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Guaranteed error estimates for finite element discretizations of Helmholtz problems

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October 8, 2021

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Motivations

Motivations

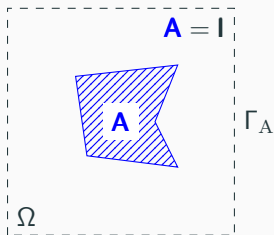
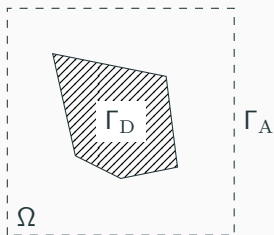
Model problem

Model problem

Given $f : \Omega \rightarrow \mathbb{C}$, find $u : \Omega \rightarrow \mathbb{C}$ such that

$$\begin{cases} -\omega^2 \mu u - \nabla \cdot (\mathbf{A} \nabla u) = \mu f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \mathbf{A} \nabla u \cdot \mathbf{n} - i\omega\gamma u = 0 & \text{on } \Gamma_A \end{cases}$$

where μ , \mathbf{A} and γ are given coefficients strictly positive coefficients.



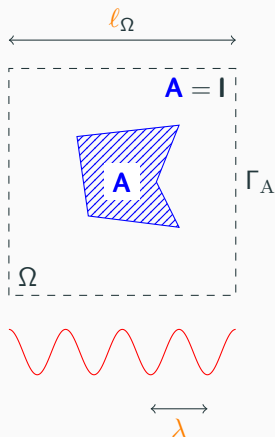
What do I mean by high-frequency?

The physical meaning of μ and \mathbf{A} depends on the application, but the wavespeed is always given by:

$$c := \sqrt{\frac{\sigma_{\min}(\mathbf{A})}{\mu}}$$

The (minimal) wavelength is then given by:

$$\lambda := \frac{2\pi}{\omega} c_{\min}.$$



The “important” quantity is $N_\lambda := \ell_\Omega / \lambda$. High-frequency means that

$$\frac{\omega \ell_\Omega}{c_{\min}} \simeq N_\lambda$$

is “large” (a few tens or hundreds).

Variational formulation

Recall the Helmholtz problem in strong form

$$\begin{cases} -\omega^2 \mu u - \nabla \cdot (\mathbf{A} \nabla u) = \mu f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \mathbf{A} \nabla u \cdot \mathbf{n} - i\omega \gamma u = 0 & \text{on } \Gamma_A. \end{cases}$$

Assuming $f \in L^2(\Omega)$, we seek $u \in H_D^1(\Omega)$ such that

$$b(u, v) = (\mu f, v) \quad \forall v \in H_D^1(\Omega),$$

with

$$b(u, v) := -\omega^2 (\mu u, v)_\Omega - i\omega (\gamma u, v)_{\Gamma_A} + (\mathbf{A} \nabla u, \nabla v)_\Omega.$$

Finite element approximation

We consider a mesh \mathcal{T}_h of Ω into tetrahedral element K .

The elements $K \in \mathcal{T}_h$ are “small” ($h_K := \text{diam } K \leq h$).

The coefficients μ, γ, \mathbf{A} are constant inside each element/face.

We introduce a “finite element” discretization space

$$V_h := \{v_h \in H_D^1(\Omega) \mid v_h|_K \in \mathbb{P}_p(K) \forall K \in \mathcal{T}_h\}$$

with $p \geq 1$.



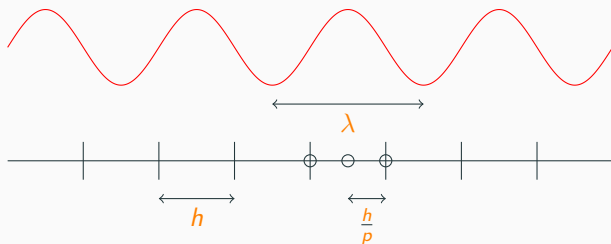
P.G. Ciarlet, 2002.

What do I mean by refined mesh?

When I am saying that “the mesh is fine” , I mean that

$$N_{\text{dofs}/\lambda} = \lambda / \frac{h}{p} \simeq \left(\frac{\omega h}{C_{\min} p} \right)^{-1}$$

is large.



Finite element approximation

Recall that u is the only element of $H_D^1(\Omega)$ such that

$$b(u, v) = (\mu f, v) \quad \forall v \in H_D^1(\Omega).$$

Analogously, we seek a discrete a discrete solution $u_h \in V_h$ such that

$$b(u_h, v_h) = (\mu f, v_h) \quad \forall v_h \in V_h. \quad (1)$$

Problem (1) corresponds to a finite dimensional linear system, that we can numerically solve.

In this talk, we are especially interested in measuring the error

$$e_h := u - u_h$$

Motivations

A priori error estimates

A priori error estimates

A priori estimates

Assume that $\omega h / c_{\min} p \leq \mathcal{C}_1$, then

$$\|\nabla e_h\|_{\mathbf{A},\Omega} \leq \mathcal{C}_2 \left(\frac{\omega h}{c_{\min} p} \right)^p.$$



F. Ihlenburg and I. Babuška, *SIAM J. Numer. Anal.*, 1997.



J.M. Melenk and S.A. Sauter, *Math. Comp.*, 2010.



T. Chaumont-Frelet and S. Nicaise, *IMA J. Numer. Anal.*, 2019.

Some limitations:

- The above result requires important regularity assumptions.
- The error estimate is not always applicable.
- The constants \mathcal{C}_1 and \mathcal{C}_2 are *not* computable in general.

A priori error estimates

A priori estimates provide qualitative upper bounds.

They are important as they show that the method converges.
They also indicate how fast the convergence happens.

They are not suited to *quantitatively* estimate the error in practice.

Motivations

A posteriori error estimation

A posteriori estimates

(ideal) A posteriori estimates

$$\|\nabla e_h\|_{\mathbf{A},\Omega} \leq \eta$$

Here η is a fully-computable real number called an “error estimator”.

This quantity is computed as a post-processing of u_h , i.e. $\eta = \eta(u_h)$.

There is *no generic constants*. We have a *guaranteed* error estimate.

Outline

- 1 Low frequencies
- 2 High frequencies
- 3 Controlling the pre-factors
- 4 Numerical illustrations

Low frequencies

The low frequency case

We first consider the low frequency limit where $\omega = 0$.

The problem then reads: find $u : \Omega \rightarrow \mathbb{C}$ such that

$$\begin{cases} -\nabla \cdot (\mathbf{A} \nabla u) &= \mu f & \text{in } \Omega, \\ u &= 0 & \text{on } \Gamma_D, \\ \mathbf{A} \nabla u \cdot \mathbf{n} &= 0 & \text{on } \Gamma_A. \end{cases}$$

For the sake of simplicity, we will assume that $f = f_h \in \mathbb{P}_p(\mathcal{T}_h)$.

Variational formulation and discrete solution

Consider the sesquilinear form

$$a(\mathbf{u}, v) = (\mathbf{A}\nabla\mathbf{u}, \nabla v)_\Omega, \quad \mathbf{u}, v \in H_{\Gamma_D}^1(\Omega).$$

We can characterize \mathbf{u} as the unique element of $H_{\Gamma_D}^1(\Omega)$ such that

$$a(\mathbf{u}, v) = (\mu f_h, v)_\Omega$$

for all $v \in H_{\Gamma_D}^1(\Omega)$.

\mathbf{u}_h is the unique element of V_h satisfying

$$a(\mathbf{u}_h, v_h) = (\mu f_h, v_h)_\Omega$$

for all $v_h \in V_h$.

Low frequencies

Key ideas behind a posteriori estimation

Key ideas

Second-order problems typically arise from two physical laws, e.g., “Faraday’s law + Gauss’ law = Poisson problem”.

The continuous solution u is uniquely determined by the condition that

$$u \in H^1(\Omega), \quad u = 0 \text{ on } \Gamma_D \quad (2a)$$

and for the “flux” $\sigma := -A\nabla u \in \mathbf{H}(\text{div}, \Omega)$

$$\sigma \cdot \mathbf{n} = 0 \text{ on } \Gamma_A, \quad \nabla \cdot \sigma = \mu f_h \text{ in } \Omega. \quad (2b)$$

The discrete solution u_h satisfies (2a) but not (2b) in general.

Key ideas

Consider the minimization problem

$$\boldsymbol{\sigma} := \arg \min_{\substack{\boldsymbol{\tau} \in \mathbf{H}(\text{div}, \Omega) \\ \boldsymbol{\tau} \cdot \mathbf{n} = 0 \text{ on } \Gamma_A \\ \nabla \cdot \boldsymbol{\tau} = \mu f_h \text{ in } \Omega}} \|\mathbf{A}^{-1} \boldsymbol{\tau} + \nabla u_h\|_{\mathbf{A}, \Omega}.$$

If the above minimum is 0, then $\boldsymbol{\sigma} = -\mathbf{A} \nabla u_h \in \mathbf{H}(\text{div}, \Omega)$ with

$$\boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \Gamma_A \quad \nabla \cdot \boldsymbol{\sigma} = \mu f_h \text{ in } \Omega$$

i.e. u_h satisfies (2b), which implies that $u = u_h$.

Otherwise, it measures how “non-conforming” u_h is.

Low frequencies

The Prager-Synge theorem

Prager-Syngé inequality

Assume that $\boldsymbol{\sigma} \in \mathbf{H}(\text{div}, \Omega)$ satisfies

$$\boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \Gamma_A, \quad \nabla \cdot \boldsymbol{\sigma} = \mu f_h \text{ in } \Omega.$$

$\boldsymbol{\sigma} = -\mathbf{A}\nabla u$ is one example.

Then

$$\begin{aligned} a(e_h, v) &= (\mu f_h, v)_\Omega - (\mathbf{A}\nabla u_h, \nabla v)_\Omega \\ &= (\nabla \cdot \boldsymbol{\sigma}, v)_\Omega - (\mathbf{A}\nabla u_h, \nabla v)_\Omega \\ &= -(\boldsymbol{\sigma} + \mathbf{A}\nabla u_h, \nabla v)_\Omega. \end{aligned}$$

Prager-Syngé inequality

$$|a(e_h, v)| \leq \|\mathbf{A}^{-1}\boldsymbol{\sigma} + \nabla u_h\|_{\mathbf{A}, \Omega} \|\nabla v\|_{\mathbf{A}, \Omega}$$

Upper bound via equilibrated flux

Recall that whenever $\nabla \cdot \boldsymbol{\sigma} = \mu f_h$ in Ω and $\boldsymbol{\sigma} \cdot \mathbf{n} = 0$ on Γ_A

$$|a(\mathbf{e}_h, v)| \leq \|\mathbf{A}^{-1} \boldsymbol{\sigma} + \nabla u_h\|_{\mathbf{A}, \Omega} \|\nabla v\|_{\mathbf{A}, \Omega} \quad \forall v \in H_{\Gamma_D}^1(\Omega).$$

Picking in particular $v = \mathbf{e}_h$, we have

$$\|\nabla \mathbf{e}_h\|_{\mathbf{A}, \Omega}^2 = |a(\mathbf{e}_h, \mathbf{e}_h)| \leq \|\mathbf{A}^{-1} \boldsymbol{\sigma} + \nabla u_h\|_{\mathbf{A}, \Omega} \|\nabla \mathbf{e}_h\|_{\mathbf{A}, \Omega}.$$

Guaranteed upper bound

$$\|\nabla \mathbf{e}_h\|_{\mathbf{A}, \Omega} \leq \|\mathbf{A}^{-1} \boldsymbol{\sigma} + \nabla u_h\|_{\mathbf{A}, \Omega}$$



W. Prager and J.L. Synge, *Quart. Appl. Math.*, 1947.

Low frequencies

Practical flux construction

Practical flux construction

Equilibrated fluxes satisfy $\nabla \cdot \boldsymbol{\sigma} = \mu f_h$ in Ω and $\boldsymbol{\sigma} \cdot \mathbf{n} = 0$ on Γ_A .
They readily provide guaranteed error bounds.

Here, because $\mu f_h \in \mathbb{P}_p(\mathcal{T}_h)$ we can actually find discrete fluxes $\boldsymbol{\sigma}_h$.

The correct tool to do that is the Raviart–Thomas finite element space

$$\mathbf{W}_h := \left\{ \mathbf{w}_h \in \mathbf{H}_{\Gamma_A}(\text{div}, \Omega) \mid \mathbf{w}_h|_K \in [\mathbb{P}_p(K)]^3 + \mathbf{x}\mathbb{P}_{p-1}(K) \right\}.$$



P.A. Raviart and J.M. Thomas, 1977.

How to select the flux?

We are going to select a discrete flux $\sigma_h \in \mathbf{W}_h$.

The “equilibration” constraint on the flux is

$$\nabla \cdot \sigma_h = \mu f_h \text{ in } \Omega.$$

The estimate the flux provides us is

$$\|\nabla e_h\|_{\mathbf{A},\Omega} \leq \|\mathbf{A}^{-1} \sigma_h + \nabla u_h\|_{\mathbf{A},\Omega}.$$

Optimal discrete flux

Recall that $\boldsymbol{\sigma}_h \in \mathbf{W}_h$ has to satisfy

$$\nabla \cdot \boldsymbol{\sigma}_h = \mu f_h \text{ in } \Omega$$

and gives us

$$\|\nabla e_h\|_{\mathbf{A},\Omega} \leq \|\mathbf{A}^{-1} \boldsymbol{\sigma}_h + \nabla u_h\|_{\mathbf{A},\Omega}.$$

The “optimal” choice is then

$$\boldsymbol{\sigma}_h := \arg \min_{\substack{\boldsymbol{\tau}_h \in \mathbf{W}_h \\ \nabla \cdot \boldsymbol{\tau}_h = \mu f_h \text{ in } \Omega}} \|\mathbf{A}^{-1} \boldsymbol{\tau}_h + \nabla u_h\|_{\mathbf{A},\Omega}.$$

How to compute it and how expensive it is?

After introducing a Lagrange multiplier, there exists a unique pair $(\boldsymbol{\sigma}_h, \mathbf{q}_h) \in \mathbf{W}_h \times \mathbb{P}_p(\mathcal{T}_h)$ such that

$$\begin{cases} (\mathbf{A}^{-1}\boldsymbol{\sigma}_h, \mathbf{w}_h)_\Omega + (\mathbf{q}_h, \nabla \cdot \mathbf{w}_h)_\Omega & = -(\nabla u_h, \mathbf{w}_h)_\Omega & \forall \mathbf{w}_h \in \mathbf{W}_h, \\ (\nabla \cdot \boldsymbol{\sigma}_h, r_h) & = (\mu f_h, r_h) & \forall r_h \in \mathbb{P}_p(\mathcal{T}_h). \end{cases}$$

This square linear system can be solved to compute the optimal flux.

Unfortunately, it is more expensive than solving the original problem, so we avoid that in practice by using a localization trick.



P. Destuynder and B. Métivet, *Math. Comp.*, 1999.

At the continuous level, the ideal flux is $\sigma := -\mathbf{A}\nabla u$.

A characterization is

$$\sigma = \arg \min_{\substack{\boldsymbol{\tau} \in \mathbf{H}_{\mathbf{r}_A}(\text{div}, \Omega) \\ \nabla \cdot \boldsymbol{\tau} = \mu f_h \text{ in } \Omega}} \|\mathbf{A}^{-1}\boldsymbol{\tau} + \nabla u\|_{\mathbf{A}, \Omega}.$$

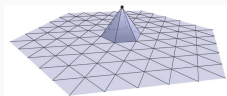
The “optimal” flux directly mimicks this definition at the discrete level

$$\sigma_h := \arg \min_{\substack{\boldsymbol{\tau}_h \in \mathbf{W}_h \\ \nabla \cdot \boldsymbol{\tau}_h = \mu f_h \text{ in } \Omega}} \|\mathbf{A}^{-1}\boldsymbol{\tau}_h + \nabla u_h\|_{\mathbf{A}, \Omega}.$$

Localization

Consider the set of “hat functions” $\{\psi^a\}_{a \in \mathcal{V}_h}$ of the mesh. We then have

$$\sum_{a \in \mathcal{V}_h} \psi^a = 1.$$



The ideal flux $\boldsymbol{\sigma} := -\mathbf{A}\nabla u$ can be decomposed as

$$\boldsymbol{\sigma} = \sum_{a \in \mathcal{V}_h} \boldsymbol{\sigma}^a, \quad \boldsymbol{\sigma}^a = -\psi^a \mathbf{A}\nabla u.$$

Easy computations show that

$$\boldsymbol{\sigma}^a \cdot \mathbf{n} = 0 \text{ on } \partial\omega^a \quad \nabla \cdot \boldsymbol{\sigma}^a = \psi^a \mu f_h - \mathbf{A}\nabla u \cdot \nabla \psi^a \text{ in } \omega^a$$

We have shown that

$$\sigma = \sum_{a \in \mathcal{V}_h} \sigma^a$$

and

$$\sigma^a = \arg \min_{\substack{\tau \in H_0(\text{div}, \omega^a) \\ \nabla \cdot \tau = \psi^a \mu f_h - \mathbf{A} \nabla u \cdot \nabla \psi^a \text{ in } \omega^a}} \|\mathbf{A}^{-1} \tau + \nabla u\|_{\mathbf{A}, \omega^a}.$$

We can mimick that on the discrete level!

Localization

We thus set

$$\boldsymbol{\sigma}_h := \sum_{a \in \mathcal{V}_h} \boldsymbol{\sigma}_h^a$$

with

$$\boldsymbol{\sigma}_h^a := \arg \min_{\substack{\boldsymbol{\tau}_h \in \mathbf{H}_0(\operatorname{div}; \omega^a) \cap \mathbf{W}_h \\ \nabla \cdot \boldsymbol{\tau}_h = \psi^a \mu f_h - \mathbf{A} \nabla u_h \cdot \nabla \psi^a \text{ in } \omega^a}} \|\mathbf{A}^{-1} \boldsymbol{\tau}_h + \nabla u_h\|_{\mathbf{A}, \omega^a}.$$

The compatibility condition

$$(\psi^a \mu f_h - \mathbf{A} \nabla u_h \cdot \nabla \psi^a, 1)_{\omega^a} = (\mu f_h, \psi^a)_{\Omega} - (\mathbf{A} \nabla u_h, \nabla \psi^a)_{\Omega} = 0$$

holds true since u_h is the discrete solution and $\psi^a \in V_h$.

Summary of the localization process

Step 1: solve a set of small, uncoupled linear systems

$$\sigma_h^a := \arg \min_{\substack{\tau_h \in \mathbf{H}_0(\operatorname{div}, \omega^a) \cap \mathbf{W}_h \\ \nabla \cdot \tau_h = \psi^a \mu_{f_h} - \mathbf{A} \nabla u_h \cdot \nabla \psi^a \text{ in } \omega^a}} \|\mathbf{A}^{-1} \tau_h + \nabla u_h\|_{\mathbf{A}, \omega^a}.$$

Step 2: assemble these local contributions

$$\sigma_h := \sum_{a \in \mathcal{V}_h} \sigma_h^a.$$

Step 3: compute the estimator

$$\eta := \|\mathbf{A}^{-1} \sigma_h + \nabla u_h\|_{\mathbf{A}, \Omega}.$$

Step 4: enjoy the guaranteed estimate

$$\|\nabla e_h\|_{\mathbf{A}, \Omega} \leq \eta.$$

Low frequencies



Efficiency

For time reasons, I will not give any proofs, but we can show that

$$\eta \leq C_{\text{eff}} \|\nabla e_h\|_{\mathbf{A}, \Omega},$$

where C_{eff} only depends on:

- the “flatness” of the tetrahedra in the mesh,
- the “contrasts” in the coefficients.

A nice aspect is that C_{eff} does not depend on p .



P. Braess, V. Pillwein and J. Schöberl, *CMAME*, 2009.



A. Ern and M. Vohralík, *Math. Comp.*, 2020.

Low frequencies

Takeaways

Takeaways

An equilibrated flux is an object $\boldsymbol{\sigma} \in \mathbf{H}(\text{div}, \Omega)$ such that

$$\boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \Gamma_A \quad \nabla \cdot \boldsymbol{\sigma} = \mu f_h \text{ in } \Omega.$$

There exist efficient algorithms to build a discrete flux $\boldsymbol{\sigma}_h \in \mathbf{W}_h$.

The *guaranteed* error estimate

$$\|\nabla e_h\|_{\mathbf{A}, \Omega} \leq \eta$$

holds true with

$$\eta := \|\mathbf{A}^{-1} \boldsymbol{\sigma}_h + \nabla u_h\|_{\mathbf{A}, \Omega}.$$

This bound cannot be too loose:

$$\eta \leq C_{\text{eff}} \|\nabla e_h\|_{\mathbf{A}, \Omega}.$$

High frequencies

The high frequency case

Back to our original problem

$$\begin{cases} -\omega^2 \mu u - \nabla \cdot (\mathbf{A} \nabla u) = \mu f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \mathbf{A} \nabla u \cdot \mathbf{n} - i\omega \gamma u = 0 & \text{on } \Gamma_A. \end{cases}$$

We introduce

$$b(\mathbf{u}, v) := -\omega^2 (\mu \mathbf{u}, v)_\Omega - i\omega (\gamma \mathbf{u}, v)_{\Gamma_A} + (\mathbf{A} \nabla \mathbf{u}, \nabla v)_\Omega.$$

Energy norm and lack of coercivity

We will consider the “balanced” norm

$$\|v\|_{\omega, \Omega}^2 := \omega^2 \|v\|_{\mu, \Omega}^2 + \|\nabla v\|_{\mathbf{A}, \Omega}^2.$$

The sesquilinear form b is not coercive.

Instead we have the “Gårding” inequality

$$\operatorname{Re} b(v, v) = \|\nabla v\|_{\mathbf{A}, \Omega}^2 - \omega^2 \|v\|_{\mu, \Omega}^2 = \|v\|_{\omega, \Omega}^2 - 2\omega^2 \|v\|_{\mu, \Omega}^2.$$

High frequencies

Flux equilibration

Definition of an equilibrated flux

Letting $\boldsymbol{\sigma} := -\mathbf{A}\nabla u$, we have

$$\boldsymbol{\sigma} \cdot \mathbf{n} = -i\omega\gamma u \text{ on } \Gamma_A \quad \nabla \cdot \boldsymbol{\sigma} = \mu f_h + \omega^2 \mu u \text{ in } \Omega.$$

Hence, natural requirements for $\boldsymbol{\sigma}_h$ are

$$\boldsymbol{\sigma}_h \cdot \mathbf{n} = -i\omega\gamma u_h \text{ on } \Gamma_A \quad \nabla \cdot \boldsymbol{\sigma}_h = \mu f_h + \omega^2 \mu u_h \text{ in } \Omega.$$

The “standard” reconstruction algorithms directly extend.

Prager-Synge inequality

Let $v \in H_{\Gamma_D}^1(\Omega)$. We have

$$\begin{aligned} b(\mathbf{e}_h, v) &= (\mu \mathbf{f}_h, v)_\Omega - b(\mathbf{u}_h, v) \\ &= (\mu \mathbf{f}_h + \omega^2 \mu \mathbf{u}_h, v)_\Omega + i\omega(\gamma \mathbf{u}_h, v)_{\Gamma_A} - (\mathbf{A} \nabla \mathbf{u}_h, \nabla v)_\Omega \\ &= (\nabla \cdot \boldsymbol{\sigma}_h, v)_\Omega - (\boldsymbol{\sigma}_h \cdot \mathbf{n}, v)_{\Gamma_A} - (\mathbf{A} \nabla \mathbf{u}_h, \nabla v)_\Omega \\ &= -(\boldsymbol{\sigma}_h + \mathbf{A} \nabla \mathbf{u}_h, \nabla v)_\Omega. \end{aligned}$$

Prager-Synge inequality

$$|b(\mathbf{e}_h, v)| \leq \eta \|\nabla v\|_{\mathbf{A}, \Omega} \quad \forall v \in H_{\Gamma_D}^1(\Omega)$$

So far, so good!

What's the matter?

Here, we do not have

$$\|\nabla e_h\|_{\mathbf{A},\Omega}^2 \leq |b(e_h, e_h)|,$$

which is a major issue!

Instead, we only have the “Gårding” inequality

$$\operatorname{Re} b(e_h, e_h) \geq \|e_h\|_{\omega,\Omega}^2 - 2\omega^2 \|e_h\|_{\mu,\Omega}^2.$$

High frequencies

A coarse error estimate

Stability constant

For $g \in L^2(\Omega)$, let \mathcal{S}^*g denote the unique element of $H_{\Gamma_D}^1(\Omega)$ such that

$$b(w, \mathcal{S}^*g) = 2\omega^2(\mu w, g)_\Omega \quad \forall w \in H_{\Gamma_D}^1(\Omega)$$

and let

$$\mathcal{C}_{\text{st}} := \frac{1}{\omega} \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu, \Omega} = 1}} \|\nabla(\mathcal{S}^*g)\|_{\mathbf{A}, \Omega}.$$

\mathcal{C}_{st} is the best constant such that

$$\|\nabla(\mathcal{S}^*g)\|_{\mathbf{A}, \Omega} \leq \mathcal{C}_{\text{st}}\omega \|g\|_{\mu, \Omega} \quad \forall g \in L^2(\Omega).$$

It is closely related to resolvent estimates.

Making up for the lack of coercivity

By definition, we have

$$b(w, \mathcal{S}^* e_h) = 2\omega^2(\mu w, e_h) \quad \forall w \in H_{\Gamma_D}^1(\Omega).$$

Hence, in particular,

$$b(e_h, \mathcal{S}^* e_h) = 2\omega^2 \|e_h\|_{\mu, \Omega}^2,$$

which is exactly the “bad” term the Gårding inequality:

$$\operatorname{Re} b(e_h, e_h) = \|e_h\|_{\omega, \Omega}^2 - 2\omega^2 \|e_h\|_{\mu, \Omega}^2.$$

Making up for the lack of coercivity

Using Prager-Syngé inequality, we have

$$\|e_h\|_{\omega,\Omega}^2 = \operatorname{Re} b(e_h, e_h + \mathcal{I}^* e_h) \leq \eta \|\nabla(e_h + \mathcal{I}^* e_h)\|_{\mathbf{A},\Omega}.$$

It follows that

$$\begin{aligned} \|e_h\|_{\omega,\Omega}^2 &\leq \eta (\|\nabla e_h\|_{\mathbf{A},\Omega} + \|\nabla(\mathcal{I}^* e_h)\|_{\mathbf{A},\Omega}) \\ &\leq \eta (\|\nabla e_h\|_{\mathbf{A},\Omega} + \mathcal{C}_{\text{st}} \omega \|e_h\|_{\mu,\Omega}) \\ &\leq \eta \max(1, \mathcal{C}_{\text{st}}) \|e_h\|_{\omega,\Omega}, \end{aligned}$$

and

$$\|e_h\|_{\omega,\Omega} \leq \max(1, \mathcal{C}_{\text{st}}) \eta.$$

Coarse error estimate

We obtained the following error estimate:

Coarse error estimate

$$\|e_h\| \leq \max(1, \mathcal{C}_{\text{st}})\eta$$

\mathcal{C}_{st} is the best constant such that:

Stability constant

$$\|\nabla(\mathcal{I}^*g)\|_{\mathbf{A},\Omega} \leq \mathcal{C}_{\text{st}}\omega \|g\|_{\mu,\Omega} \quad \forall g \in L^2(\Omega).$$

High frequencies

Efficiency

We can show that

$$\eta \leq C_{\text{eff}} \left(1 + \max_{K \in \mathcal{T}_h} \frac{\omega h_K}{c_{\min K} \rho} \right) \|e_h\|_{\omega, \Omega},$$

where $c_{\min K}$ is the wavespeed in the element K .

For any reasonable discretization, we have

$$\frac{\omega h_K}{c_{\min K} \rho} \leq 1,$$

so that in practice

$$\eta \leq C_{\text{eff}} \|e_h\|_{\omega, \Omega},$$

where C_{eff} only depends on the elements “flatness” and the contrasts.



T. Chaumont-Frelet, A. Ern and M. Vohralík, *Numer. Math.*, 2021.



W. Dörfler, S. Sauter, *Comput. Meth. Appl. Math.*, 2013.

The problem with the coarse error estimate

Recall that

$$\eta \leq C_{\text{eff}} \|e_h\|_{\omega, \Omega} \quad \|e_h\|_{\omega, \Omega} \leq \max(1, \mathcal{C}_{\text{st}}) \eta.$$

We have $C_{\text{eff}} \simeq 1$ and $\mathcal{C}_{\text{st}} \gtrsim \omega \ell_{\Omega} / c_{\text{min}}$, so that

$$\eta \lesssim \|e_h\|_{\omega, \Omega} \lesssim \frac{\omega \ell_{\Omega}}{c_{\text{min}}} \eta.$$

In practice, the coarse error estimate will largely overestimate the error in the high frequency regime.

High frequencies

Sharp error estimate

The approximation factor

We introduce

$$\mathcal{C}_{\text{ap}} := \frac{1}{\omega} \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu, \Omega} = 1}} \min_{v_h \in V_h} \|\nabla(\mathcal{I}^* g - v_h)\|_{\mathbf{A}, \Omega}.$$

Approximability

For all $g \in L^2(\Omega)$, there exists $v_h^* \in V_h$ such that

$$\|\nabla(\mathcal{I}^* g - v_h^*)\|_{\mathbf{A}, \Omega} \leq \mathcal{C}_{\text{ap}} \omega \|g\|_{\mu, \Omega}.$$

This was called η in Markus' talk.

It's better than the stability constant!

Recall that

$$\mathcal{C}_{\text{ap}} := \max_{\substack{\mathbf{g} \in L^2(\Omega) \\ \|\mathbf{g}\|_{\mu, \Omega} = 1}} \min_{\mathbf{v}_h \in V_h} \omega \|\mathcal{I} \mathbf{g} - \mathbf{v}_h\|_{\omega, \Omega}$$

since we can take $\mathbf{v}_h = 0$, we have

$$\mathcal{C}_{\text{ap}} \leq \max_{\substack{\mathbf{g} \in L^2(\Omega) \\ \|\mathbf{g}\|_{\mu, \Omega} = 1}} \omega \|\mathcal{I} \mathbf{g}\|_{\omega, \Omega} =: \mathcal{C}_{\text{st}}.$$

Besides, standard approximability results for FEM show that

$$\mathcal{C}_{\text{ap}} \leq \mathcal{C} \left(\frac{1}{p} \frac{h}{\ell_{\Omega}} \right)^s$$

for some $s > 0$, so that $\mathcal{C}_{\text{ap}} \rightarrow 0$.

Using Galerkin orthogonality

Recall that

$$\|e_h\|_{\omega, \Omega}^2 = \operatorname{Re} b(e_h, e_h + \mathcal{I}^* e_h).$$

By Galerkin orthogonality, we have

$$\begin{aligned} \|e_h\|_{\omega, \Omega}^2 &= \operatorname{Re} b(e_h, e_h) + \operatorname{Re} b(e_h, \mathcal{I}^* e_h) \\ &= \operatorname{Re} b(e_h, e_h) + \operatorname{Re} b(e_h, \mathcal{I}^* e_h - v_h^*) \\ &\leq \eta (\|\nabla e_h\|_{\mathbf{A}, \Omega} + \|\nabla(\mathcal{I}^* e_h - v_h^*)\|_{\mathbf{A}, \Omega}) \\ &\leq \eta \max(1, \mathcal{C}_{\text{ap}}) \|e_h\|_{\omega, \Omega}. \end{aligned}$$

Sharp error estimate

Sharp error estimate

$$\|e_h\|_{\omega, \Omega} \leq \max(1, \mathcal{C}_{\text{ap}})\eta.$$

Approximation factor

$$\mathcal{C}_{\text{ap}} := \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu, \Omega} = 1}} \min_{v_h \in V_h} \omega \| \mathcal{I}g - v_h \|_{\omega, \Omega} \rightarrow 0.$$



T. Chaumont-Frelet, A. Ern and M. Vohralík, *Numer. Math.*, 2021.



W. Dörfler, S. Sauter, *Comput. Meth. Appl. Math.*, 2013.

High frequencies

Takeaways

Takeways

The “equilibration” technology is the same than for low frequencies.

Coarse error estimate

$$\|e_h\|_{\omega, \Omega} \leq \max(1, \mathcal{C}_{st}) \eta \quad \mathcal{C}_{st} \gtrsim \omega \ell_{\Omega} / c_{\min}$$

Sharp error estimate

$$\|e_h\|_{\omega, \Omega} \leq \max(1, \mathcal{C}_{ap}) \eta \quad \mathcal{C}_{ap} \rightarrow 0$$

Efficiency

$$\eta \leq C_{\text{eff}} \left(1 + \frac{\omega h}{c_{\min} p} \right) \|e_h\|_{\omega, \Omega}$$

Controlling the pre-factors

Controlling the pre-factors

The stability constant \mathcal{C}_{st}

The stability constant

The stability constant is defined by

$$\mathcal{C}_{\text{st}} := \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu, \Omega} = 1}} \|\nabla(\mathcal{I}^* g)\|_{\mathbf{A}, \Omega}.$$

It is only related to the PDE, and independent of the numerical scheme.

Qualitative behaviour

It is known that we have “at least”:

$$\mathcal{C}_{\text{st}} \gtrsim \frac{\omega l \Omega}{c_{\text{min}}}.$$

For non-trapping settings (the “easier” scenario), we have

$$\mathcal{C}_{\text{st}} \lesssim \frac{\omega l \Omega}{c_{\text{min}}}.$$

If strong trapping happens, “extreme” behaviors can occur

$$\mathcal{C}_{\text{st}} \gtrsim \exp\left(\alpha \frac{\omega l \Omega}{c_{\text{min}}}\right)$$

for “some” frequencies. For “most frequency”

$$\mathcal{C}_{\text{st}} \gtrsim \left(\frac{\omega l \Omega}{c_{\text{min}}}\right)^\beta.$$



D. Lafontaine, E.A. Spence and J. Wunsch, *Comm. Pure Appl. Math.* 2021

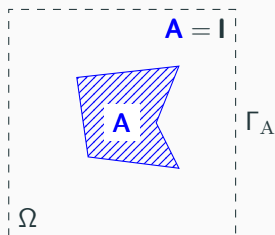
Quantitative estimate for star-shaped non-trapping obstacles

$\Omega := (-\ell/2, \ell/2)^3$ is a cube centered at the origin.

$D \subset \Omega$ is star shaped with respect to the origin.

Assume that $\gamma = 1$ and that

$\mu = 1$ and $\mathbf{A} = \mathbf{I}$ in $\Omega \setminus D$.



Assume that $\mu = \mu_D \geq 1$ and $\mathbf{A} = \mathbf{A}_D \preceq \mathbf{I}$ in D .

This describes an obstacle made of a material with a “slow” wavespeed.

Guaranteed upper bound

$$\mathcal{C}_{\text{st}} \leq 6 + \frac{3 + \sqrt{3}}{\sqrt{3}} \frac{\omega l_{\Omega}}{C_{\text{min}}}$$

The proof relies on a “Morawetz multiplier”:
multiply the PDE by $\mathbf{x} \cdot \nabla u$ and integrate by parts until it works!



C.S. Morawetz, *Comm. Pure Appl. Math.*, 1962.



J.M. Melenk, *PhD thesis*, 1995.



H. Barucq, T. Chaumont-Frelet and C. Gout, *Math. Comp.*, 2016.



T. Chaumont-Frelet, A. Ern, M. Vohralík, *Numer. Math.* 2021.

Controlling the pre-factors

The approximation factor \mathcal{C}_{ap}

The approximation factor

The approximation factor is defined by

$$\mathcal{C}_{\text{ap}} := \max_{\substack{\mathbf{g} \in L^2(\Omega) \\ \|\mathbf{g}\|_{\mu, \Omega} = 1}} \min_{\mathbf{v}_h^* \in V_h} \|\nabla(\mathcal{I}^* \mathbf{g} - \mathbf{v}_h^*)\|_{\mathbf{A}, \Omega}.$$

It depends on both the PDE and the approximation space V_h .

Assuming that $\mathbf{A} = \mathbf{I}$, Ω is convex, and \mathcal{C}_{st} is known, we can control it.

Idea one: explicit interpolation error



R. Arcangeli and J.L. Gout, RAIRO Numer. Anal., 1976.

If $v \in H^2(\Omega)$, let $I_h^1 v \in V_h$ denotes its first-order Lagrange interpolant:

$$\|\nabla(v - I_h^1 v)\|_{\mathbf{A},\Omega} \leq \mathcal{C}_{\mathcal{T},i} h \|\nabla^2 v\|_{\Omega},$$

with a constant $\mathcal{C}_{\mathcal{T},i}$ that is easily computable.

We then have

$$\begin{aligned} \mathcal{C}_{\text{ap}} &:= \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu,\Omega}=1}} \min_{v_h^* \in V_h} \|\nabla(\mathcal{S}^* g - v_h^*)\|_{\mathbf{A},\Omega} \\ &\leq \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu,\Omega}=1}} \|\nabla(\mathcal{S}^* g - I_h^1(\mathcal{S}^* g))\|_{\mathbf{A},\Omega} \\ &\leq \mathcal{C}_{\mathcal{T},i} h \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu,\Omega}=1}} \|\nabla^2(\mathcal{S}^* g)\|_{\Omega}. \end{aligned}$$

Idea two: estimation of the Hessian norm



P. Grisvard, 1985.



T. Chaumont-Frelet, S. Nicaise and J. Tomezyk, *Comm. Pure Appl. Anal.*, 2020.

Because Ω is convex and $\gamma = 1$, we have

$$\|\nabla^2(\mathcal{I}^*g)\|_{\Omega} \leq \|\Delta(\mathcal{I}^*g)\|_{\Omega}.$$

Then, we use the facts that

$$-\Delta(\mathcal{I}^*g) = 2\mu\omega^2g + \mu\omega^2\mathcal{I}^*g$$

and

$$\omega\|\mathcal{I}^*g\|_{\mu,\Omega} \leq 2\mathcal{C}_{\text{st}}\|g\|_{\mu,\Omega},$$

to show that

$$\|\nabla^2(\mathcal{I}^*g)\|_{\Omega} \leq 2\frac{\omega}{c_{\min}}(1 + \mathcal{C}_{\text{st}})\|g\|_{\mu,\Omega}.$$

Explicit control of the approximation factor

Recall that

$$\mathcal{C}_{\text{ap}} \leq \mathcal{C}_{\mathcal{T},i} h \max_{\substack{g \in L^2(\Omega) \\ \|g\|_{\mu,\Omega}=1}} \|\nabla^2(\mathcal{I}^* g)\|_{\Omega}$$

and

$$\|\nabla^2(\mathcal{I}^* g)\|_{\Omega} \leq 2 \frac{\omega}{c_{\min}} (1 + \mathcal{C}_{\text{st}}) \|g\|_{\mu,\Omega} \quad \forall g \in L^2(\Omega).$$

Guaranteed bound

$$\mathcal{C}_{\text{ap}} \leq 2(1 + \mathcal{C}_{\mathcal{T},i}) \frac{\omega h}{c_{\min}} \mathcal{C}_{\text{st}}$$

Controlling the pre-factors

Takeaways

Takeaways

The estimator η needs to be “pre-factored” by \mathcal{C}_{st} or \mathcal{C}_{ap} .

The “qualitative” behaviors of both quantities are relatively well known.

The behaviour of \mathcal{C}_{st} is only dictated by the PDE.

Explicit bounds are available for non-trapping star-shaped obstacles.

The approximation factor \mathcal{C}_{ap} depends on the PDE and V_h .

When $\mathbf{A} = \mathbf{I}$, Ω is convex and \mathcal{C}_{st} is known, we can bound it nicely.

Numerical illustrations

Numerical illustrations

A validation experiment

Propagation of a plane wave

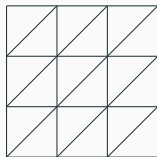
We consider the propagation of a plane wave in $\Omega = (-1, 1)^2$

$$\begin{cases} -\omega^2 \mathbf{u} - \Delta \mathbf{u} = 0 & \text{in } \Omega, \\ \nabla \mathbf{u} \cdot \mathbf{n} - i\omega \mathbf{u} = \mathbf{g} & \text{on } \Gamma_A, \end{cases}$$

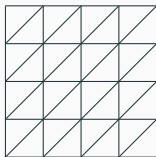
where

$$\mathbf{g} := \nabla \xi_\theta \cdot \mathbf{n} - i\omega \xi_\theta \quad \xi_\theta := e^{i\omega \mathbf{d} \cdot \mathbf{x}}$$

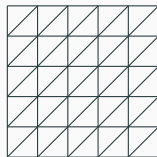
with $\mathbf{d} := (\cos \theta, \sin \theta)$ and $\theta = \pi/12$. The solution is $\mathbf{u} = \xi_\theta$.



$$h = \sqrt{2} \times 2/3$$

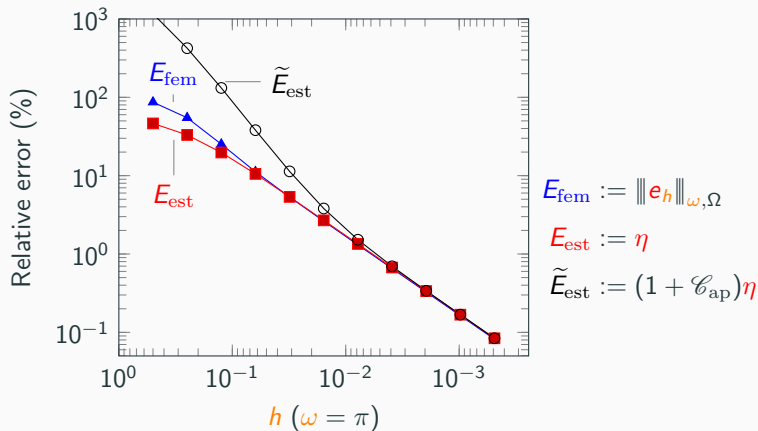


$$h = \sqrt{2} \times 1/2$$

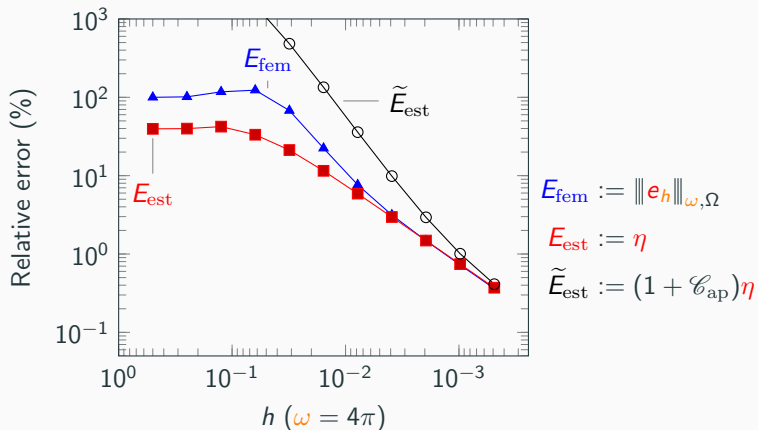


$$h = \sqrt{2} \times 2/5$$

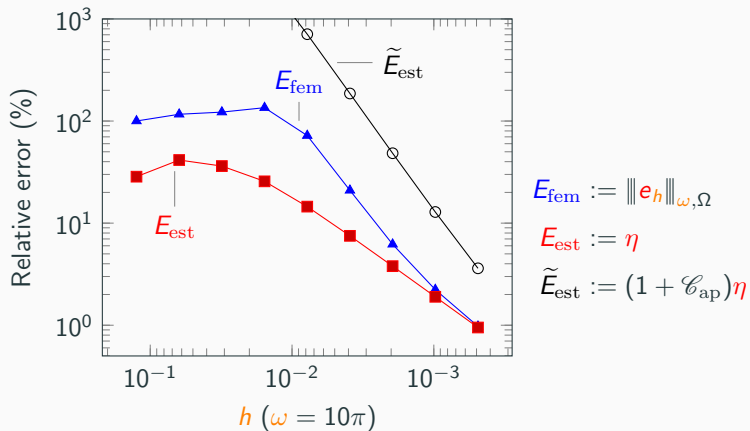
Plane wave experiment $\rho = 1$ and $\omega = \pi$



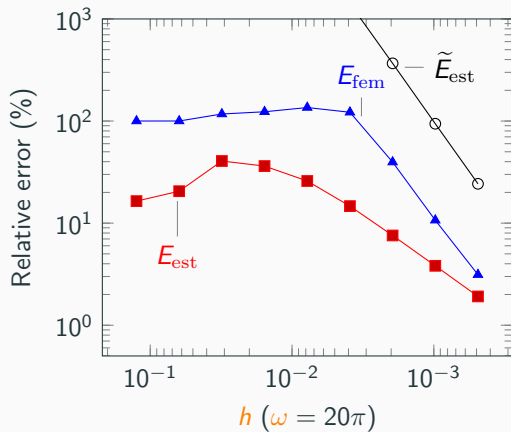
Plane wave experiment $\rho = 1$ and $\omega = 4\pi$



Plane wave experiment $\rho = 1$ and $\omega = 10\pi$



Plane wave experiment $p = 1$ and $\omega = 20\pi$

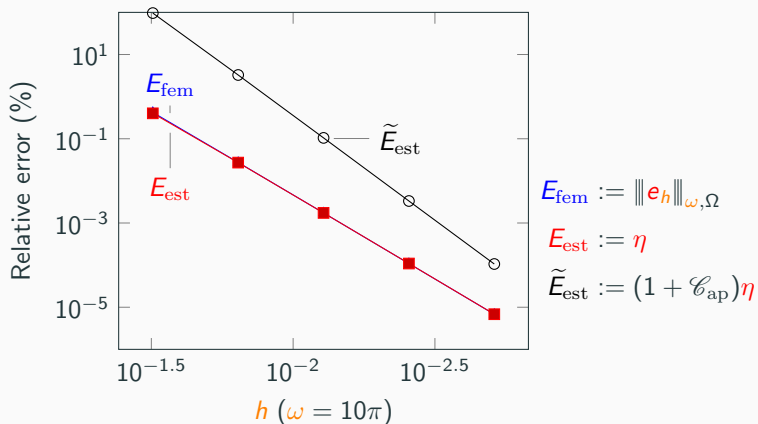


$$E_{\text{fem}} := \|e_h\|_{\omega, \Omega}$$

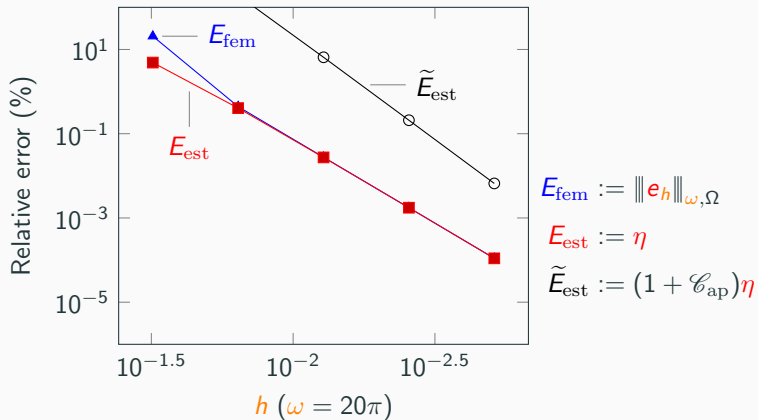
$$E_{\text{est}} := \eta$$

$$\tilde{E}_{\text{est}} := (1 + \mathcal{C}_{\text{ap}})\eta$$

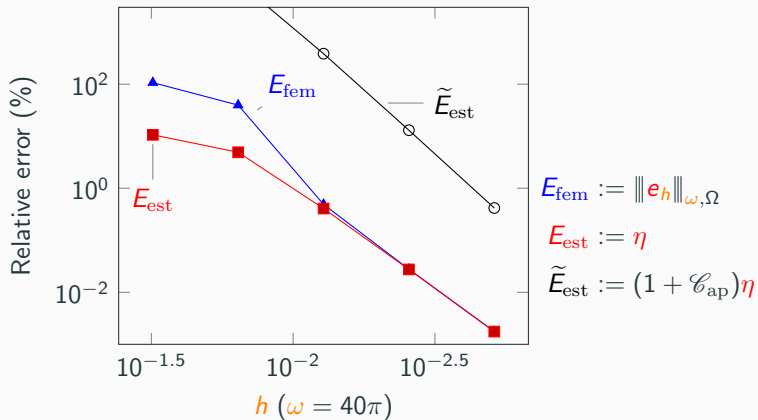
Plane wave experiment $\rho = 4$ and $\omega = 10\pi$



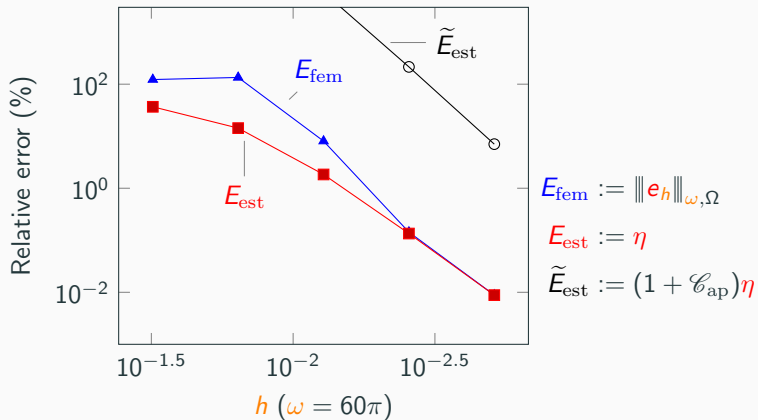
Plane wave experiment $\rho = 4$ and $\omega = 20\pi$



Plane wave experiment $\rho = 4$ and $\omega = 40\pi$



Plane wave experiment $\rho = 4$ and $\omega = 60\pi$



Numerical illustrations

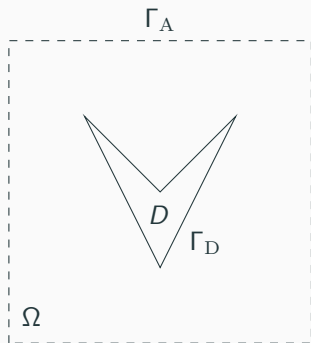
A more realistic example

Scattering by an non-trapping obstacle

We now consider a scattering problem

$$\begin{cases} -\omega^2 \mathbf{u} - \Delta \mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_D, \\ \nabla \mathbf{u} \cdot \mathbf{n} - i\omega \mathbf{u} = \mathbf{g} & \text{on } \Gamma_A, \end{cases}$$

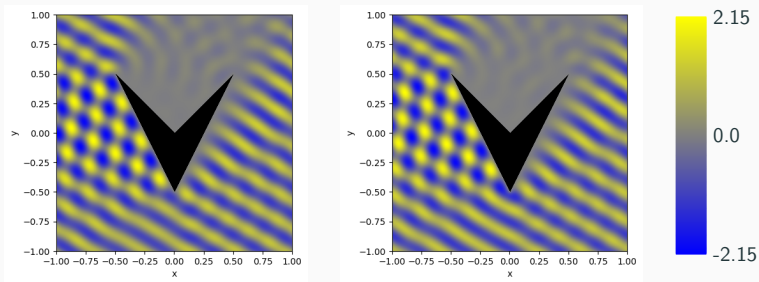
where again $\mathbf{g} = \nabla \xi_\theta \cdot \mathbf{n} - i\omega \xi_\theta$.



We fix the wavenumber $\omega = 10\pi$ and employ \mathbb{P}_3 elements.

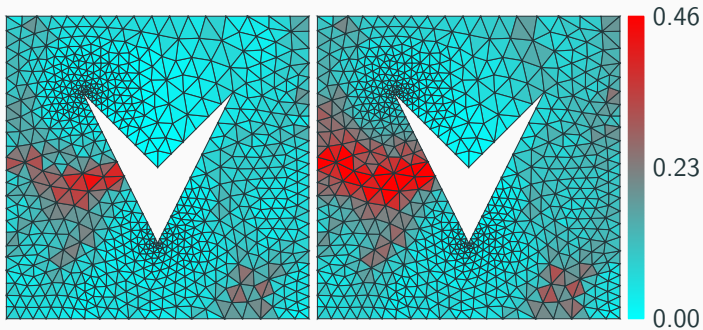
We consider a sequence of meshes that are adaptively refined using η_K .

Solution of the scattering problem



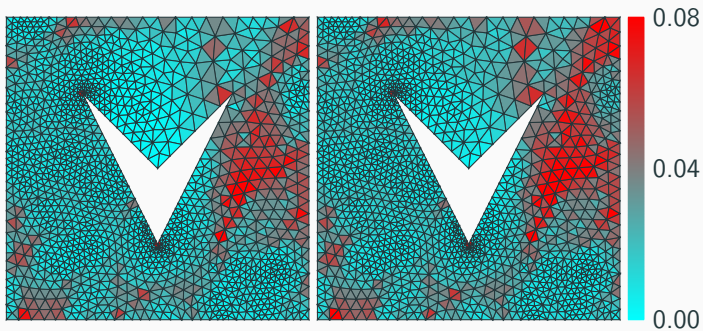
Real (left) and imaginary (right) parts of the solution

Estimated error in mesh #1



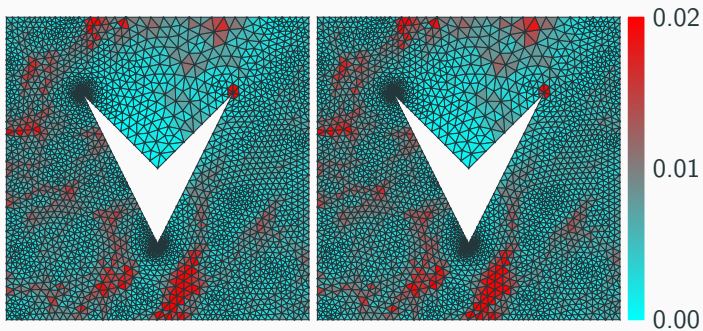
Estimator η_K (left) and elementwise error $\|e_h\|_{\omega,K}$ (right)

Estimated error in mesh #2



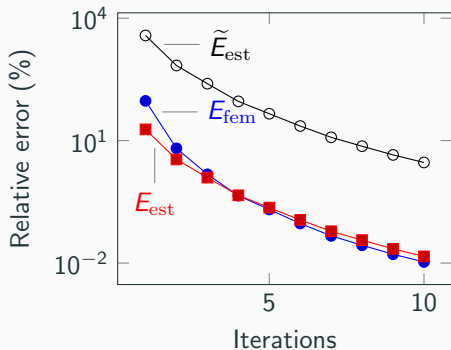
Estimator η_K (left) and elementwise error $\|e_h\|_{\omega,K}$ (right)

Estimated error in mesh #3



Estimator η_K (left) and elementwise error $\|e_h\|_{\omega,K}$ (right)

Behavior of the estimator through the adaptive procedure



$$E_{fem} := \|e_h\|_{\omega, \Omega}$$

$$E_{est} := \eta$$

$$\tilde{E}_{est} := (1 + \mathcal{C}_{st})\eta$$

Behaviors of the estimated and analytical errors in the adaptive procedure

Concluding remarks

Concluding remarks

Takeaways

Takeaways

We construct an a posteriori error estimator η via flux equilibration.
It directly provides guaranteed error estimates at low frequencies.

For high frequencies, η has to be pre-factored, either by \mathcal{C}_{st} and \mathcal{C}_{ap} .
The estimates are asymptotically constant-free.

In specific situations, we can provide guaranteed bounds on \mathcal{C}_{st} and \mathcal{C}_{ap} .

There is still a long way toward fully reliable error estimation for high-frequency problems!



T. Chaumont-Frelet, A. Ern and M. Vohralík, *Numer. Math.*, 2021.

Concluding remarks

Extensions

We can obtain guaranteed bounds on \mathcal{C}_{st} in weakly trapping geometry with “directional” Morawetz multiplier

$$(\mathbf{x}_d \mathbf{e}^d) \cdot \nabla u.$$



S.N. Chandler-Wilde et. al., *SIAM J. Math. Anal.*, 2020.



T. Chaumont-Frelet and E.A. Spence, *submitted*.



T. Chaumont-Frelet and Z. Kassali, *in progress*.

It is possible to obtain approximations for \mathcal{C}_{ap} in more general situations.

Everything I presented (painfully) extends to Maxwell's equations:



T. Chaumont-Frelet, A. Ern and M. Vohralík, *C.R. Math. Acad. Sci.*, 2020.



T. Chaumont-Frelet, A. Ern and M. Vohralík, *Math. Comp.*, 2021.



T. Chaumont-Frelet and M. Vohralík, *submitted*.



T. Chaumont-Frelet, *will be submitted soon!*

Thanks for your attention! :-)