Séminaire du Centre de Mathématiques Appliquées

A curious instability phenomenon for rounded corners in plasmonic metamaterials

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Coll. with A.-S. Bonnet-Ben Dhia[2], P. Ciarlet[2], C. Carvalho[2], X. Claeys[3], S.A. Nazarov[4]

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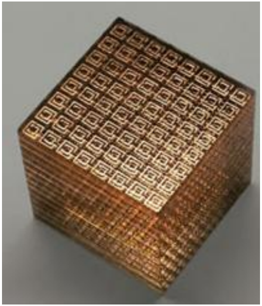
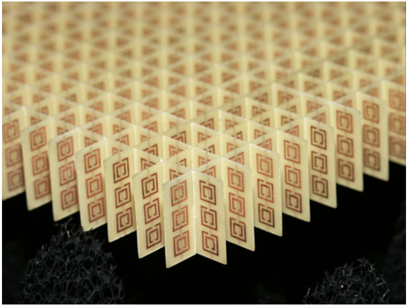
Introduction: physical context

- Electromagnetism in presence of metamaterials.





Zoom on a metamaterial (NASA)

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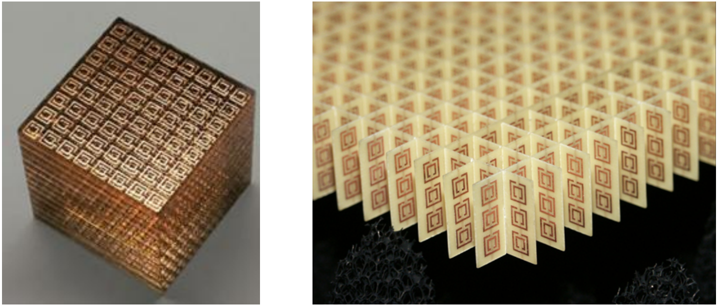


ZOOM ON A METAMATERIAL (NASA)

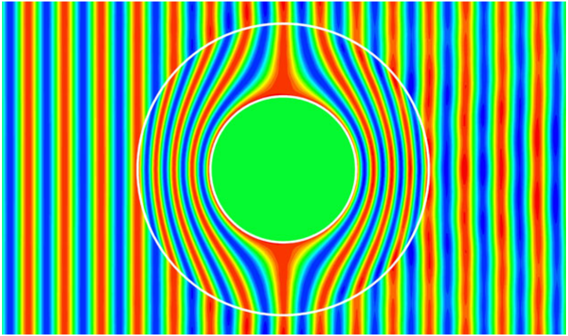
"*Metamaterials are artificial materials engineered to have properties that may not be found in nature. [...] Metamaterials gain their properties not from their composition, but from their exactingly-designed structures.*"

One example in nature

- For certain butterflies, bright colors are not due chemical pigments but rather to a geometric arrangement of tissues.

☛ The general idea is to design structures to control light.

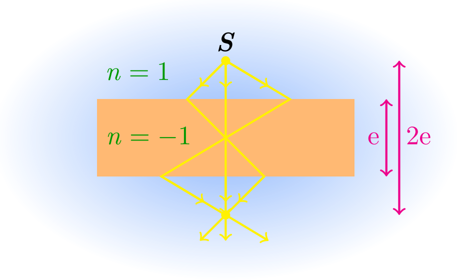
- Realization of cloaking devices (*capes d'invisibilité*).



Remark: a priori, one could use the same idea to bend tsunami and seismic waves.

Some applications of metamaterials 2/2

- Realization of negative refractive index materials ($n < 0$).



$\Rightarrow$ The negative refraction at the interface metamaterial/dielectric could allow the realization of perfect lenses, photonic traps...

Negative metamaterials

- To design a material with a negative refractive index ($n < 0$), it is necessary to have both $\varepsilon < 0$ and $\mu < 0$.

- Here, ε and μ denote the permittivity and the permeability appearing in the Maxwell's equations:

$$\left|\begin{array}{l} \operatorname{div} \boldsymbol{E} = \rho/\varepsilon \\ \operatorname{div} \boldsymbol{B} = 0 \\ \operatorname{curl} \boldsymbol{E} + \dfrac{\partial \boldsymbol{B}}{\partial t} = 0 \\ \mu^{-1} \operatorname{curl} \boldsymbol{B} - \varepsilon \dfrac{\partial \boldsymbol{E}}{\partial t} = \boldsymbol{J}, \end{array}\right.$$

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where

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\begin{array}{l}
\boldsymbol{E} \text{ is the electric field} \\
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\rho \text{ is the charge density} \\
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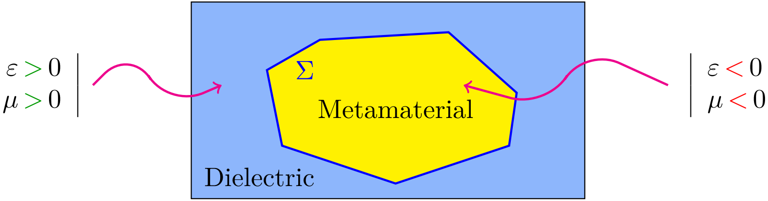

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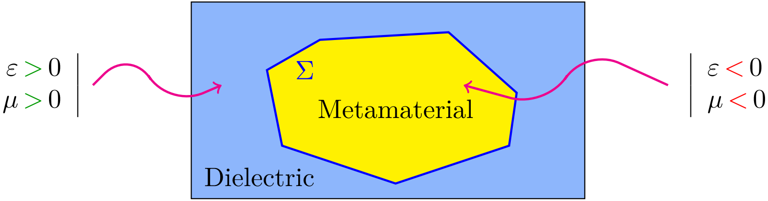

- In this talk, we consider only the homogenized model of the metamaterial (mathematical justification: `Bouchitté, Bourel, Felbacq 09`...).

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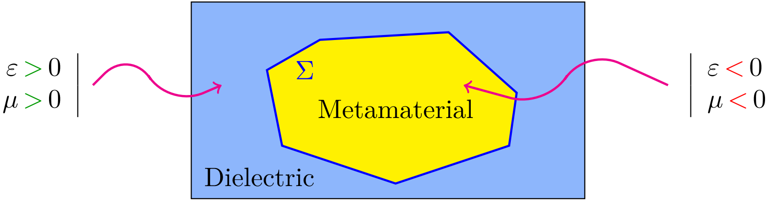

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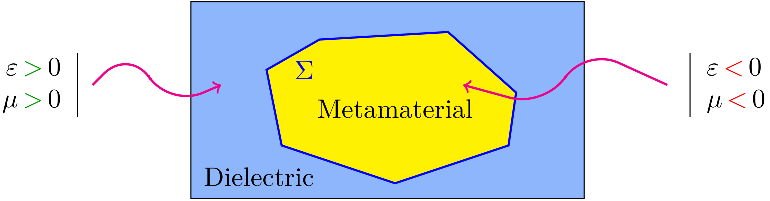

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- Broadly speaking, I investigate the following questions:
  - Do these problems with sign-changing coefficients have a unique solution?
  - If not, why (link with physics)?
  - Numerical methods to approximate the solution?

Outline of the talk

1. The coerciveness issue for the scalar case

2. A new functional framework in the critical interval

3. A curious instability phenomenon for a rounded corner

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2. A new functional framework in the critical interval
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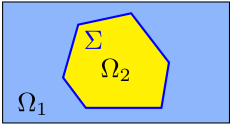
A scalar model problem

► Under appropriate assumptions, the study of Maxwell's equations reduces to the study of the following problem:

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ such that:} \\ -\mathrm{div}(\sigma \nabla u) = f \text{ in } \Omega. \end{array} \right.$$



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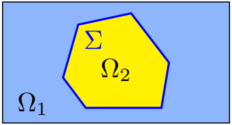

- $\mathrm{H}^1_0(\Omega) = \{v \in \mathrm{L}^2(\Omega) \,|\, \nabla v \in \mathbf{L}^2(\Omega);\ v|_{\partial\Omega} = 0\}$
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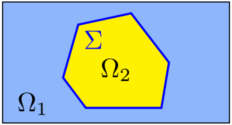

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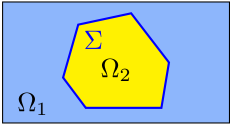

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$$(\mathscr{P}) \quad \Leftrightarrow \quad (\mathscr{P}_V) \quad \left| \begin{array}{l} \text{Find } u \in \mathrm{H}_0^1(\Omega) \text{ such that:} \\ a(u, v) = \ell(v),\ \forall v \in \mathrm{H}_0^1(\Omega), \end{array} \right.$$

with $a(u, v) = \displaystyle\int_\Omega \sigma \, \nabla u \cdot \nabla v \, d\boldsymbol{x}$ and $\ell(v) = \langle f, v \rangle$.

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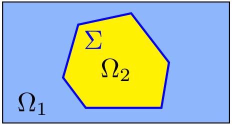

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Definition. We will say that the problem $(\mathscr{P})$ is well-posed if the operator $\mathrm{div}\,(\sigma\nabla\cdot)$ is an isomorphism from $\mathrm{H}^1_0(\Omega)$ to $\mathrm{H}^{-1}(\Omega)$.

Mathematical difficulty

- Classical case $\sigma > 0$ everywhere:

$$a(u,u) = \int_\Omega \sigma\,|\nabla u|^2\,d\boldsymbol{x} \geq \min(\sigma)\,\|u\|^2_{\mathrm{H}^1_0(\Omega)} \qquad \text{coercivity}$$

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- The case σ changes sign:

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? How to study $(\mathscr{P})$ when σ changes sign?

Idea of the $\mathtt{T}$-coercivity 1/2

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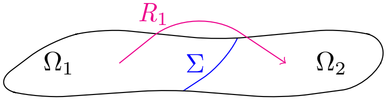

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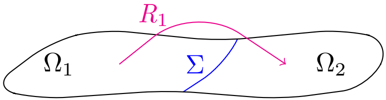

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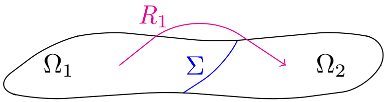

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On Σ, we have $-u + 2R_1 u = -u + 2u = u \Rightarrow \mathtt{T}_1 u \in \mathrm{H}^1_0(\Omega)$.

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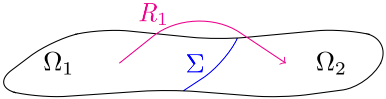

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2 $\mathtt{T}_1 \circ \mathtt{T}_1 = Id$ so $\boxed{\mathtt{T}_1 \text{ is an isomorphism of } \mathrm{H}^1_0(\Omega)}$

Idea of the $\mathtt{T}$-coercivity 2/2

3. We find $a(u, \mathtt{T}_1 u) = \displaystyle\int_\Omega |\sigma|\,|\nabla u|^2\, d\boldsymbol{x} - 2\int_{\Omega_2} \sigma_2\, \nabla u \cdot \nabla(R_1(u|_{\Omega_1}))\, d\boldsymbol{x}$.

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Young's inequality: $\Rightarrow$ a is T-coercive when $\sigma_1 > \|R_1\|^2 \, |\sigma_2|$.

Idea of the T-coercivity 2/2

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Idea of the $\mathtt{T}$-coercivity

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5 Conclusion:

THEOREM. If the contrast $\kappa_\sigma = \sigma_2/\sigma_1 \notin [-\|R_2\|^2; -1/\|R_1\|^2]$, then Problem $(\mathscr{P})$ is well-posed.

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5. Conclusion:

The interval depends on the norms of the transfer operators

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Choice of R_1, R_2?

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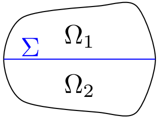

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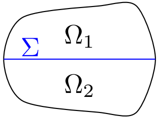

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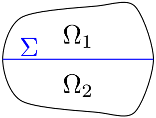

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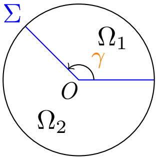

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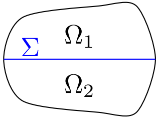

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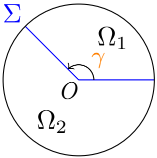

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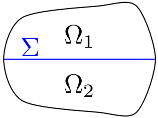

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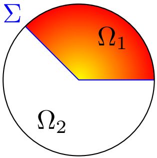

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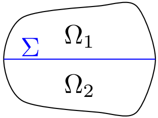

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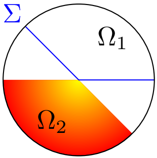

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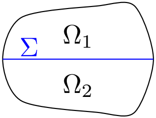

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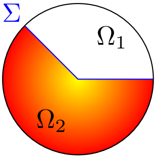

Action of R_1: symmetry + dilatation in θ

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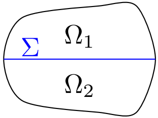

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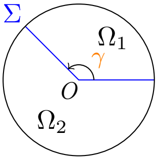

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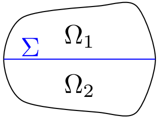

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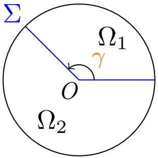

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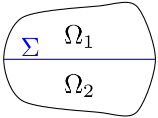

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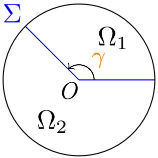

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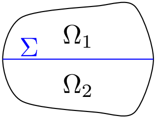

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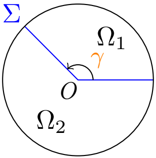

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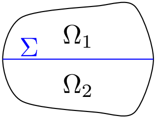

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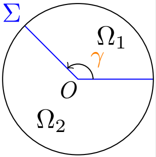

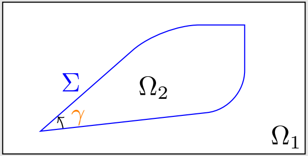

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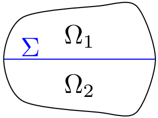

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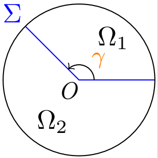

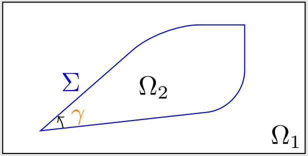

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- Using localization techniques, we can prove the

> Proposition. $(\mathscr{P})$ is well-posed in the Fredholm sense for a curvilinear polygonal interface iff $\kappa_\sigma \notin [-\mathcal{R}_\gamma; -1/\mathcal{R}_\gamma]$ where γ is the smallest angle.

$\Rightarrow$When Σ is smooth, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\sigma \neq -1$.

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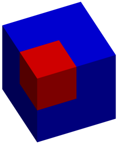

Fichera corner. Using some symmetries, we can build R_1, R_2 such that $\|R_1\|^2 = \|R_2\|^2 = 7$

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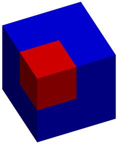

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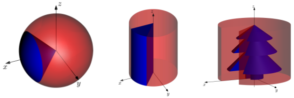
More cases in 3D than in 2D:  ...

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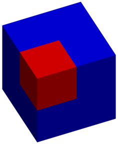

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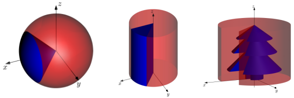

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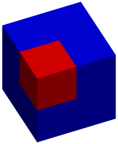

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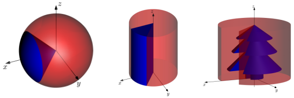
More cases in 3D than in 2D:  ...

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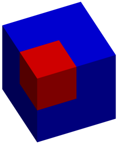

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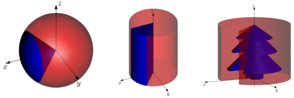
More cases in 3D than in 2D:  ...

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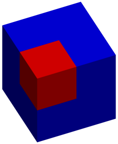

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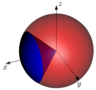
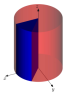
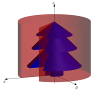
More cases in 3D than in 2D:    ...

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1. The coerciveness issue for the scalar case

2. A new functional framework in the critical interval

3. A curious instability phenomenon for a rounded corner

Problem considered in this section

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ such that:} \\ -\mathrm{div}(\sigma \nabla u) = f \quad \text{ in } \Omega. \end{array} \right.$$

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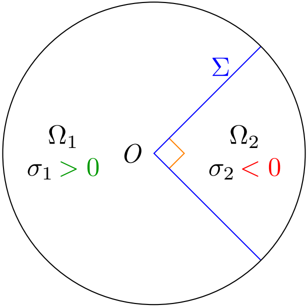

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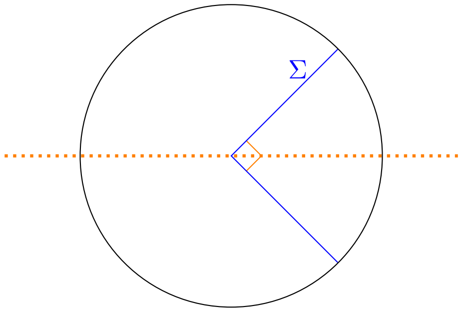

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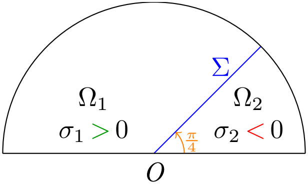

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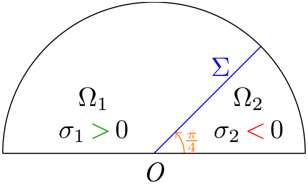

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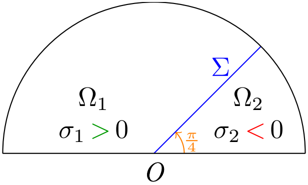

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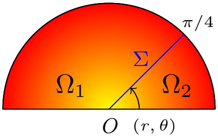
What happens when $\kappa_\sigma \in (-1; -1/3]$?

Analogy with a waveguide problem

- Bounded sector Ω

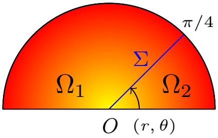


- Equation:

$$\underbrace{-\mathrm{div}(\sigma\nabla u)}_{-r^{-2}(\sigma(r\partial_r)^2+\partial_\theta\sigma\partial_\theta)u} \qquad = f$$

Analogy with a waveguide problem

- Bounded sector Ω



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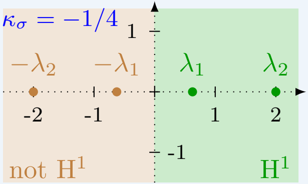
- Singularities in the sector

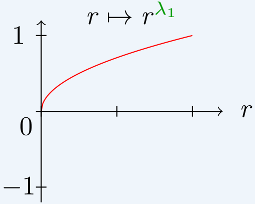
$$s(r,\theta) = r^\lambda\varphi(\theta)$$

Analogy with a waveguide problem

We compute the singularities $s(r,\theta) = r^\lambda \varphi(\theta)$ and we observe two cases:

- Outside the critical interval





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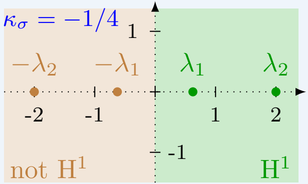

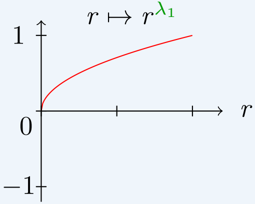

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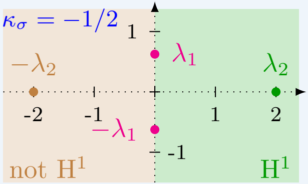

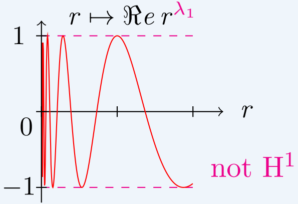

Inside the critical interval: message 1

For a contrast κ_σ inside the critical interval, there are singularities of the form $s(r,\theta) = r^{\pm i\eta}\varphi(\theta)$ with $\eta \in \mathbb{R} \setminus \{0\}$.

- Using these singularities, we can show that the following *a priori* estimate does not hold

$$\xcancel{\|u\|_{\mathrm{H}^1_0(\Omega)} \leq C\,(\|Au\|_{\mathrm{H}^1_0(\Omega)} + \|u\|_{\mathrm{L}^2(\Omega)}), \qquad \forall u \in \mathrm{H}^1_0(\Omega),}$$

where $A : \mathrm{H}^1_0(\Omega) \to \mathrm{H}^1_0(\Omega)$ is the operator such that

$$(Au, v)_{\mathrm{H}^1_0(\Omega)} = (\sigma\nabla u, \nabla v)_\Omega, \qquad \forall u, v \in \mathrm{H}^1_0(\Omega).$$

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Proposition. For $\kappa_\sigma \in (-1; -1/3)$, the operator A is not of Fredholm type ($\Im m\, A$ is not closed in $\mathrm{H}^1_0(\Omega)$).

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Let's see how to change the functional framework to recover a well-posed problem ...

Analogy with a waveguide problem

We compute the singularities $s(r,\theta) = r^\lambda \varphi(\theta)$ and we observe two cases:

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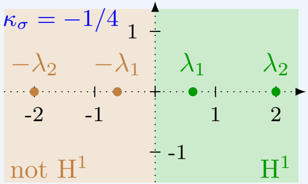

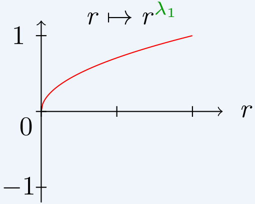

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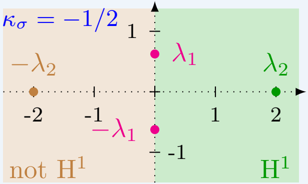

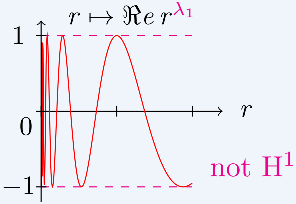

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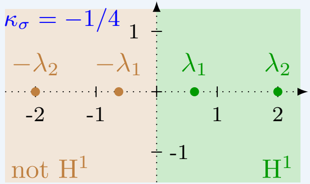

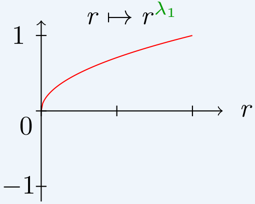

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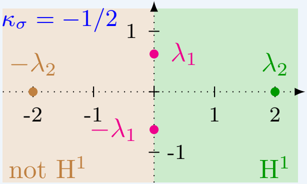
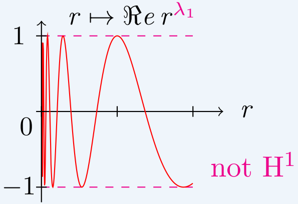
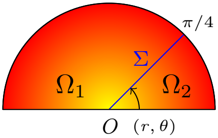




How to deal with the propagative singularities inside the critical interval?

Analogy with a waveguide problem

- Bounded sector Ω



- Equation:

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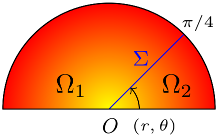
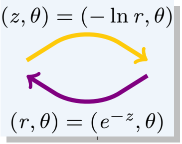
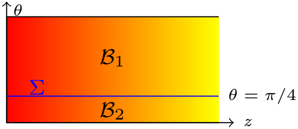




- Half-strip $\mathcal{B}$



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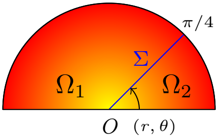

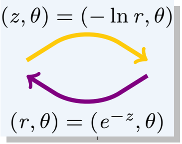

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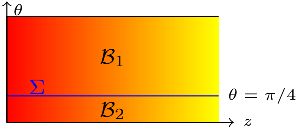

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- Equation:

$$\underbrace{-\mathrm{div}(\sigma\nabla u)}_{-(\sigma\partial_z^2+\partial_\theta\sigma\partial_\theta)u} = e^{-2z} f$$

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Analogy with a waveguide problem

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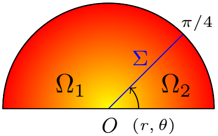

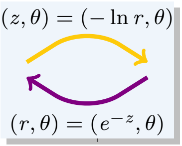

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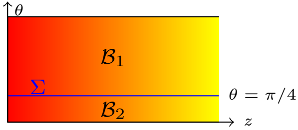

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- Modes in the strip

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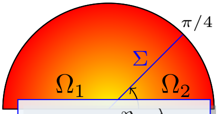
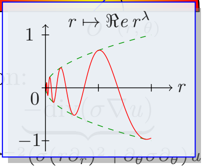
Analogy with a waveguide problem

- Bounded sector Ω





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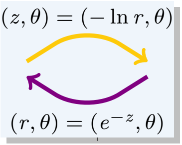

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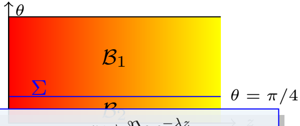

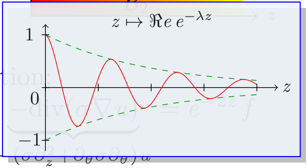

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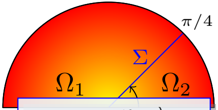
- Modes in the strip

$m(z,\theta) = e^{-\lambda z}\varphi(\theta)$

$s \in \mathrm{H}^1(\Omega)$ $\qquad$ $\Re e\,\lambda > 0$ $\qquad$ m is evanescent

Analogy with a waveguide problem

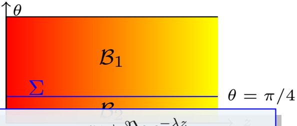
- Bounded sector Ω



$(z,\theta) = (-\ln r, \theta)$

$(r,\theta) = (e^{-z}, \theta)$

- Half-strip $\mathcal{B}$



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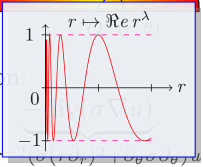

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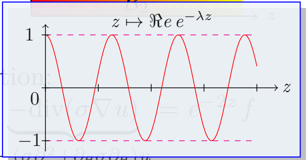

- Singularities in the sector

$$s(r,\theta) = r^{\lambda}\varphi(\theta)$$
$$= \cancel{r^{a}}\,(\cos b\ln r + i\sin b\ln r)\varphi(\theta)$$

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$(\Re e\,\lambda = a,\ \Im m\,\lambda = b)$

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Analogy with a waveguide problem

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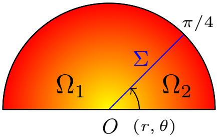

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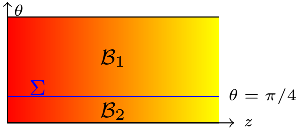

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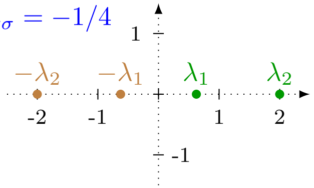
- This encourages us to use modal decomposition in the half-strip.

Modal analysis in the waveguide

$\kappa_\sigma = -1/4$



- Outside the critical interval. All the modes are exponentially growing or decaying.

$\rightarrow$ We look for an exponentially decaying solution. $\boxed{\mathrm{H}^1 \text{ framework}}$

Modal analysis in the waveguide

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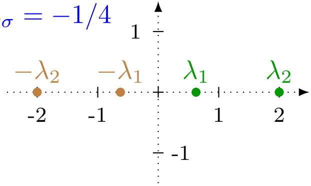

- Outside the critical interval. All the modes are exponentially growing or decaying.

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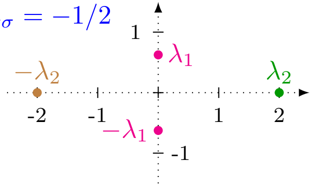
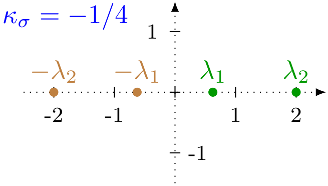
$\kappa_\sigma = -1/2$



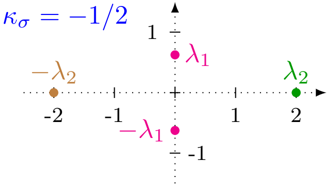
- Inside the critical interval. There are exactly two propagative modes.

Modal analysis in the waveguide



▶ Outside the critical interval. All the modes are exponentially growing or decaying.

→ We look for an exponentially decaying solution. $\boxed{\text{H}^1 \text{ framework}}$



▶ Inside the critical interval. There are exactly two propagative modes.

→ The decomposition on the outgoing modes leads to look for a solution of the form

$$u = \underbrace{c\,\varphi_1\, e^{\lambda_1 z}}_{\text{propagative part}} + \underbrace{u_e}_{\text{evanescent part}}.$$

$\boxed{\text{non H}^1 \text{ framework}}$

Inside the critical interval: message 2

✉ There is a functional framework, different from $\mathrm{H}_0^1(\Omega)$, involving one singularity, where existence and uniqueness of the solution holds.

How to numerically approximate the solution

in this new framework ?

Naive approximation

- Let us try a usual Finite Element Method (P1 Lagrange Finite Element). We solve the problem

$$\left| \begin{array}{l} \text{Find } u_h \in \mathrm{V}_h \text{ s.t.:} \\ \displaystyle\int_\Omega \sigma \nabla u_h \cdot \nabla v_h = \int_\Omega f v_h, \quad \forall v \in \mathrm{V}_h, \end{array} \right.$$

where V_h approximates $\mathrm{H}^1_0(\Omega)$ as $h \to 0$ (h is the mesh size).

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- We display u_h as $h \to 0$.

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THE SEQUENCE (u_h) DOES NOT CONVERGE AS $h \to 0$!!!

where V_h appr… $_0(\Omega)$ as $h \to 0$ (h is the mesh size).

- We display u_h as $h \to 0$.

(. . .)

Contrast $\kappa_\sigma = -0.999 \in (-1; -1/3)$.

Remark

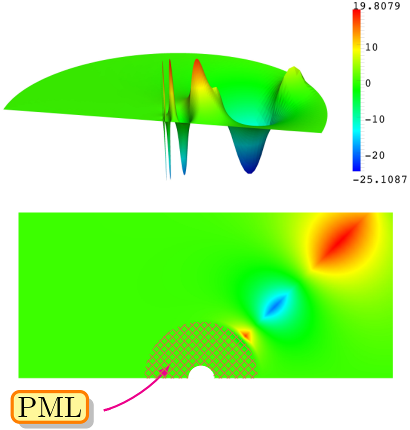
- Outside the critical interval, for the classical approximation method, the sequence (u_h) converges.

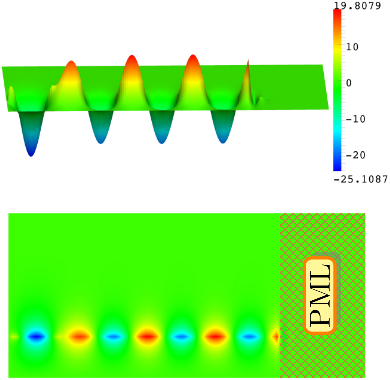
$$(\dots)$$

Contrast $\kappa_\sigma = -1.001 \notin (-1; -1/3)$.

How to approximate the solution?

- We use a PML (*Perfectly Matched Layer*) to bound the domain $\mathcal{B}$ + finite elements in the truncated strip ($\kappa_\sigma = -0.999 \in (-1; -1/3)$).

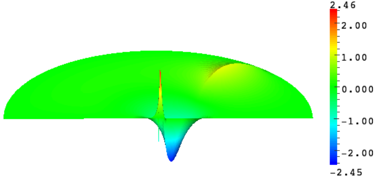


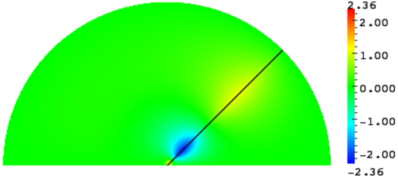


A curious black hole phenomenon

- For the Helmholtz equation $\operatorname{div}(\sigma\nabla u) + \omega^2 u = f$, analogously, it is necessary to modify the functional framework to have a well-posed problem.

- In time domain, the solution adopts a curious behaviour.





$$(\boldsymbol{x}, t) \mapsto \Re e\left(u(\boldsymbol{x})e^{-i\omega t}\right) \quad \text{for } \kappa_\sigma = -1/1.3$$

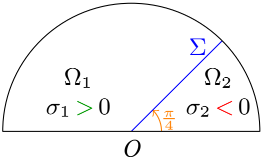
- Everything happens like if a waves was absorbed by the corner point.

- Analogous phenomena occur in cuspidal domains in the theory of water-waves and in elasticity (`Cardone, Nazarov, Taskinen`).

Summary of the results

Problem

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ s.t.:} \\ -\mathrm{div}\,(\sigma \nabla u) = f \qquad \text{in } \Omega. \end{array} \right.$$



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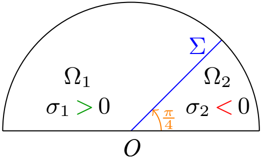
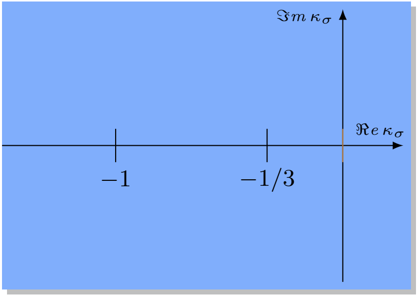


Results

For $\kappa_\sigma \in \mathbb{C}\backslash\mathbb{R}_-$, $(\mathscr{P})$ well-posed in $\mathrm{H}^1_0(\Omega)$ (Lax-Milgram)



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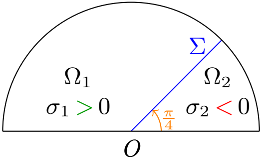

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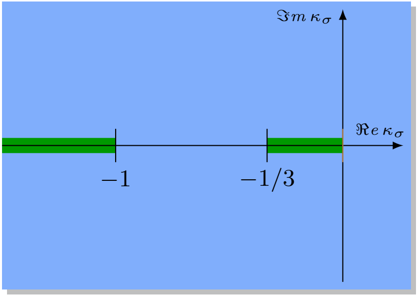

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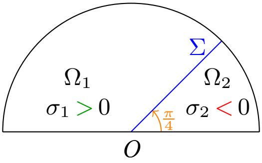

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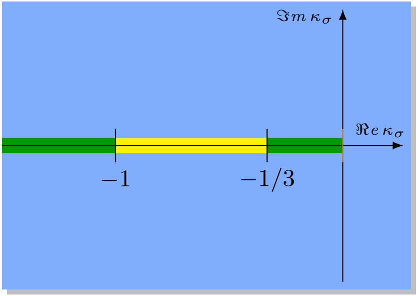

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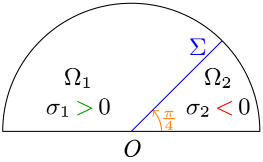

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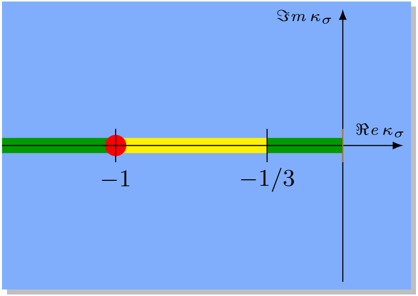
$\kappa_\sigma = -1$, $(\mathscr{P})$ ill-posed in $\mathrm{H}^1_0(\Omega)$



1. The coerciveness issue for the scalar case

2. A new functional framework in the critical interval

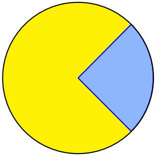
3. A curious instability phenomenon for a rounded corner

The problematic of the rounded corner

- We recall the problem under consideration

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ such that:} \\ -\mathrm{div}(\sigma \nabla u) = f \quad \text{ in } \Omega. \end{array} \right.$$

- When the interface has a corner, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\sigma \notin I_c$ (the critical interval).



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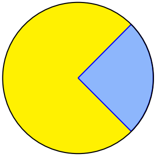

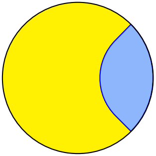

- When the interface is smooth, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\sigma \neq -1$.

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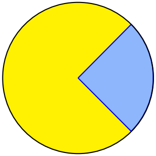
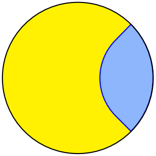
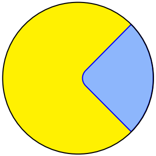




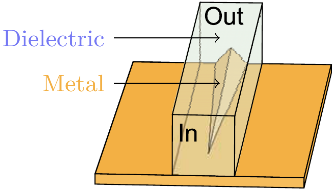
- When the interface is smooth, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\sigma \neq -1$.

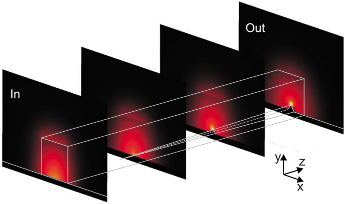
What happens for a slightly rounded corner when $\kappa_\sigma \in I_c \setminus \{-1\}$?

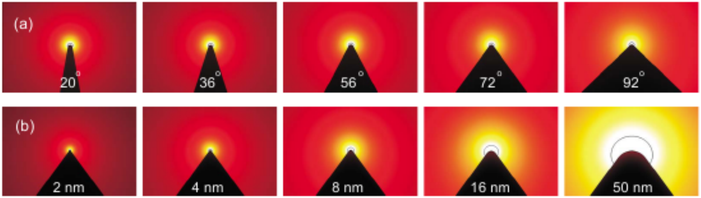


Physical context

- For metals at optical frequency, $\varepsilon(\omega) < 0$.





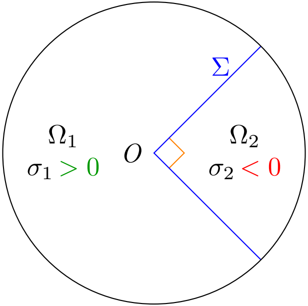


Figures from `O'Connor` *`et al.`*`, Appl. Phys. Lett. 95, 171112 (2009)`

- Physicists use singular geometries to focus energy. It allows to stock information.

Numerical experiment 1/2

- For the numerical experiments, we round the corner in a particular way



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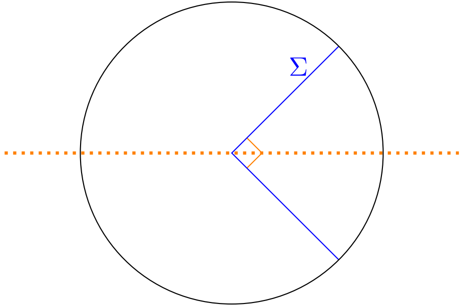

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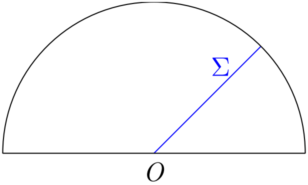

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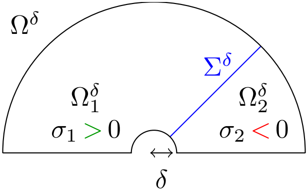

δ is the rounding parameter

Numerical experiment 1/2

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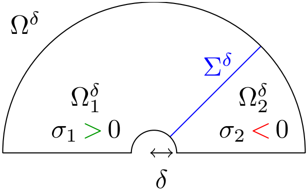

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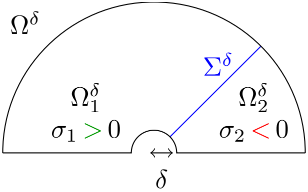

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- Our goal is to study the behaviour of the solution, *if it is well-defined*, of

$$(\mathscr{P}^\delta) \quad \left| \begin{array}{l} \text{Find } u^\delta \in \mathrm{H}^1_0(\Omega^\delta) \text{ such that:} \\ -\mathrm{div}(\sigma^\delta \nabla u^\delta) = f \quad \text{in } \Omega^\delta. \end{array} \right.$$

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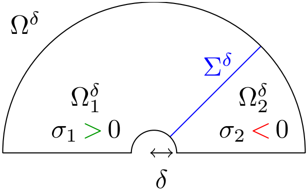

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- We approximate u^δ, *assuming it is well-defined*, by a usual P1 Finite Element Method. We compute the solution u_h^δ of the discretized problem with *FreeFem++*.

We display the behaviour of u_h^δ as $\delta \to 0$.

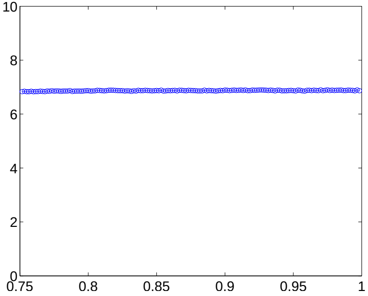
Numerical experiments 1/2

$\sigma_1 = 1$ and $\sigma_2 = 1$ (positive materials)

Numerical experiments 1/2

$\boxed{\sigma_1 = 1 \text{ and } \sigma_2 = 1 \text{ (positive materials)}}$

$(\dots)$



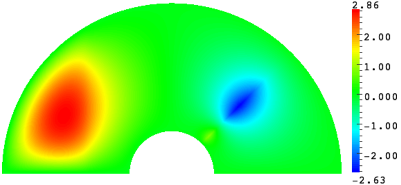
u_h^δ w.r.t. δ $\qquad$ $\|\nabla u_h^\delta\|_{\Omega^\delta}$ w.r.t. $1-\delta$

- For positive materials, it is well-known that $(u^\delta)_\delta$ converges to u, the solution in the limit geometry.
- The rate of convergence depends on the regularity of u.
- To avoid to mesh Ω^δ, we can approximate u^δ by u_h.

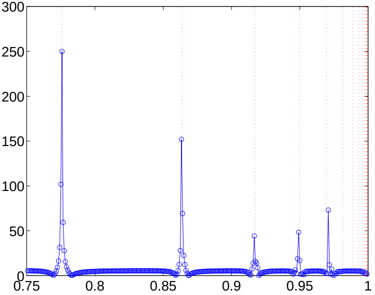
Numerical experiments 2/2

... and what about for a sign-changing σ???

$$\boxed{\sigma_1 = 1 \text{ and } \sigma_2 = -0.9999}$$



u_h^δ w.r.t. δ



$\|\nabla u_h^\delta\|_{\Omega^\delta}$ w.r.t. $1-\delta$

- For this configuration, u^δ seems to depend critically on δ.

Numerical experiments 2/2

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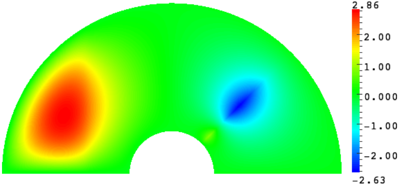

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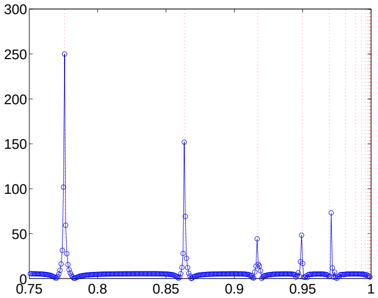

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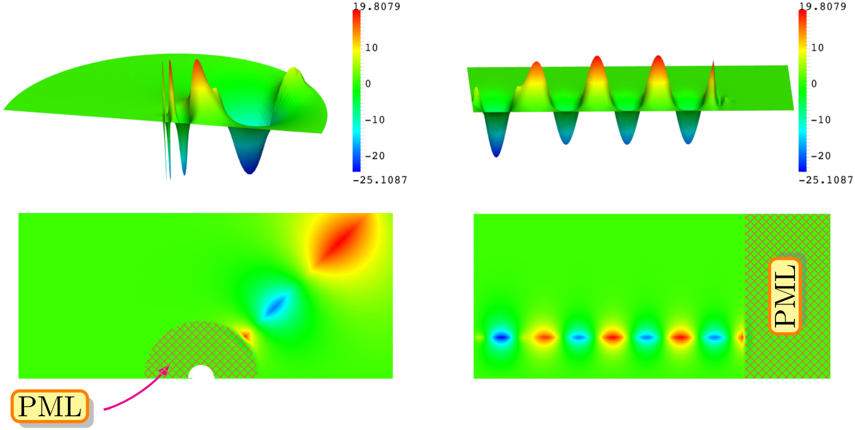
- For this configuration, u^δ seems to depend critically on δ.

Why???

How to approximate the solution?

- We use a PML (*Perfectly Matched Layer*) to bound the domain $\mathcal{B}$ + finite elements in the truncated strip ($\kappa_\sigma = -0.999 \in (-1; -1/3)$).



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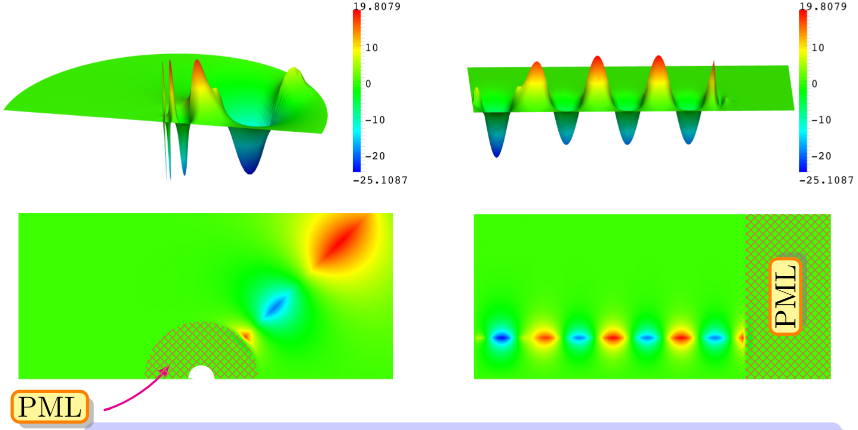
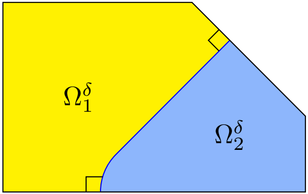
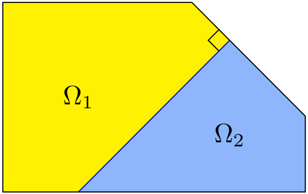


Without the PML, the solution in the truncated strip of length L does not converge when $L \to \infty$. This is what we observe in our numerical experiment for the rounded corner.

Source term problem





$$(\mathscr{P}^\delta)\ \left|\ \begin{array}{l}\text{Find } u^\delta \in \mathrm{H}_0^1(\Omega) \text{ s.t.:}\\ -\mathrm{div}(\sigma^\delta \nabla u^\delta) = f \text{ in } \Omega.\end{array}\right.$$

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- The behaviour of $(u^\delta)_\delta$ depends on the properties of the limit problem.

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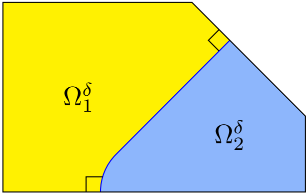

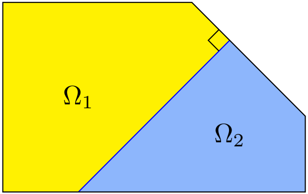

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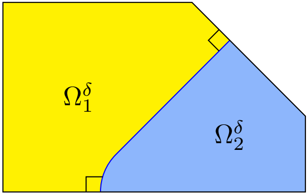
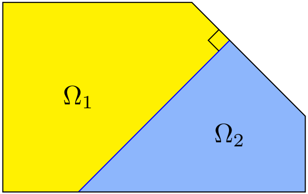
- The behaviour of $(u^\delta)_\delta$ depends on the properties of the limit problem.

If $(\mathscr{P})$ well-posed (in $\mathrm{H}^1_0(\Omega)$), then u^δ is uniquely defined for δ small enough and $(u^\delta)_\delta$ converges to u (as for positive materials).

Source term problem





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Idea of the approach:

1. We prove the *a priori* estimate $\|u^\delta\|_{\mathrm{H}^1_0(\Omega)} \le c\,|\ln\delta|^{1/2}\|f\|_\Omega$ for all δ in some set $\mathscr{S}$ which excludes a discrete set accumulating in zero (♠ hard part of the proof, `Nazarov's` technique).

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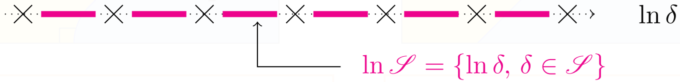

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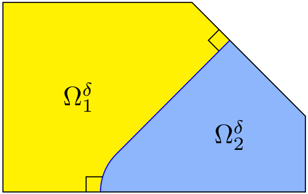

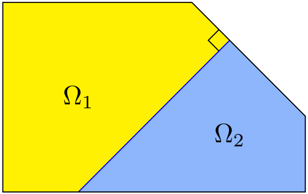

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- The $\mathtt{T}$-coercivity approach can be adapted to consider other problems (Maxwell equations, bilaplacian,...). Example:

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► Our new model in the critical interval raises a lot of questions, related to the physics of plasmonics and metamaterials.

> Can we observe this black-hole effect in practice? Is it possible that almost identical geometries leads to two different solutions?

More generally, can we reconsider the homogenization process to take into account interfacial phenomena?

Thank you for your attention!!!