencia 2017) $W(\mathsf{A}) := \{\mathsf{x}^T \mathsf{A} \mathsf{x} \,|\, \mathsf{x} \in \mathbb{C}^n,\, \mathsf{x} \neq 0,\, \|\mathsf{x}\|_2 = 1\}$

$$\min_{\substack{p_m \in \mathbb{P}_m,\\ p_m(0)=1}} \|p_m(\mathsf{A})\| \leq (1+\sqrt{2}) \min_{\substack{p_m \in \mathbb{P}_m,\\ p_m(0)=1}} \max_{x \in W(\mathsf{A})} |p_m(x)|$$

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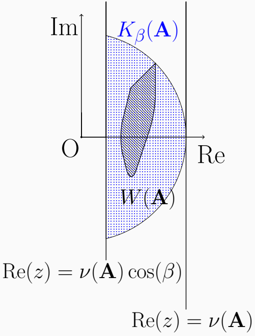
- $\nu(\mathsf{A}) := \max(|z| \,|\, z \in W(\mathsf{A})) \leq \|\mathsf{A}\|$
- (Beckermann, Goreinov, and Tyrtyshnikov 2005)

$$\min_{\substack{p_m \in \mathbb{P}_m, \\ p_m \text{Faber polynomial}, \\ p_m(0)=1}} \max_{x \in K_\beta(\mathsf{A})} |p_m(x)| \leq (2+\gamma)\gamma^m,$$

$$\gamma := 2 \sin\left(\frac{\beta}{4 - 2\beta/\pi}\right) < \sin(\beta)$$



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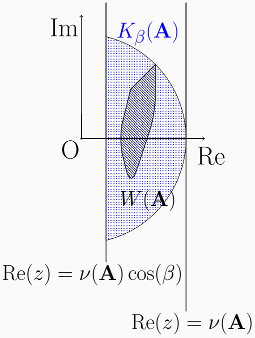

Hard to use with outliers near origin

Cluster+outlier model

Assumptions:

- $\sigma(\mathsf{A}) = \{\lambda_j\}_{j=1,\dots,n}$
- $|\lambda_j| < 1/2$ for $j = 1, \dots, l$ (outliers)
- $\Re(\lambda_j) > S > 0$ for $j = l+1, \dots, n$ (cluster)

Definitions

- Resolvent: $\mathsf{R}(\mathsf{x}) := (z\mathsf{I}_{\mathrm{d}} - \mathsf{A})^{-1}$
- Γ encloses the cluster in the complex plane, while Γ_j is a circle centered on λ_j for $j = 1 \dots, l$

Cluster+outlier model

- Spectral projectors:

$$P_{\mathrm{cl}} := \frac{1}{2\pi i}\int_{\Gamma} \mathsf{R}(\mathsf{x})\,\mathrm{d}x, \quad \text{and} \quad P_{\mathrm{out}} := \sum_{j=1}^{l} \frac{1}{2\pi i}\int_{\Gamma_j} \mathsf{R}(\mathsf{x})\,\mathrm{d}x$$

- $q_l(z) := \prod_{j=1}^{l}(1-\lambda_j^{-1}z)$, minimal polynomial associated with outliers

We use

$$\begin{aligned} p_m(\mathsf{A}) &= q_l(\mathsf{A})p_{m-l}(\mathsf{A}) = (P_{\mathrm{cl}} + P_{\mathrm{out}})q_l(\mathsf{A})p_{m-l}(\mathsf{A}) \\ &= \underbrace{P_{\mathrm{out}}q_l(\mathsf{A})}_{=0}p_{m-l}(\mathsf{A}) + P_{\mathrm{cl}}q_l(\mathsf{A})p_{m-l}(\mathsf{A}) \end{aligned}$$

Cluster+outlier model

Spectral projector: $P_{\mathrm{cl}} := \frac{1}{2\pi i}\int_\Gamma \mathsf{R}(x)\,\mathrm{d}x$

$$\frac{\|\mathsf{r}_m(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2}{\|\mathsf{r}_0(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2} \le \min_{\substack{p_{m-l}\in\mathbb{P}_{m-l},\\ p_{m-l}(0)=1}} \|P_{\mathrm{cl}} q_l(\mathsf{A}) p_{m-l}(\mathsf{A})\|$$

$$\le \frac{1}{2\pi}|\Gamma| \min_{\substack{p_{m-l}\in\mathbb{P}_{m-l},\\ p_{m-l}(0)=1}} \max_{z\in\Gamma} \left(\prod_{j=1}^{l} \frac{|\lambda_j - z|}{|\lambda_j|} \|\mathsf{R}(z)\| |p_{m-l}(z)|\right)$$

(Campbell, Ipsen, Kelley, and Meyer 1996)

How to choose Γ and p_{m-l}?

Guidelines:

- Γ should not cross $\Lambda_\delta := \left\{z \in \mathbb{C} \mid \|\mathsf{R}\| \geq \delta^{-1}\right\}$
- We should control the distance between Γ and the outliers
- We need to choose p_{m-l} to bound $\min \max |p_{m-l}(z)|$
- We should bound the length of Γ

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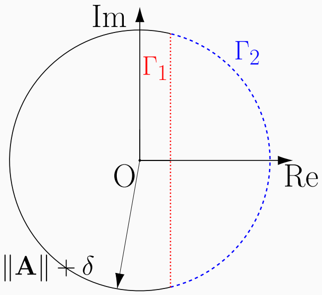
Solutions:

- Define Γ as a D-shaped domain to use Faber polynomials for p_{m-l}
- For Γ_2, we have $\Lambda_\delta(\mathbf{A}) \subset W(\mathbf{A}) + \delta \subset B(O, \|\mathbf{A}\| + \delta)$
- For Γ_1, Bauer-Fike theorem: $\Lambda_\delta \subseteq \cup_j B(\lambda_j, O(\delta))$



Algebraic bound

For $S > L > 0$, there exists $\delta > 0$ so that

$$\frac{\|\mathsf{r}_m(\mathsf{A}, \mathsf{b}, \mathsf{x}_0)\|_2}{\|\mathsf{r}_0(\mathsf{A}, \mathsf{b}, \mathsf{x}_0)\|_2} \lesssim \prod_{j=1}^{l} \frac{1}{|\lambda_j|} \cdot (D)^{l+1} \cdot \delta^{-1}(\gamma_\beta + 2)\gamma_\beta^{m-l}$$

where

- $D = \|\mathsf{A}\| + \delta$
- $\cos(\beta) = L/(\|\mathsf{A}\| + \delta)$
- $\gamma_\beta := 2\sin\left(\frac{\beta}{4 - 2\beta/\pi}\right) < \sin(\beta)$

Application to BEM

Properties of $A'_{k,k}$

Assumptions:

- $|\lambda_j| < 1/2$ for $j = 1, \ldots, l$, correspond to resonant frequencies, and move at $k-$independent speed
- $\Re(\lambda_j) > S > 0$ for $j = l + 1, \ldots, n$ are in a cluster
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A priori results:

- $\|A'_{k,k}\| \lesssim k^{1/3} \log(k+2)$ if $\partial\Omega$ does not contain a straight line, $\|A'_{k,k}\| \lesssim k^{1/2} \log(k+2)$ otherwise
- $\|(A'_{k,k})^{-1}\| \sim e^{Ck_\alpha}$ for resonant frequencies
- Bauer-Fike theorem: $\Lambda_\delta \subseteq \cup_j B(\lambda_j, \delta n \kappa(\lambda_j))$
- We choose $\delta^{-1} \sim k^{2d-2} \max_j \kappa(\lambda_j)$ to compensate for increasing density of outliers and non-normality

Bound on the number of iterations

We suppose eigenvalues and singular values are well-approximated by the Galerkin discretization $M^{-1}A'_{k,k}$.

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Theorem

With previous hypotheses, for $\varepsilon > 0$ and $L > 0$ with $L < S$, we have

$$m_{convergence} \gtrsim k_\alpha^{d-1} + k_\alpha^{1/2}\log(k_\alpha)(k_\alpha^d + k_\alpha^{d-1}\log(k_\alpha) + \log(\max_{1\le j\le n_k}(\kappa(\lambda_j)))) + O(\log(k_\alpha)),$$

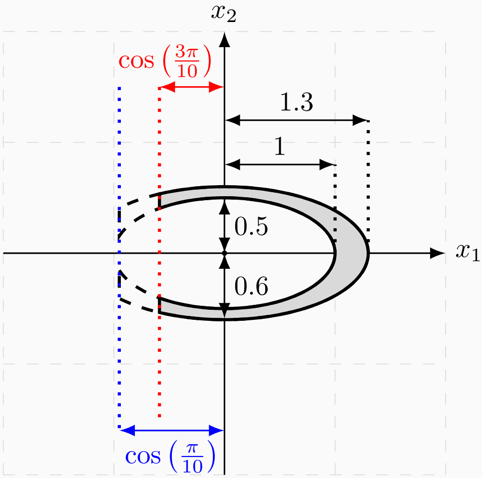
where

- *the factor $k_\alpha^{1/2}\log(k_\alpha)$ comes from the growth of the operator norm,*
- *k_α^{d-1} comes from the growth of the outlier density,*
- *k_α^d comes from the exponentially decreasing eigenvalues and their density growth.*

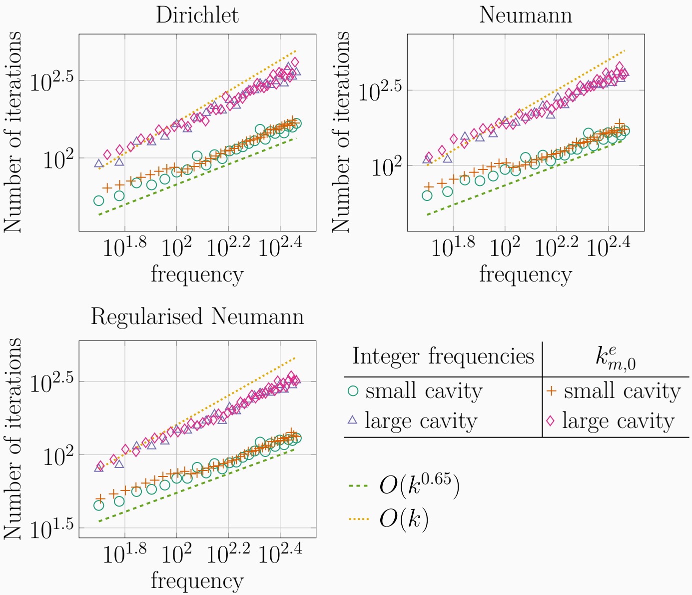
Numerical experiments

Considered problem

$$\mathsf{M}^{-1}\mathsf{A}'_{k,k}\mathsf{x} = \frac{\partial}{\partial \mathsf{n}}\mathsf{u}^I - ik\mathsf{u}^I$$



Number of iterations



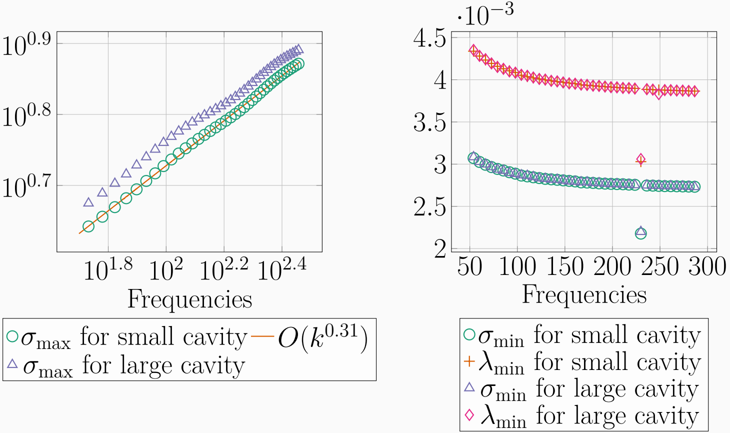


Figure 5: Singular values and eigenvalues of $M^{-1}A'_{k,k}$ for bouncing ball modes

Strong trapping has a weak effect for most frequencies[1]

[1]Lafontaine, E. A. Spence, and Wunsch 2020.

Result without exponentially decreasing eigenvalues

Corollary

With previous hypotheses, for $\varepsilon > 0$ and $L > 0$ with $L < S$, we have

$$m_{convergence} \gtrsim k^{d-1} + k^{1/2}\log(k)(k^{d-1} + k^{d-1}\log(k\log(k)) + \log(\max_{1\leq j\leq n_k}(\kappa(\lambda_j)))) + O(\log(k)),$$

where

- *the factor* $k^{1/2}\log(k)$ *comes from the growth of the operator norm,*
- k^{d-1} *comes from the growth of the outlier density,*

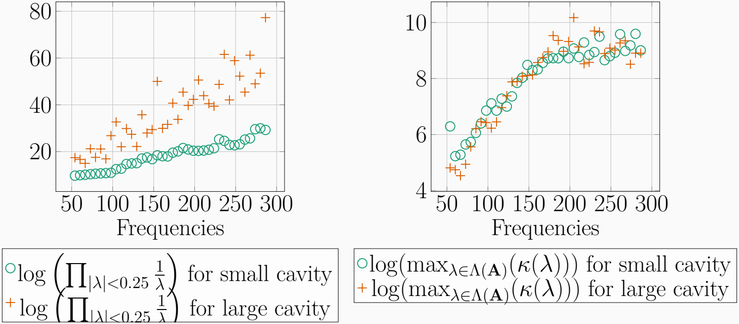


Figure 6: Outliers and eigenvalue conditioning of $M^{-1}A'_{k,k}$ for bouncing ball modes

3D results

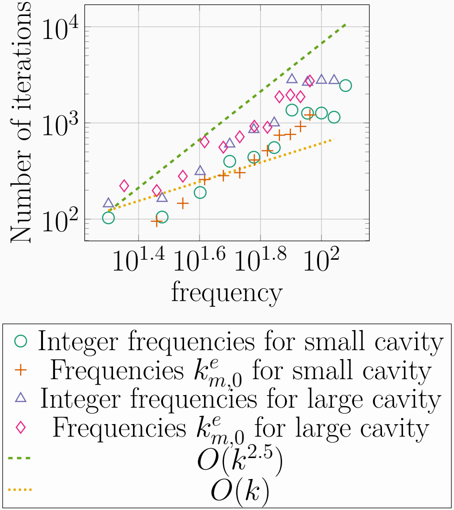


Figure 7: Number of iterations for incident angle $\theta = 4\pi/10$ and a 3D ellipsoid cavity

Why is it not sharp?

- What we define as a cluster, is itself a “cluster+outlier”
- GMRes has a super linear convergence, we have

$$\frac{\|\mathsf{r}_m(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2}{\|\mathsf{r}_0(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2} \lesssim \theta^m, \quad \theta < 1$$

but it should be

$$\frac{\|\mathsf{r}_m(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2}{\|\mathsf{r}_0(\mathsf{A},\mathsf{b},\mathsf{x}_0)\|_2} \lesssim \theta(m)^m, \quad \theta_m \to 0$$

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See videos

Why is it not sharp?

- The right-hand side has a great influence

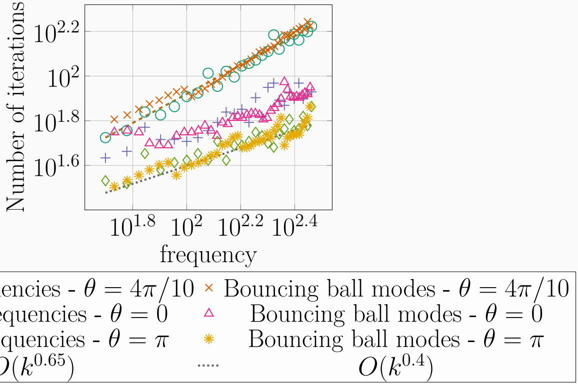


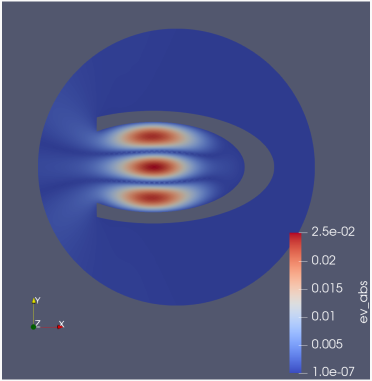
Figure 8: Number of iterations for Dirichlet problem with a small cavity

Conclusion

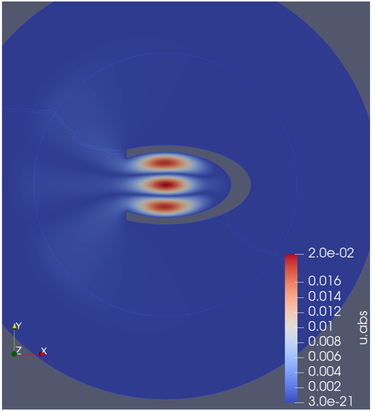
What does this approach bring?

- It shows what are the features that makes the number of iterations increases,
- It gives a tool to analyze new formulation,
- The GMRes bound can be used in other situations
- (Quasimodes implies small eigenvalues) does not depend on integral formulation

Quasimodes everywhere



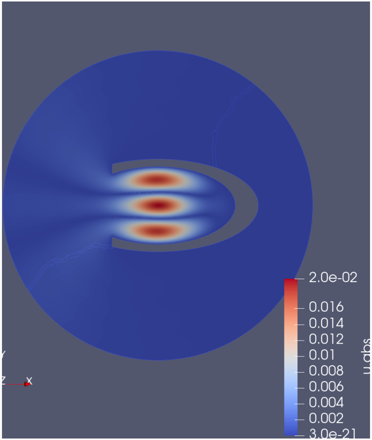
(a) BEM (FreeFEM)



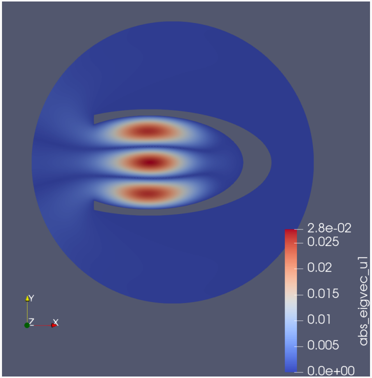
(b) FEM with PML (FreeFEM)

Figure 9: Absolute value of the eigenvector associated with the smallest eigenvalue for $k = 9.977120156613617$ and small cavity

Quasimodes everywhere



(a) FEM with impedance condition (FreeFEM)



(b) FEM BEM coupling (Xlife++)

Figure 10: Absolute value of the eigenvector associated with the smallest eigenvalue for $k = 9.977120156613617$ and small cavity

Conclusion

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Marchand, Galkowski, A. Spence, and E. A. Spence 2021

Outlook

- Influence of right-hand side
- Regularised Neumann problem
- Build robust preconditioners

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Thank you for your attention!