Padé approximation for Helmholtz frequency response problems

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Model Reduction for Parametrized Systems IV
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Parametric Helmholtz BVP

We consider the Helmholtz problem

$$-\Delta u - k^2 u = f \quad \text{in } D$$

coupled with either Dirichlet or Neumann homogeneous b.c. on ∂D, where

- D is a open bounded regular domain in $\mathbb{R}^d$, $d = 1, 2, 3$
- the wavenumber k^2 is parametric and belongs to the interval of interest $K := [k^2_{min}, k^2_{max}] \subset \mathbb{R}_{>0}$
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- $f \in L^2(D)$

We denote with V either $H^1(D)$ or $H^1_0(D)$ and assume the functions in V to be complex-valued.

Weak formulation: given $f \in L^2(D)$ and $k^2 \in K$, find $u_{k^2} \in V$ such that

$$\int_D \nabla u_{k^2}(x) \cdot \overline{\nabla v(x)} dx - k^2 \int_D u_{k^2}(x) \overline{v(x)} dx = \int_D f(x) \overline{v(x)} dx \quad \forall v \in V$$

Helmholtz frequency response problem

We introduce the Helmholtz frequency response function (solution map)

$$\mathcal{S} : K \to V, \quad k^2 \mapsto \mathcal{S}(k^2) = u_{k^2}$$

Goal: to know $\mathcal{S}(k^2)$ for any $k^2 \in K$, where K contains high wavenumbers (mid- and high-frequency regime)

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Due to the oscillatory behavior of the solutions, the finite element approximation is accurate only on fine meshes or with high polynomial degrees. Hence, the direct numerical computation of u_{k^2} for a whole range of frequencies is out of reach.

Method: to reduce the computational cost by approximating $\mathcal{S}$ using a Padé-type technique

OFFLINE: compute evaluations of $\mathcal{S}$ (and of its derivatives) only at few frequencies

ONLINE: given a new frequency $\bar{k}^2$, estimate $\mathcal{S}(\bar{k}^2)$ by evaluating the constructed approximation of $\mathcal{S}$

Outline

1. Regularity of the frequency response function
2. Rational (Padé) approximation of the solution map
3. Numerical results

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Frequency response function - complex wavenumbers

We extend the solution map $\mathcal{S}$ to the complex plane $\mathbb{C}$. $\mathcal{S}$ associates each complex wavenumber $z \in \mathbb{C}$ with $u_z \in V$, where u_z solves

$$\int_D \nabla u_z(x) \cdot \overline{\nabla v(x)} dx - z \int_D u_z(x) \overline{v(x)} dx = \int_D f(x) \overline{v(x)} dx \quad \forall v \in V$$

Remark: extending $\mathcal{S}$ to the complex plane is equivalent to perturb the Helmholtz problem adding the damping term $i\mathrm{Im}\,(z)\, u$.

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Denote with Λ the set of eigenvalues of the Laplace bvp with the considered boundary conditions. Then $\mathcal{S}$ is well-defined on $\mathbb{C} \setminus \Lambda$ (see [Bonizzoni–Nobile–Perugia2016]).

A-priori bound for the Helmholtz solution

Given a positive real weight $w > 0$, we introduce the $H^1(D)$-weighted norm

$$\|v\|_{1,w} := \sqrt{\|\nabla v\|_{L^2(D)}^2 + w^2 \|v\|_{L^2(D)}^2}$$

Remark: $\|\cdot\|_{1,w}$ is equivalent to the standard $H^1(D)$-norm $\|\cdot\|_1$ (with $w = 1$).

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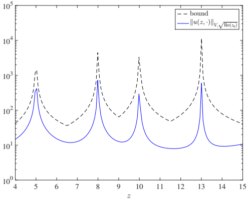
Proposition [Bonizzoni–Nobile–Perugia 2016]

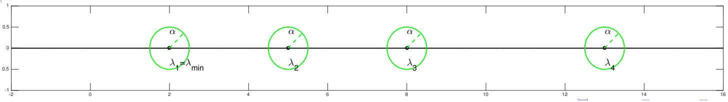
Let $z \in \mathbb{C} \setminus \Lambda$. Consider the Helmholtz problem with wavenumber z

$$-\Delta u_z(x) - z\, u_z(x) = f(x), \quad x \in D$$

with either Dirichlet or Neumann hom. b.c. on ∂D. Let $\lambda_{min} := \min\{\lambda \in \Lambda\}$. If $\min_{\lambda_j \in \Lambda} |\lambda_j - z| > \alpha > 0$ then the unique solution $u_z \in V$ satisfies the a-priori bound

$$\|u_z\|_{1,w} \leq \frac{\sqrt{|z-\lambda_{min}| + |\mathrm{Re}(z)| + w^2}}{\alpha} \|f\|_{L^2(D)}.$$





Regularity of the frequency response function

- $\mathcal{S}$ is continuous in $\mathbb{C} \setminus \Lambda$, i.e. $\lim_{h\to 0} \|\mathcal{S}(z+h) - \mathcal{S}(z)\|_{1,w} = 0$
- $\mathcal{S}$ admits a complex derivative $\dfrac{d\mathcal{S}}{dz}(z) := \lim\limits_{h\to 0} \dfrac{\mathcal{S}(z+h) - \mathcal{S}(z)}{h}$ for $z \in \mathbb{C} \setminus \Lambda$, which is the unique solution of

$$\int_D \nabla \frac{d\mathcal{S}}{dz} \cdot \overline{\nabla v}\, dx - z \int_D \frac{d\mathcal{S}}{dz} \overline{v}\, dx = \int_D \mathcal{S}(z)\overline{v}\, dx \quad \forall v \in V$$

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Moreover, $\mathcal{S}$ is meromorphic in $\mathbb{C}$ with poles of order 1.

Indeed, let μ_j be the (finite) multiplicity of each eigenvalue of the Laplacian $\lambda_j \in \Lambda$, and $\{\varphi_j\}_{j=1}^{\mu_j}$ the corresponding eigenfunctions. Then, the frequency response function can be expanded as

$$\mathcal{S}(z) = u_z = \sum_{j=1}^{\infty} \sum_{i=1}^{\mu_j} \frac{f_{j,i}}{\lambda_j - z} \varphi_{j,i}$$

Outline

Rational approximation of Hilbert space-valued functions

For Hilbert space-valued functions a rational (Padé) approximation $S_{[M/N]} : \mathbb{C} \to V$ is the ratio of two polynomials of degree M and N respectively

$$\mathcal{S}_{[M/N]}(z) = \frac{\mathcal{P}_{[M/N]}(z)}{\mathcal{Q}_{[M/N]}(z)}$$

with

- numerator: $\mathcal{P}_{[M/N]} \in \mathbb{P}_M(\mathbb{C}; V)$, i.e., $\mathcal{P}_{[M/N]}(z) = \sum_{i=0}^{M} p_i(z) z^i$, with coefficients $p_i(z) \in V$
- denominator: $\mathcal{Q}_{[M/N]} \in \mathbb{P}_N(\mathbb{C})$, i.e., $\mathcal{Q}_{[M/N]}(z) = \sum_{i=0}^{N} q_i z^i$, with coefficients $q_i \in \mathbb{C}$.

Least Square Padé approximant for $\mathcal{S}$

[Guillame–Huard–Robin1997], [Huard–Robin1999]

Notation: we denote with $\mathcal{S}_\alpha$ the α-th order Taylor coeff. of $\mathcal{S}$ in z_0, and with $(\mathcal{S}(z))^E$ the Taylor pol. of degree E, i.e. $(\mathcal{S}(z))^E = \sum_{\alpha=0}^{E} \mathcal{S}_\alpha (z - z_0)^\alpha$

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Functional $j_{\rho,E}$: given $P(z) = \sum_{i=0}^{M} p_i(z)(z-z_0)^i \in \mathbb{P}_M(\mathbb{C}; V)$, $Q(z) = q_i(z-z_0)^i \in \mathbb{P}_N(\mathbb{C})$, $\rho \in \mathbb{R}^+$ and $E \in \mathbb{N}$, we define

$$j_{\rho,E}(P,Q) := \left(\sum_{\alpha=0}^{E} \left\| (Q(z)\mathcal{S}(z) - P(z))_\alpha \right\|_{1,w}^2 \rho^{2\alpha} \right)^{1/2}$$

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Normalization of Q: $\mathbb{P}_N^\star(\mathbb{C}) = \left\{ Q(z) = \sum_{i=0}^{N} q_i z^i \in \mathbb{P}_N(\mathbb{C}) : \ \sum_{i=0}^{N} |q_i|^2 = 1 \right\}$

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Least squares Padé approximant: Let $E \geq M+N$.

$$\mathcal{S}_{[M/N]}(z) = \frac{\mathcal{P}(z)}{\mathcal{Q}(z)}, \quad (\mathcal{P}, \mathcal{Q}) = \operatorname{argmin}_{\substack{P \in \mathbb{P}_M(\mathbb{C};V) \\ Q \in \mathbb{P}_N^\star(\mathbb{C})}} j_{\rho,E}(P,Q)$$

The Padé minimization problem admits at least one solution (minimization of a continuous functional on a compact set).

Construction of the least squares Padé approximant

Starting point: Compute $\mathcal{S}(z_0)$ and the first E derivatives $\mathcal{S}_\alpha$, $\alpha = 1, 2, \ldots, E$ by

$$\int_D \nabla \mathcal{S}_\alpha(z) \cdot \overline{\nabla v} \; dx - z \int_D \mathcal{S}_\alpha(z) \overline{v} \; dx = \alpha \int_D \mathcal{S}_{\alpha-1}(z) \overline{v} \; dx \quad \forall \; v \in V$$

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Reduced functional:

$$j_{\rho,E}(P,Q)^2 \quad = \sum_{\alpha=0}^{E} \left\| (Q\mathcal{S} - P)_\alpha \right\|_{1,w}^2 \rho^{2\alpha}$$

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$$\begin{aligned} j_{\rho,E}(P,Q)^2 &= \textstyle\sum_{\alpha=0}^{E} \|(Q\mathcal{S}-P)_\alpha\|_{1,w}^2\, \rho^{2\alpha} \\ &= \textstyle\sum_{\alpha=0}^{M} \|(Q\mathcal{S}-P)_\alpha\|_{1,w}^2\, \rho^{2\alpha} + \sum_{\alpha=M+1}^{E} \|(Q\mathcal{S}-P)_\alpha\|_{1,w}^2\, \rho^{2\alpha} \end{aligned}$$

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Take P such that $P_\alpha = (Q\mathcal{S})_\alpha$ for $0 \leq \alpha \leq M$, and define the reduced functional $\bar{j}_{\rho,E}(Q)^2 = \sum_{\alpha=M+1}^{E} \|(Q\mathcal{S})_\alpha\|_{1,w}^2\, \rho^{2\alpha}$ (quadratic form in $\{q_i\}$)

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Eigenvalue problem: $\mathcal{Q}$ corresponds to the "smallest" eigenvector of $\bar{j}_{\rho,E}(Q)$

$$\min_{Q \in \mathbb{P}_N(\mathbb{C})} \bar{j}_{\rho,E}(Q), \quad \text{s.t. } \textstyle\sum_{i=0}^{N} |q_i|^2 = 1$$

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A fast version of the algorithm is under investigation: see the poster presented by D. Pradovera!

Convergence result

Theorem [Bonizzoni–Nobile–Perugia 2016]

Let $N \in \mathbb{N}$ be fixed, and $R > 0$ s.t. $\overline{B(z_0, R)}$ contains exactly N poles $\lambda_l, \dots, \lambda_{l+N}$ of $\mathcal{S}$. Denote $G = \{\lambda_l, \dots, \lambda_{l+N}\}$. Then

$$\lim_{M\to\infty} \left\|\mathcal{S}(z) - \mathcal{S}_{[M/N]}(z)\right\|_{1,w} = 0$$

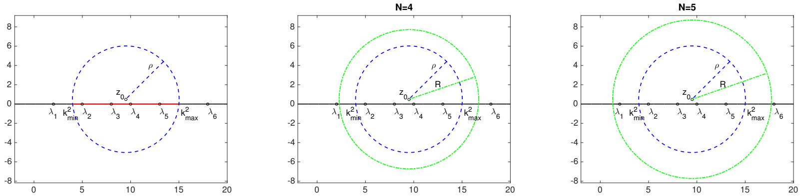
uniformly on all compact subsets of $B(z_0, R) \setminus G$.

In particular, let $K_\alpha := \cup_{\lambda\in\Lambda\cap K}(\lambda-\alpha, \lambda+\alpha) \subset K$, where $K = [k^2_{min}, k^2_{max}]$ is the interval of interest, and $\alpha > 0$. Then $\exists\, M^\star$ s.t. $\forall\, M \geq M^\star$,

$$\left\|\mathcal{S}(z) - \mathcal{S}_{[M/N]}(z)\right\|_{1,w} \leq C\frac{1}{\alpha}\left(\frac{\rho}{R}\right)^{M+1}, \quad \forall z \in K \setminus K_\alpha$$

where $\rho_K < \rho < R$, with $\rho_K = \min_{z\in K}|z_0 - z|$, and C depends on ρ_K, ρ, R, N, $g_{K,\alpha} := \min_{z\in K\setminus K_\alpha}|g(z)|$, z_0, $\lambda_{min} = \min \lambda \in \Lambda$ and $\|f\|_{L^2(D)}$.

Example to clarify the ideas...



1. $K = [k^2_{min}, k^2_{max}]$ interval of interest, which contains 4 poles
2. Fix z_0 with $\mathrm{Im}(z_0) \neq 0$ and $\rho > 0$ s.t. $K \subset B(z_0, \rho)$
3. Take $N = 4$ and $R > \rho$ s.t. $\overline{B(z_0, R)}$ contains exactly 4 poles
4. Construct the Padé approximant $\mathcal{S}_{[M/N]}$. The convergence rate is $\left(\frac{\rho}{R}\right)^{M+1}$
5. If $N = 5$, we can choose R larger s.t. $\overline{B(z_0, R)}$ contains exactly 5 poles. The convergence is faster!

Geometrical interpretation:

- ρ: it is the radius of the smallest disk $B(z_0, \rho)$ which contains the interval of interest.
- R: it is the radius of the biggest disk $B(z_0, R)$ which contains N poles of $\mathcal{S}$ (i.e. N eigenvalues of the Laplacian).

Random wave number - Convergence result

- Consider $k^2 \in K := [k^2_{min}, k^2_{max}]$ random with given distribution μ
- QoI: $X(k^2) = \mathcal{L}(\mathcal{S}(k^2))$, with $\mathcal{L} : V \to \mathbb{R}$ a linear and bounded functional
- Approximate QoI: $X_P(k^2) = \mathcal{L}(\mathcal{S}_{[M/N]}(k^2))$
- Characteristic function $\phi_X(t) = \mathbb{E}\left[e^{iXt}\right]$; cdf $F_X(t) = \mathbb{P}\{X \leq t\}$

From the uniform convergence of the Padé approximant $\mathcal{S}_{[M/N]}$ on compact subsets of $K \setminus G$, we infer the convergence of ϕ_{X_P} and F_{X_P} :

- for any $t \in \mathbb{R}_+$

$$|\phi_X(t) - \phi_{X_P}(t)| \leq 2\,|K_\alpha| + tLC\frac{1}{\alpha}\left(\frac{\rho}{R}\right)^{M+1}|K \setminus K_\alpha|$$

- for any $0 < p < +\infty$ and $\delta \in \mathbb{R}$

$$|F_X(\delta) - F_{X_P}(\delta)| \leq 2\,|K_\alpha| + 3\left(\frac{D_X(\delta LC)}{\alpha}\left(\frac{\rho}{R}\right)^{M+1}\right)^{\frac{p}{p+1}}|K \setminus K_\alpha|^{\frac{1}{p+1}}$$

where $0 < D_X(\delta) \leq sup_x f_X(x)$, with f_X the pdf of X.

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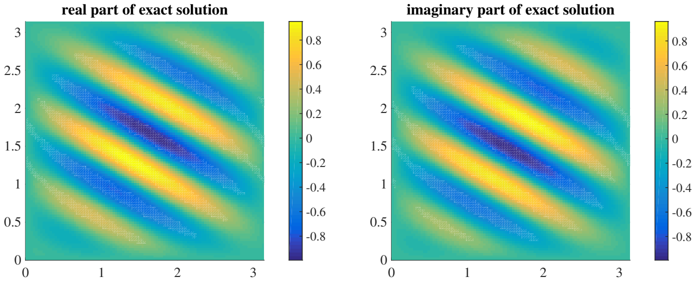
Test 1: Setting

Let $D = [0,\pi] \times [0,\pi]$, and consider the Helmholtz problem with homogeneous Dirichlet boundary conditions on ∂D.
Let $\nu^2 \in \mathbb{R}^+ \setminus \Lambda$, and $\mathbf{d} = (d_1, d_2) \in \mathbb{R}^2$.
The loading term $f(\mathbf{x}) = f(x_1, x_2)$ is such that the unique solution of the considered Helmholtz problem with wavenumber ν^2 is the product between the plane wave traveling along the direction $\mathbf{d}$, $v(\mathbf{x}) = e^{-i\nu \mathbf{d}\cdot\mathbf{x}}$, and the bubble $w(\mathbf{x}) = \frac{16}{\pi^2} x_1 x_2 (x_1 - \pi)(x_2 - \pi)$.

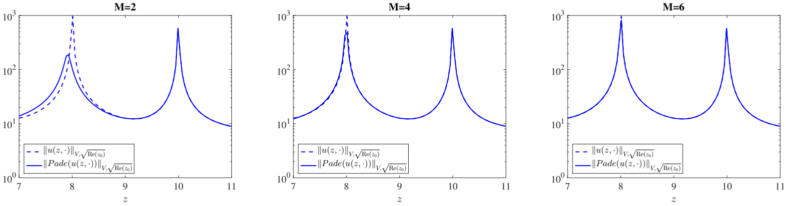


$$\nu = \sqrt{12}, \mathbf{d} = (\cos(\pi/6), \sin(\pi/6))$$

Test 1

Consider $K = [7, 11]$, which contains two eigenvalues of the Laplace operator: $\lambda = 8$ (multiplicity one) and $\lambda = 10$ (multiplicity two), i.e. K contains two simple poles of $\mathcal{S}$.

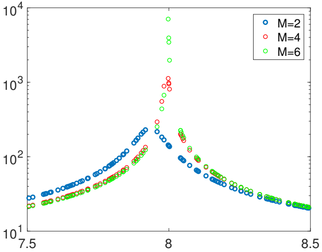
- Given $N = 2$ we construct the Padé approximant $\mathcal{S}_{[M/N]}$ centered in $z_0 = 10 + 0.5i$.
- We partition uniformly K in 100. At each point z of the mesh, the solution $\mathcal{S}_h(z) = u_h(z, \cdot)$ is computed vie the $\mathbb{P}^3$ continuous FE method.



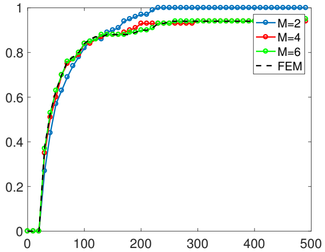
Comparison between the norm of the FE solution $\|u_h(z, \cdot)\|_{1,w}$ (dashed line), and the norm of the Padé approximant $\|u_{P,h}(z, \cdot)\|_{1,w}$ (solid line).

Test 1: Random wavenumber

Here $k^2 \sim \mathcal{U}([7.5; 8, 5])$; QoI $X(k^2) = \|u_{k^2}\|_{1,w}$



sampled X_P



cumulative distribution function

Test 2: Transmission/Reflection problem

Consider the square domain $D = (-1, 1)^2$ with two different refractive indices. The interface is located in $y = 0$. Problem: find $u \in H^1(D)$ s.t.

$$\begin{cases} -\Delta u - k^2 \varepsilon_r u = 0 & \text{in } \Omega \\ u|_{\partial D} = g_\theta \end{cases} \qquad \text{where } \varepsilon_r = \begin{cases} 4, & \text{if } y < 0 \\ 1, & \text{if } y > 0 \end{cases}$$

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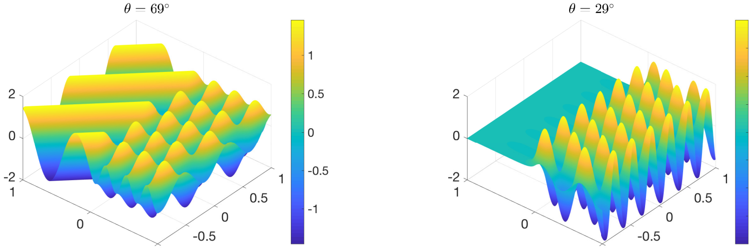
Incident plane wave $u^i = e^{iz\mathbf{d}\cdot\mathbf{x}}$, with $\mathbf{d} = (\cos(\theta), \sin(\theta))$.
Depending on the value of the parameter θ, the solution u behaves differently.
There exists a critical value θ_c s.t.

- if $\theta > \theta_c$, the wave is refracted
- if $\theta < \theta_c$, we have internal reflection



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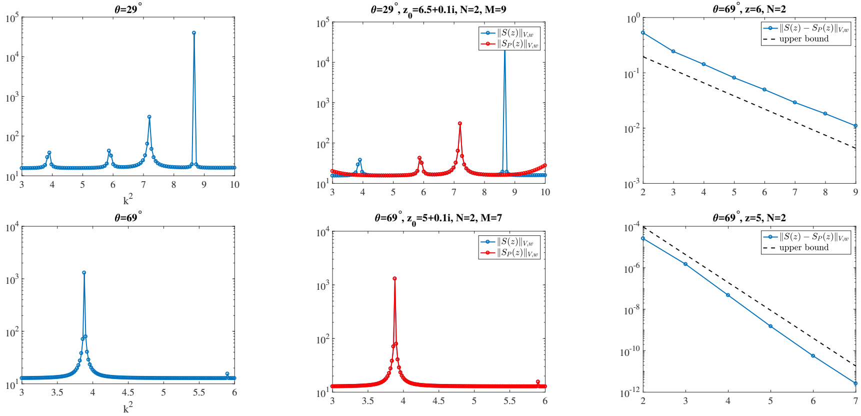
We let k vary in the interval of interest K



- The frequency response map is meromorphic in $\mathbb{C}$, with (real) poles of order one (see [Bonizzoni–Nobile–Perugia–Pradovera2018])
- The Padé approximant $\mathcal{S}_{[M/N]}$ is able to catch the singularities of $\mathcal{S}$
- The approximation error decays as the predicted rate $\frac{\rho}{R}^{(M+1)}$

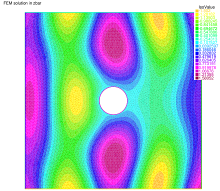
Test 3: Scattering problem

Consider the scattering of acoustic waves at a scatterer occupying the domain $\mathcal{B}(0, 0.5) \subset \mathbb{R}^2$. Let g be the impedance trace of the incident plane wave $u^i = e^{iz\mathbf{d}\cdot\mathbf{x}}$, i.e., $g = \frac{\partial u^i}{\partial n} - izu^i$. Problem: find $u \in H^1_{\Gamma_D}(D)$ ($\Gamma_D = \partial\mathcal{B}(0, 0.5)$) s.t.

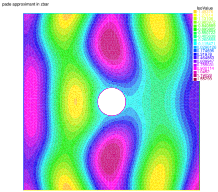
$$\begin{cases} -\Delta u - z^2 u = 0 & \text{in } D \\ u = 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} - izu = g & \text{on } \Gamma_N \end{cases} \tag{1}$$

- Problem (1) admits a unique solution for any z with $\mathrm{Im}\,(z) \geq 0$
- The frequency response map $\mathcal{S} : z \to u_z$ is meromorphic in $\mathbb{C}$, with poles in the half-plane $\{\mathrm{Im}\,(z) < 0\}$ (see [Bonizzoni–Nobile–Perugia–Pradovera2018])

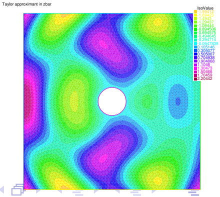
FEM solution



Padé approx.



Taylor approx.



Conclusions

- We have designed a Least-Square Padé-type approximation for Hilbert space-valued meromorphic maps
- We have proved that the Padé approximation error converges exponentially in the degree of the denominator
- Numerical examples which show the effectiveness of our approach are provided

Thank you for your attention!

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