Mathematical and Numerical study of plasmonic structures with corners

Camille Carvalho

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About

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- The modeling of plasmonic waveguides: characterization of the guided modes

Both theoretical and numerical aspects are investigated.

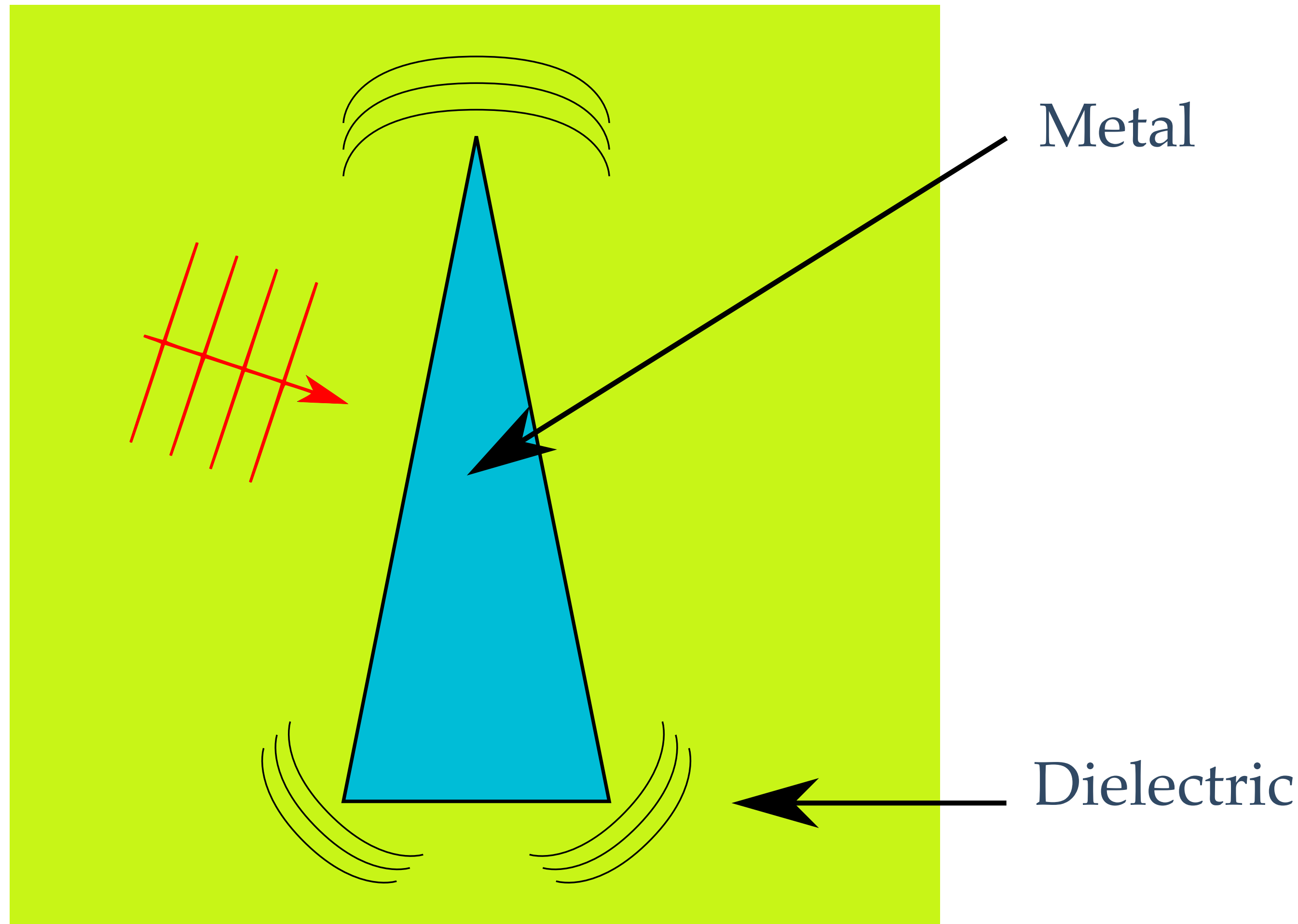
Both problems are tackled in the **time-harmonic regime.**

I'm more a mathematician than a physicist, I make some approximations in the model.

Motivations of this work

The goal is to compute the scattered field by a polygonal metallic obstacle.

$$u^{inc} = e^{i\overrightarrow{k}\cdot\overrightarrow{x}}$$



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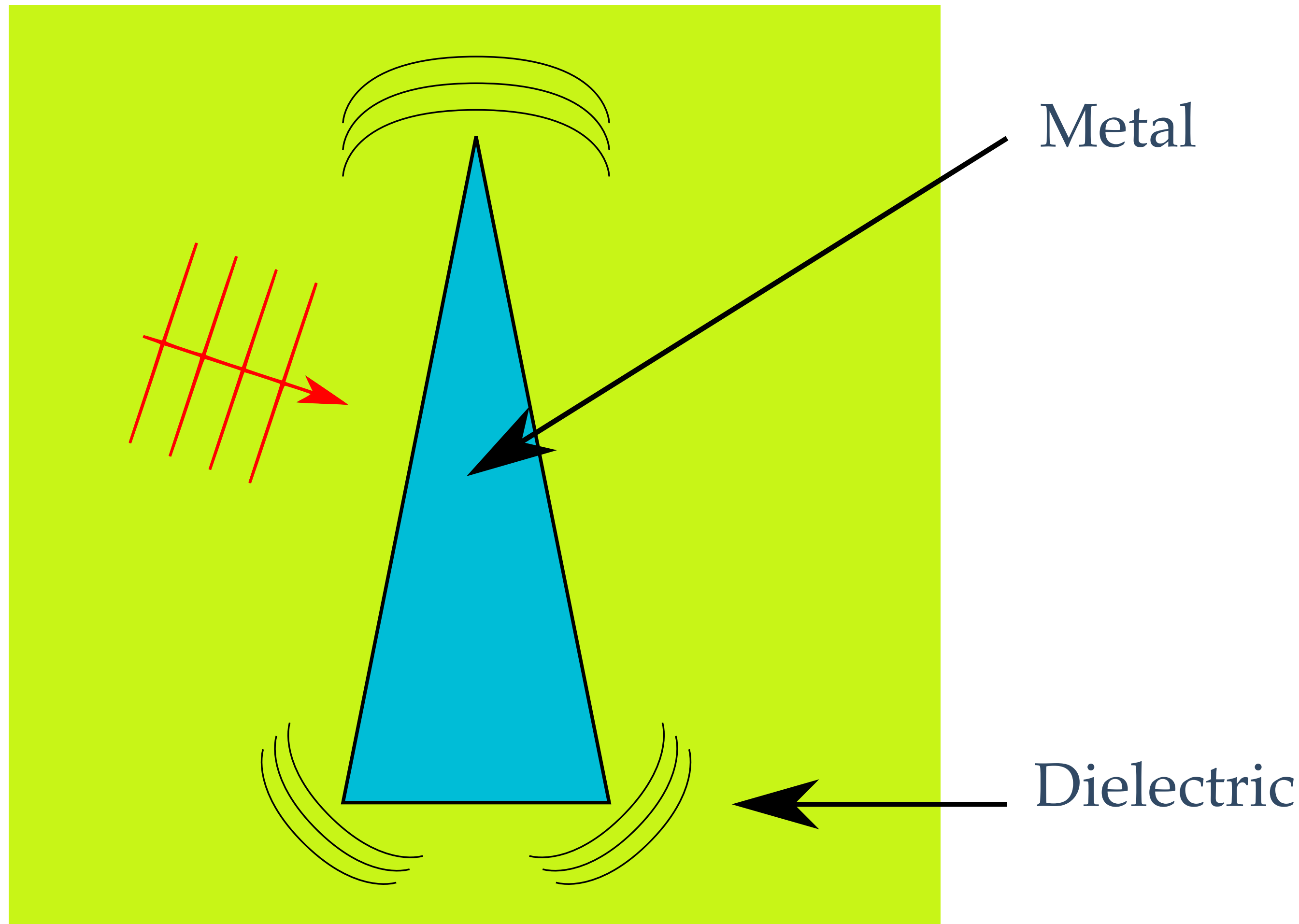

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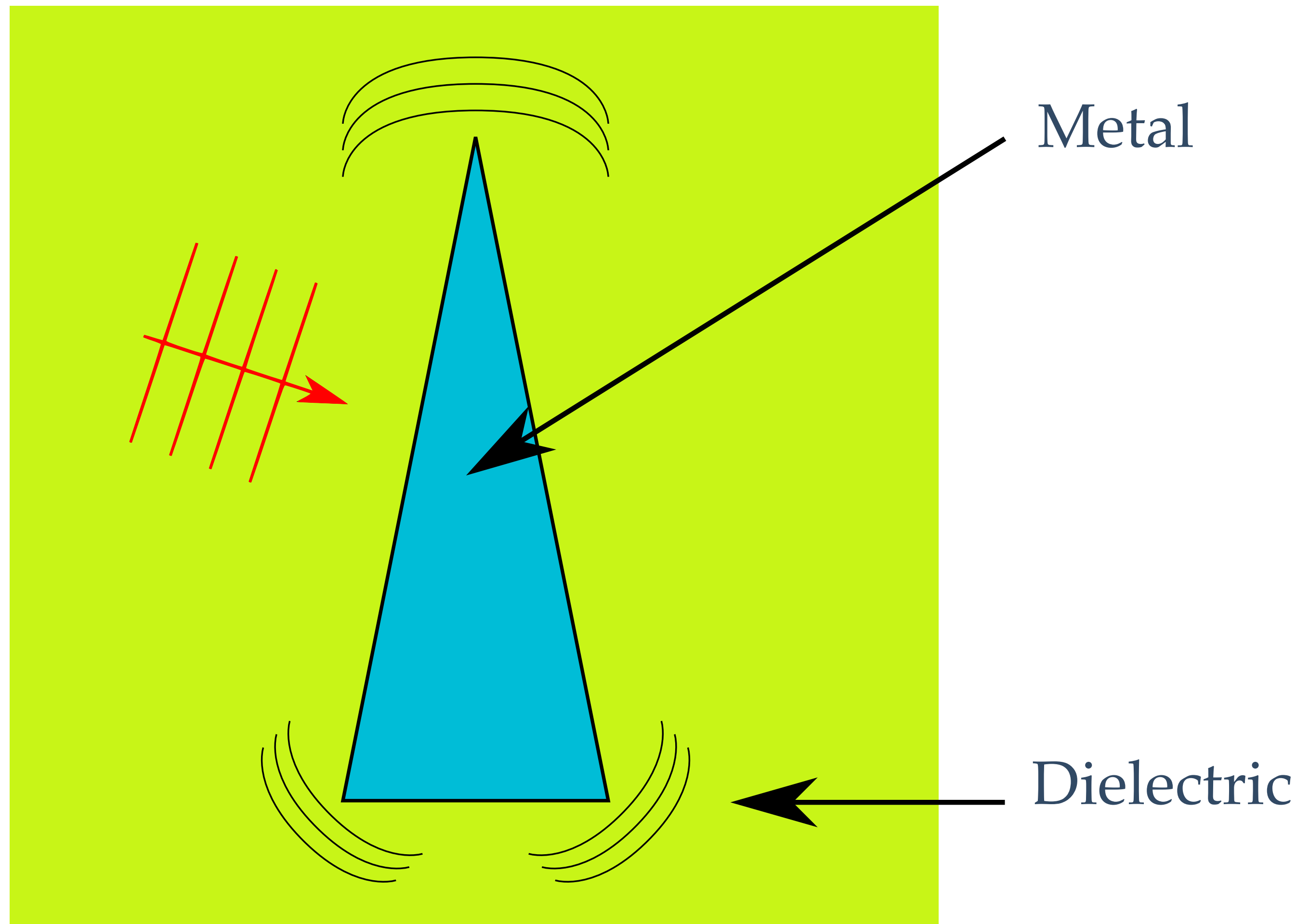

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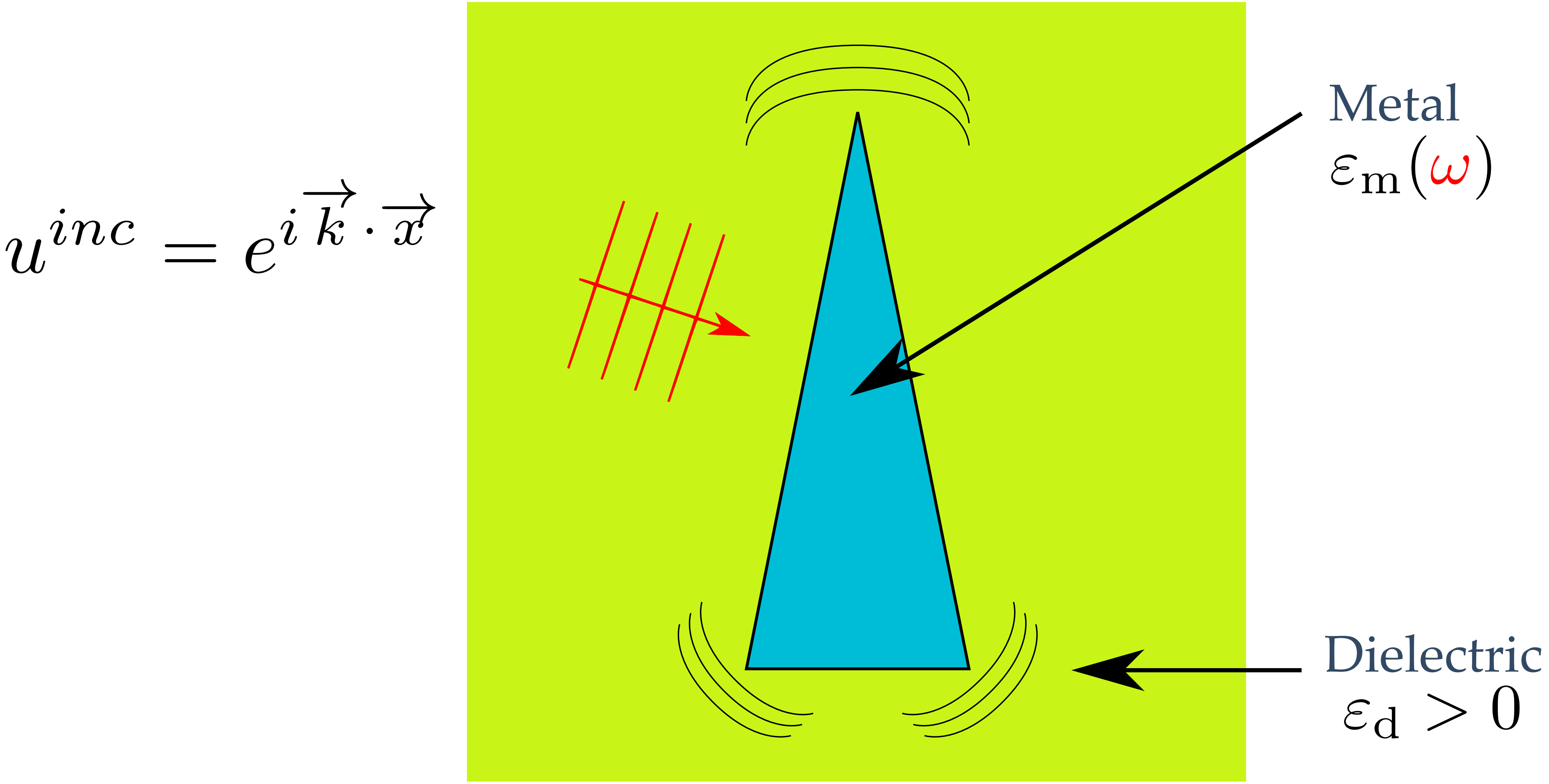

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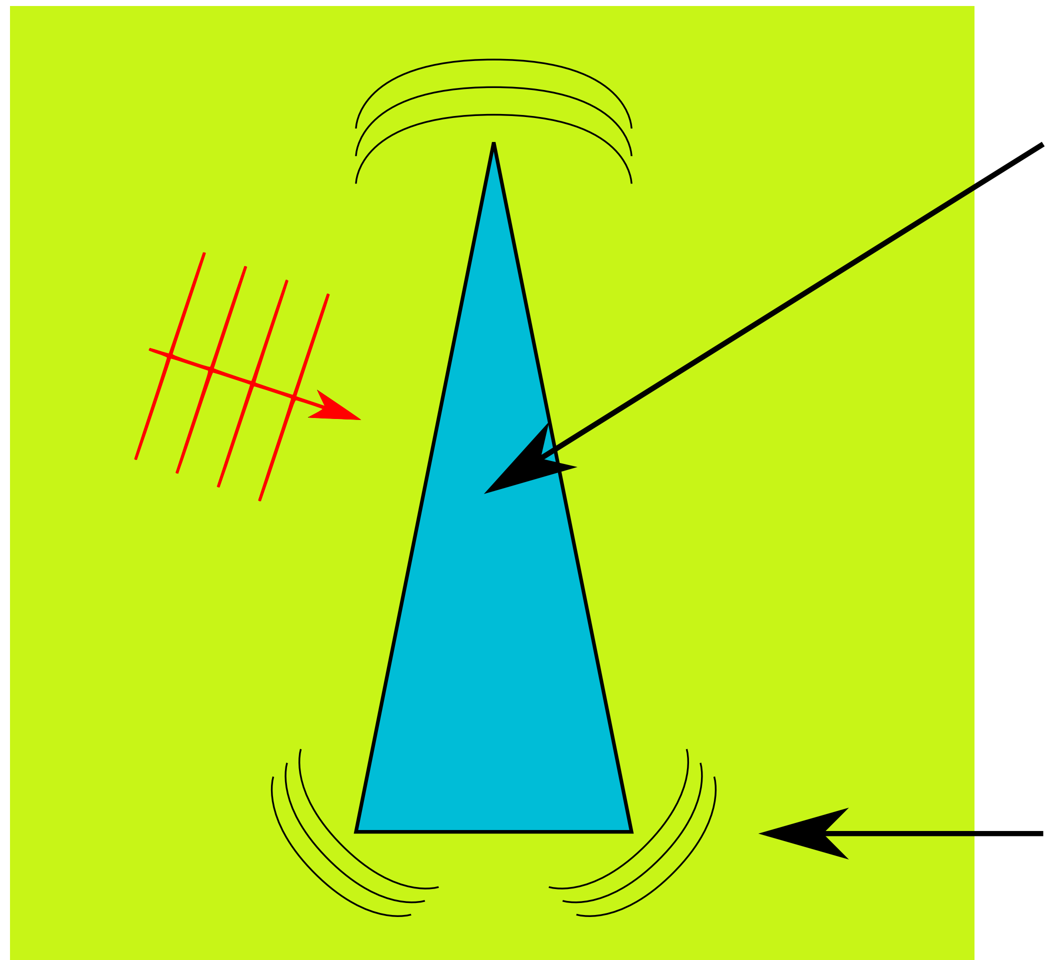

Metal
$\varepsilon_{\mathrm{m}}(\omega) \quad \mu_{\mathrm{m}} > 0$

Dielectric
$\varepsilon_{\mathrm{d}} > 0 \quad \mu_{\mathrm{d}} > 0$

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Time harmonic equations for the TM polarization

$$H_z = u^{\text{inc}} + u^{\text{sca}} \qquad k = \frac{\omega}{c}\sqrt{\varepsilon_{\text{d}}\mu_{\text{d}}}$$

$$\boxed{\begin{aligned} &\text{div}\left(\frac{1}{\varepsilon(\omega)}\nabla H_z\right) + \frac{\omega^2}{c^2}\mu H_z = 0 \text{ in } B_R \\ &\partial_n H_z - ikH_z = \partial_n u^{\text{inc}} - iku^{\text{inc}} \text{ on } \Gamma_R \end{aligned}}$$

- Radiation condition at finite distance

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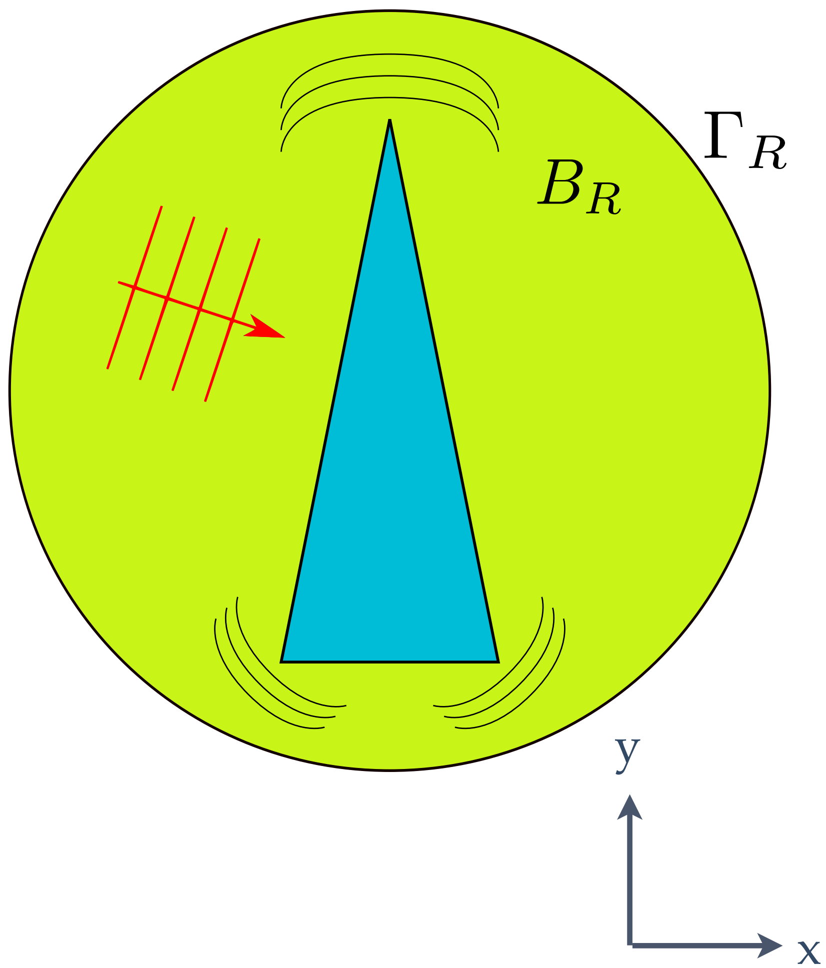

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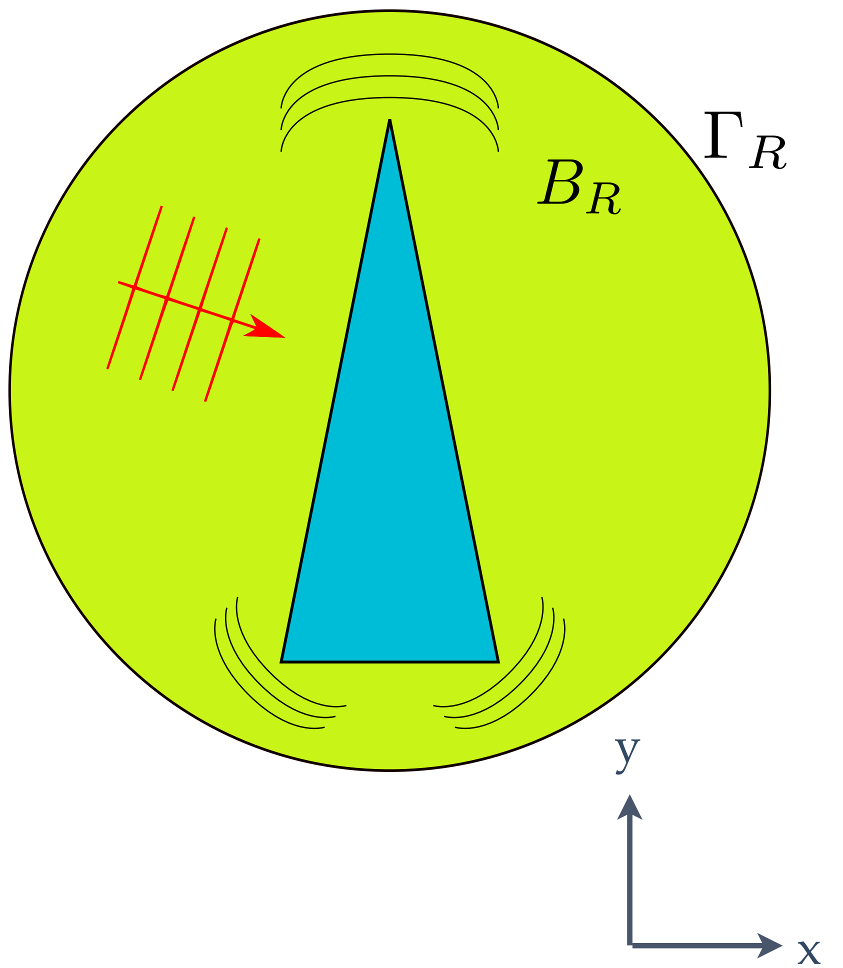

Mathematically:
-due to the dissipation, the problem has a unique solution
-one can approximate the solution with Finite Elements Methods

Numerical illustrations

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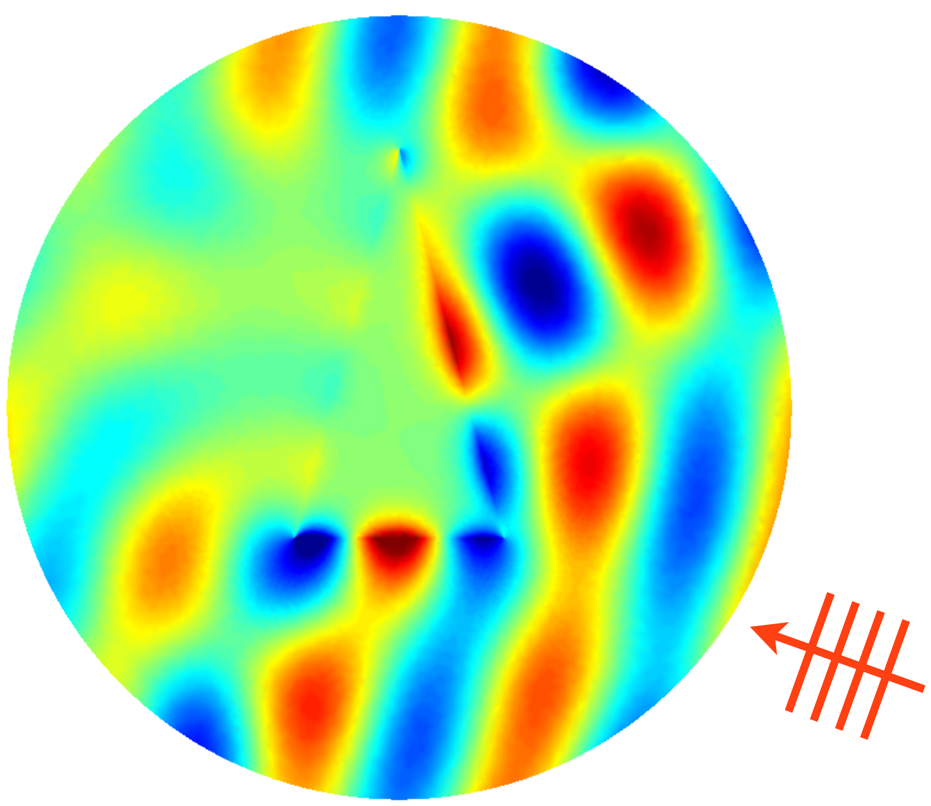

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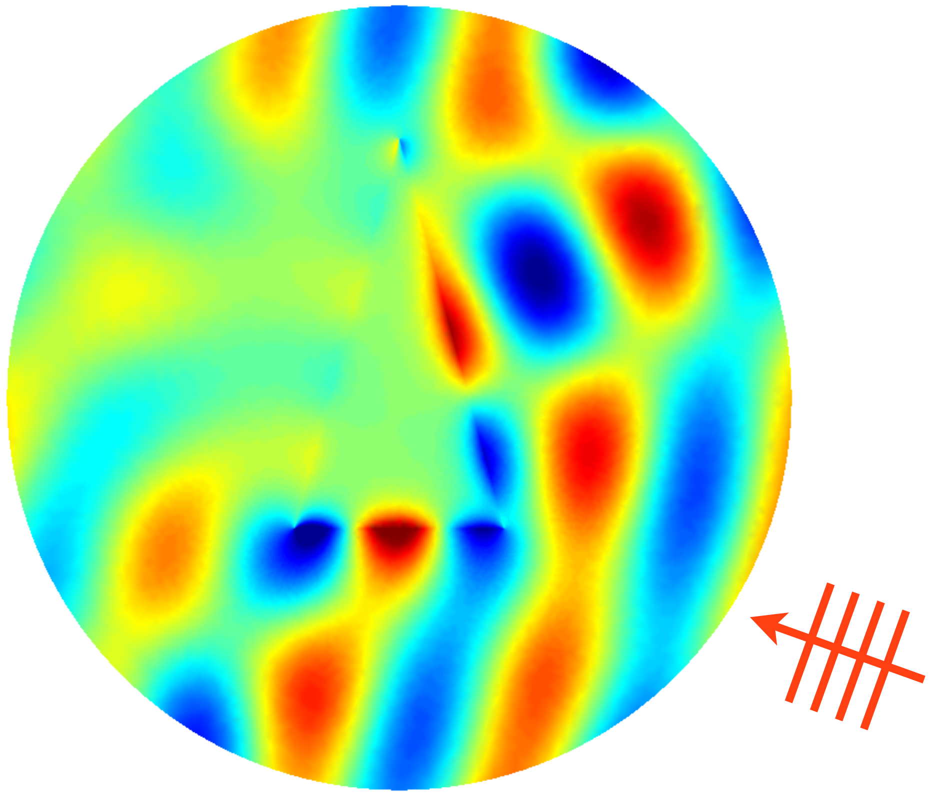

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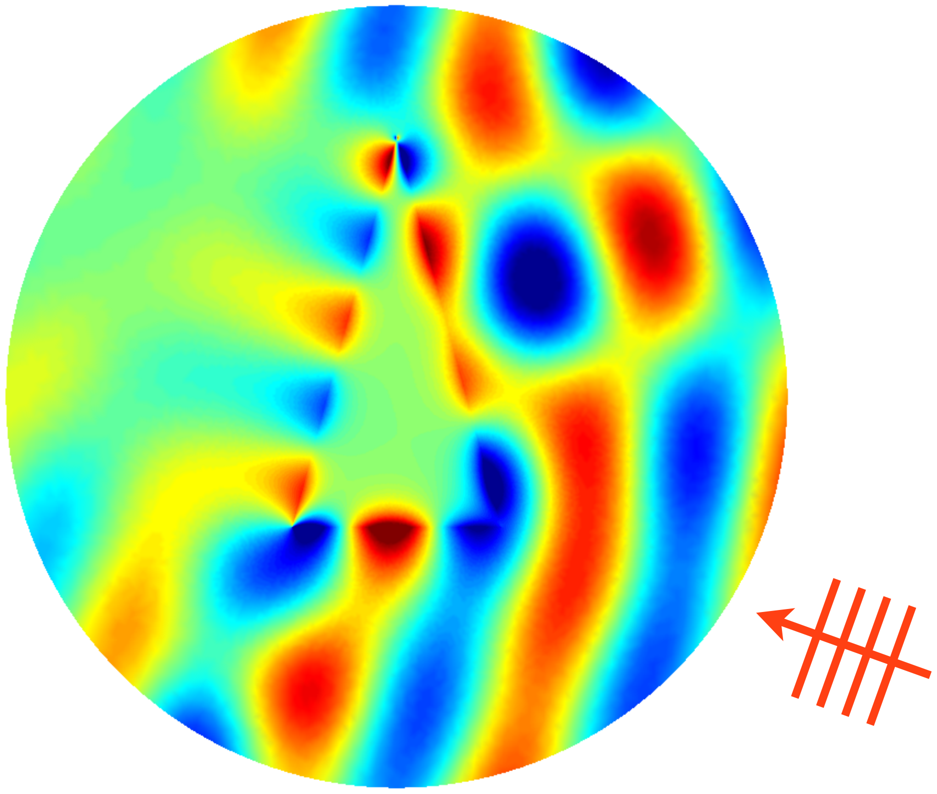

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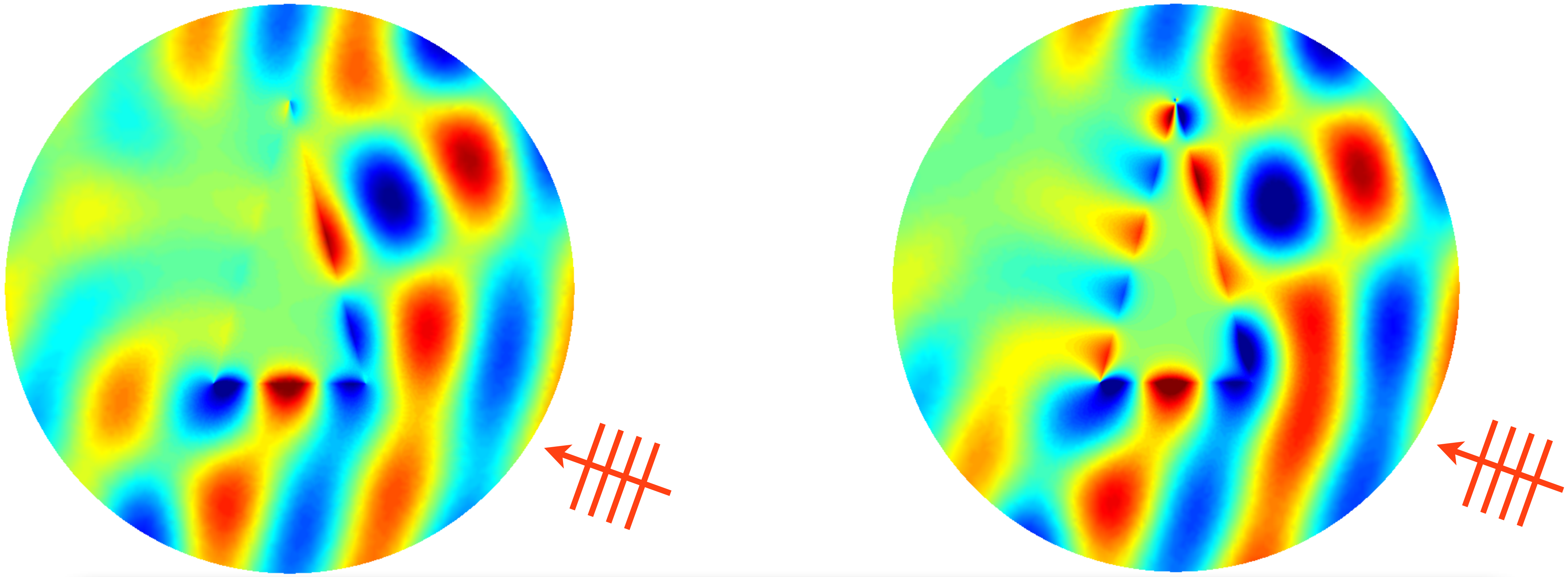

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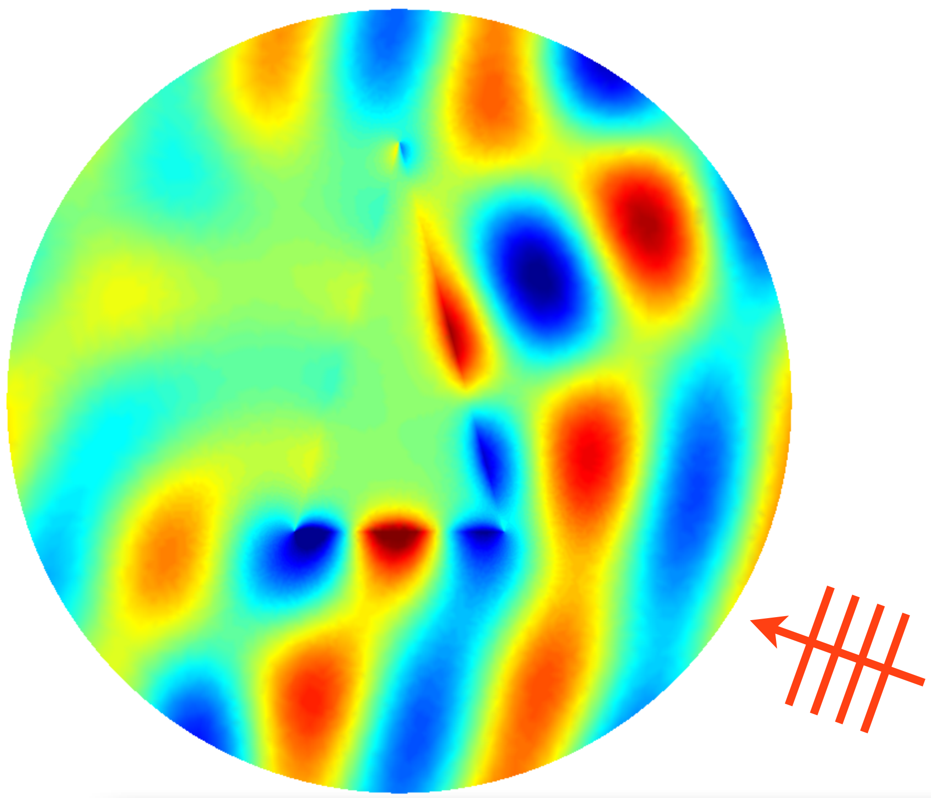

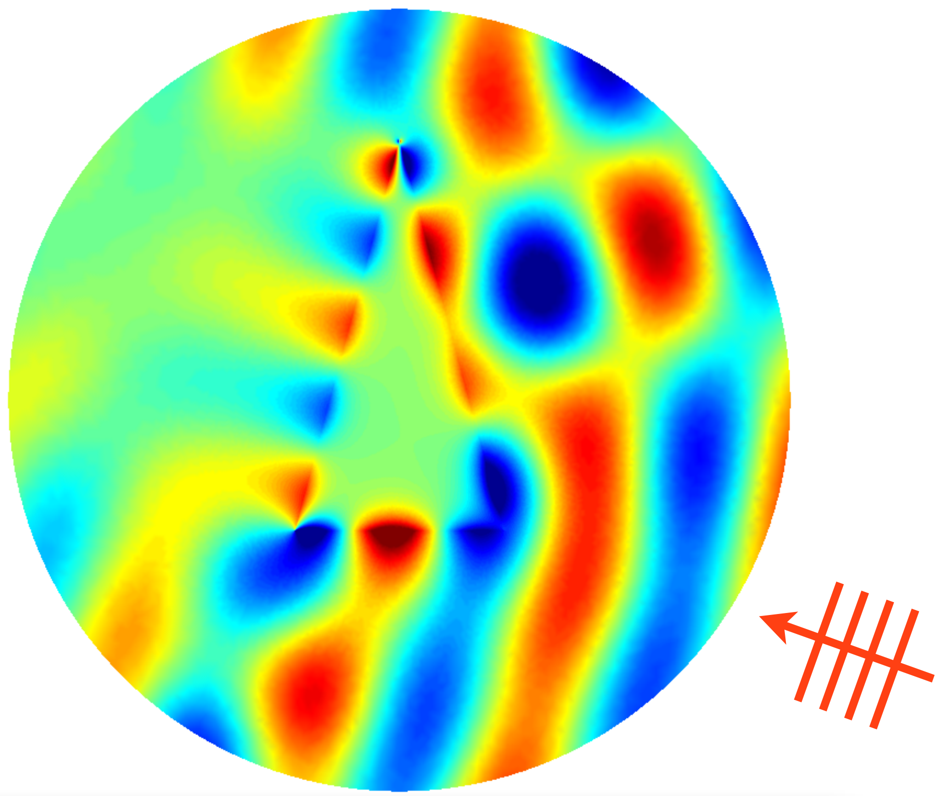

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To understand the reasons of such instabilities and how to avoid them, we study a **limit problem by neglecting dissipation.**

The dissipationless Drude's model

At optical frequencies ($\gamma \ll \omega < \omega_p$), one can neglect dissipation so that the metal's permittivity follows the law:

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-difficulties to prove existence and uniqueness of the solution
-the corners of the inclusion may cause strong singular behavior
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Once some answers have been given, we studied the guided modes of a dissipationless plasmonic waveguide.

Outline

- Introduction
- **Scattering problem with sign-changing coefficients**
- Guided modes in a plasmonic waveguide

Variational formulation

$$
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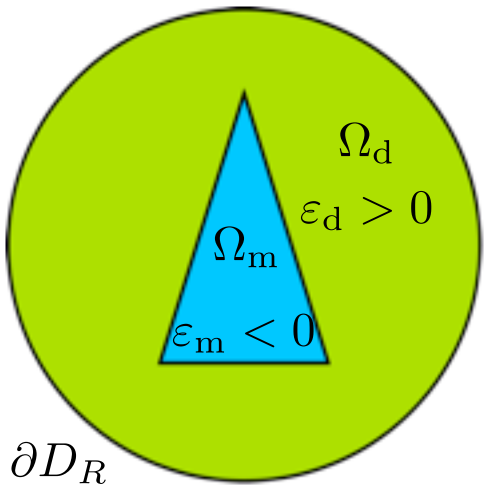

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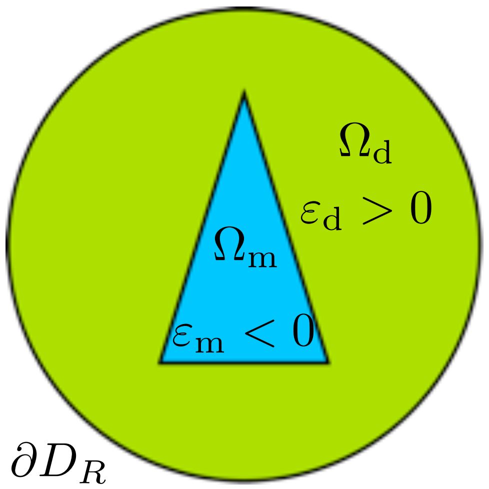

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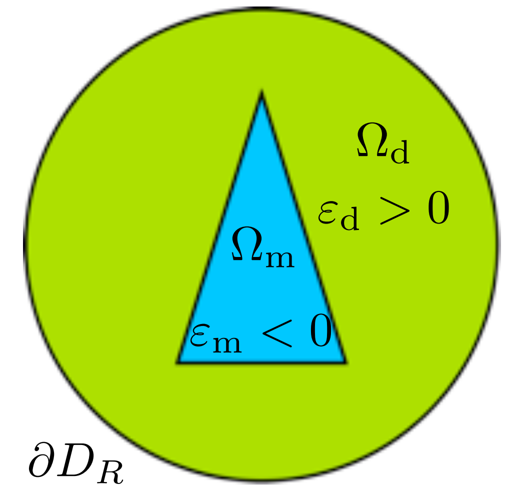

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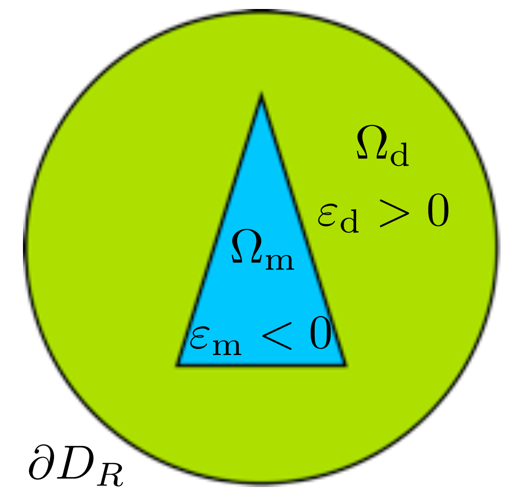

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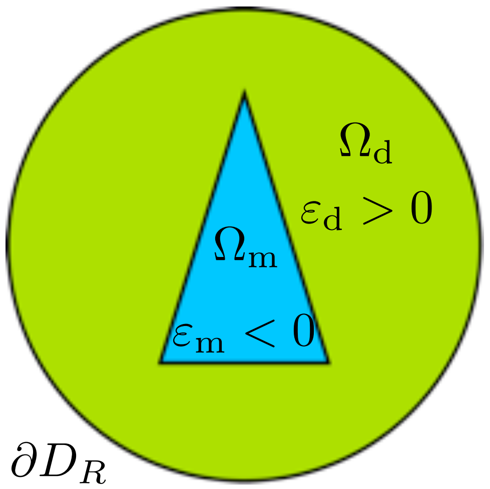

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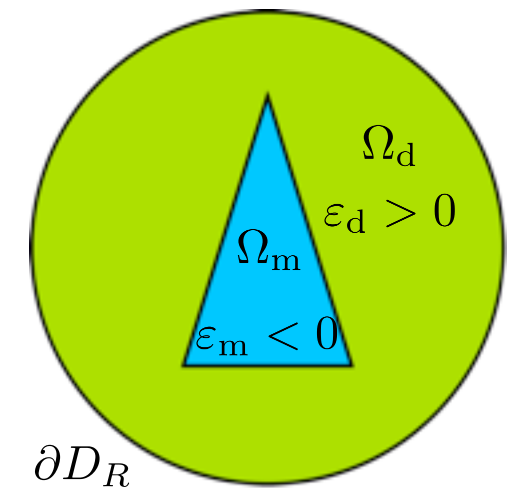

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Due to sign-changing coefficient, it is not guaranteed !

Study of non coercive forms

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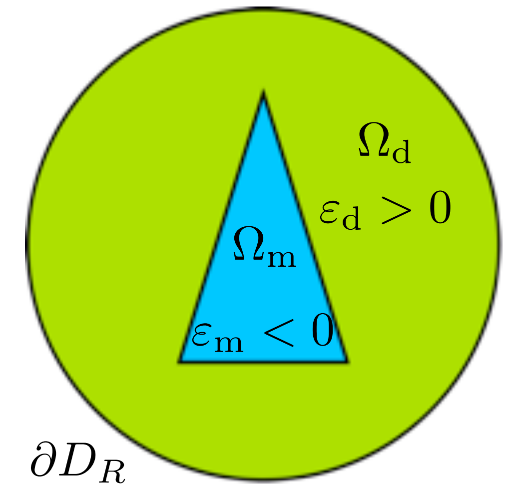

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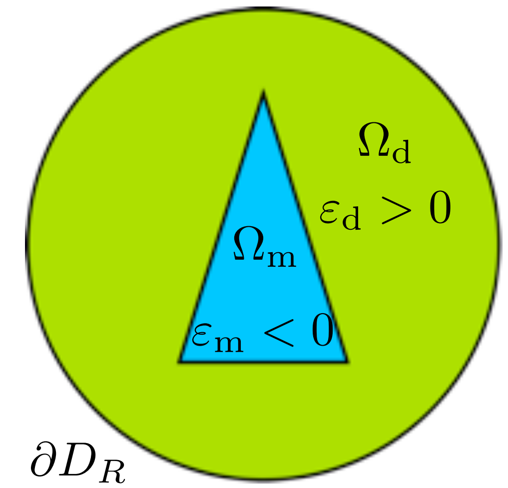

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T-coercivity for scalar interface problems between dielectrics and metamaterials,
Anne-Sophie Bonnet-Ben Dhia, Lucas Chesnel, Patrick Ciarlet, M2AN, 2012

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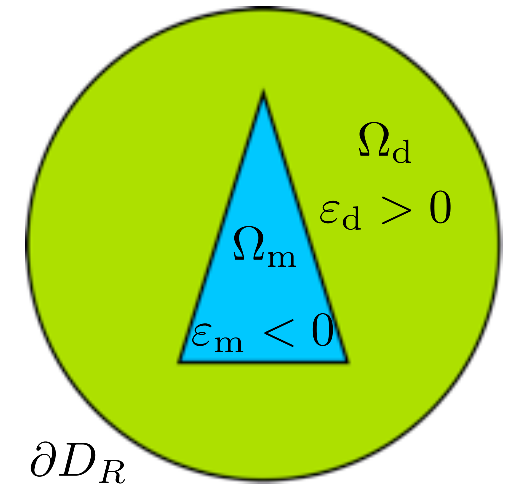

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In our case: YES if and only if $\kappa_\varepsilon := \dfrac{\varepsilon_{\text{m}}}{\varepsilon_{\text{d}}} \notin I_c$

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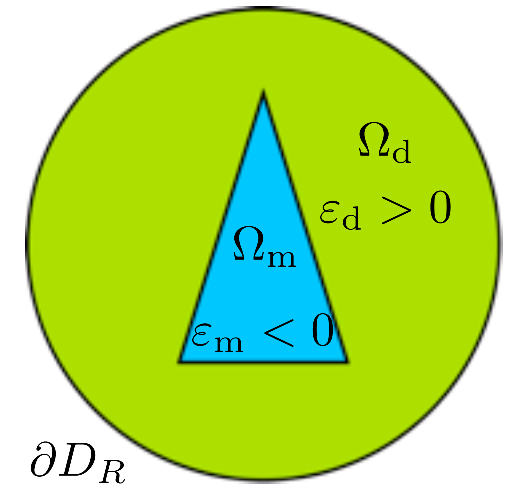

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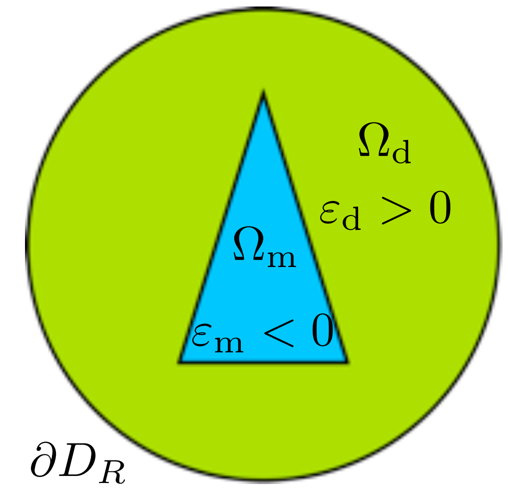

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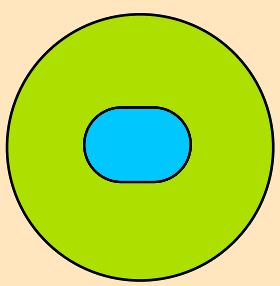

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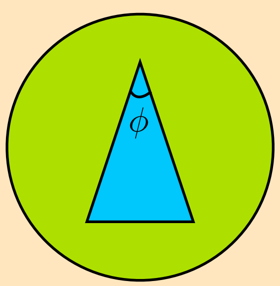

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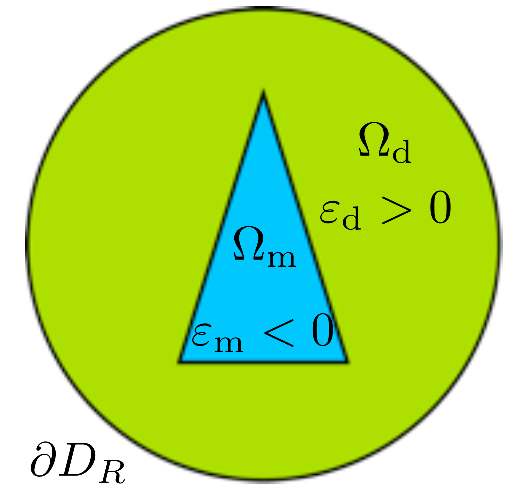

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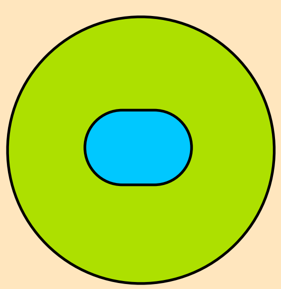

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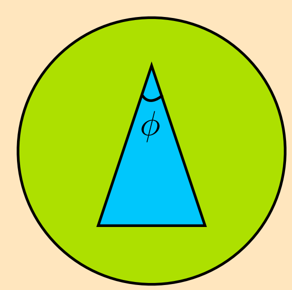

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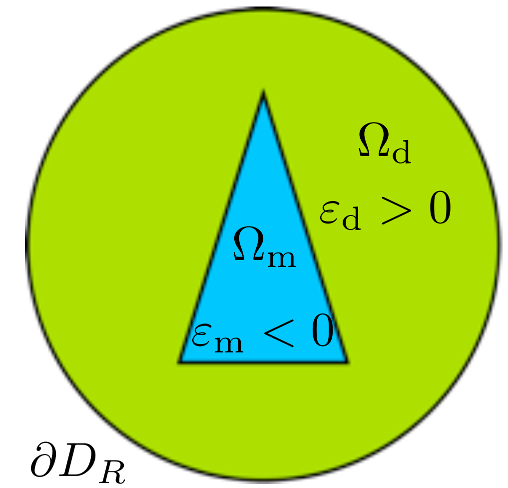

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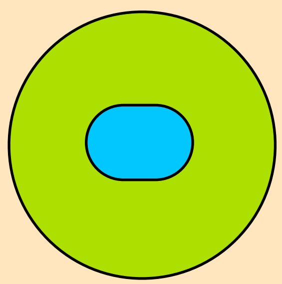

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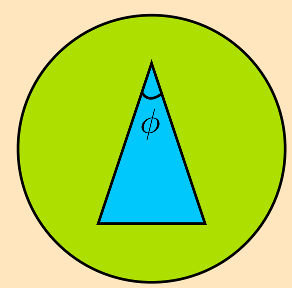

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Two configurations

Outside I_c
(YES)

Inside I_c
(NO)

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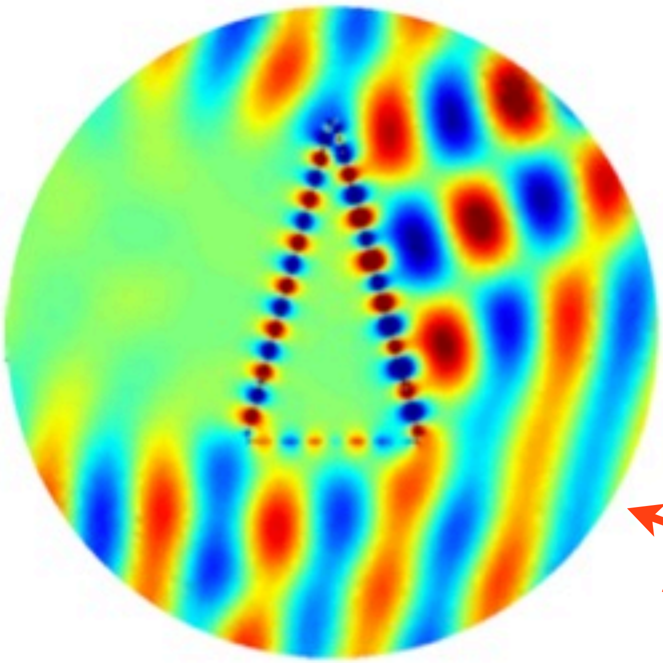
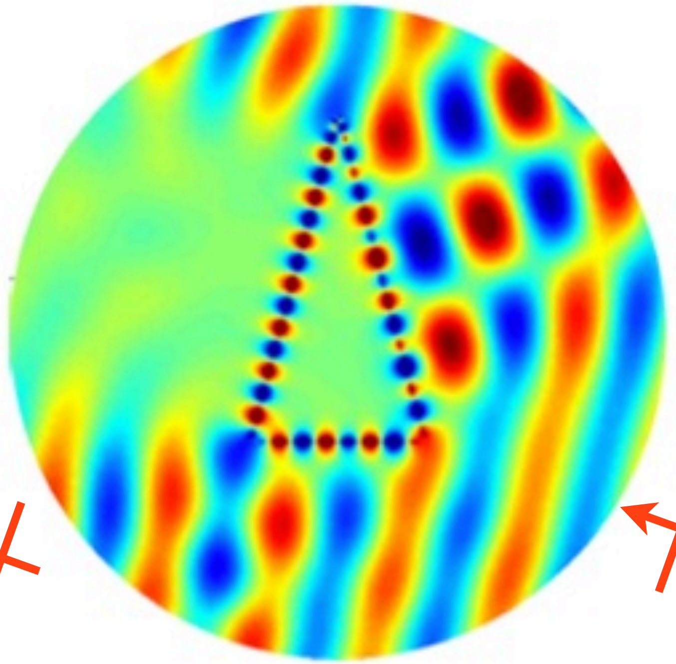
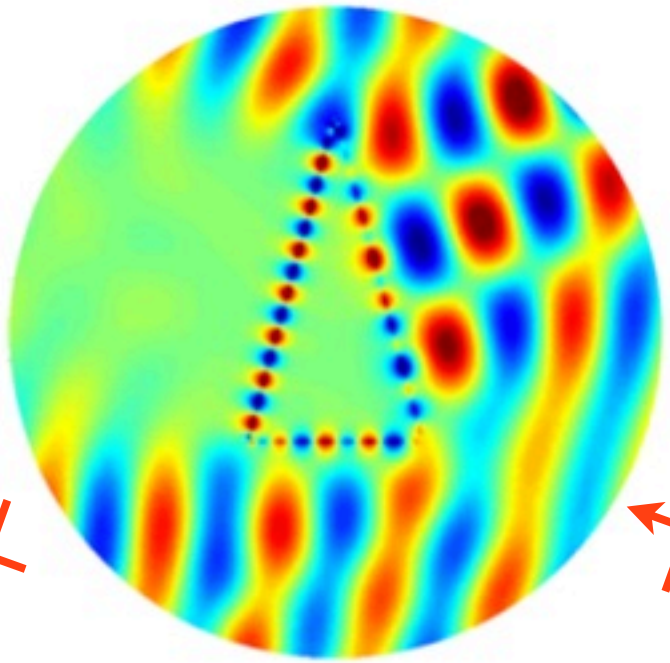


coarse mesh



intermediate mesh



refined mesh

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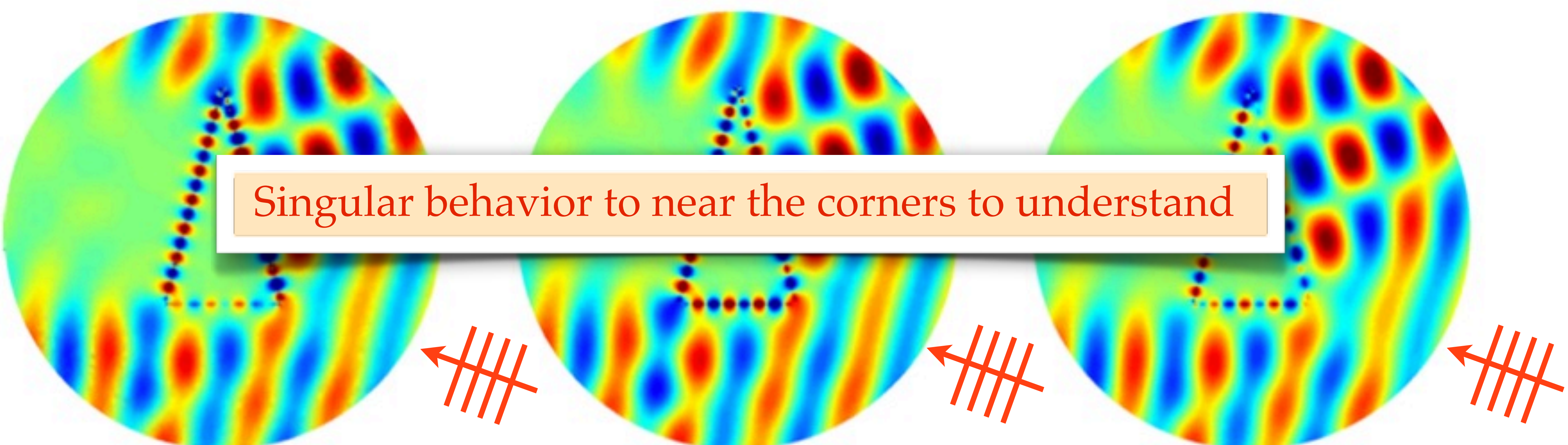


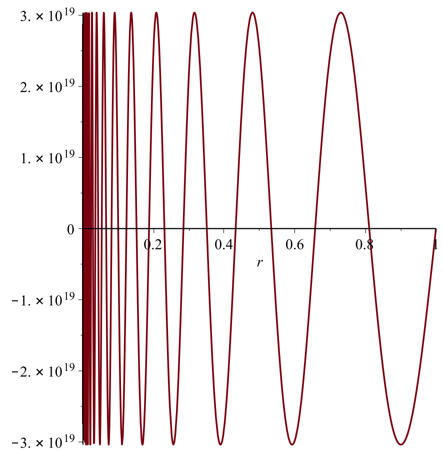
Singular behavior to near the corners to understand

coarse mesh — intermediate mesh — refined mesh

The appearance of black-hole waves

One proves that for a frequency inside the critical frequency range, oscillating singularities appear at the corners called black-hole waves. They can be interpreted as plasmonic waves propagating at the corners but never reach it:

$$s^{\pm}(r,\theta) = e^{i(\pm\eta \ln r - \omega t)}\Phi(\theta)$$



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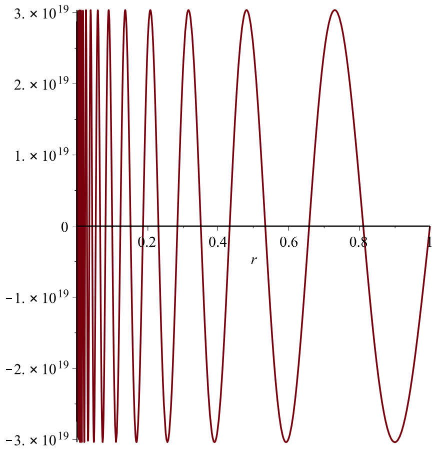

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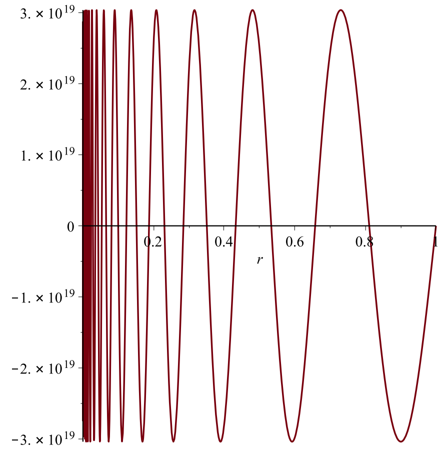

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Near the corners the solution decomposes as

$$u = b^+ s^+ + b^- s^- + \tilde{u}, \quad \tilde{u} \in H^1(D_R),\ s^{\pm} \notin H^1(D_R),\ b^{\pm} \in \mathbb{C}$$

Zoom at the corner

To simplify, let us consider a metallic inclusion with only one corner.

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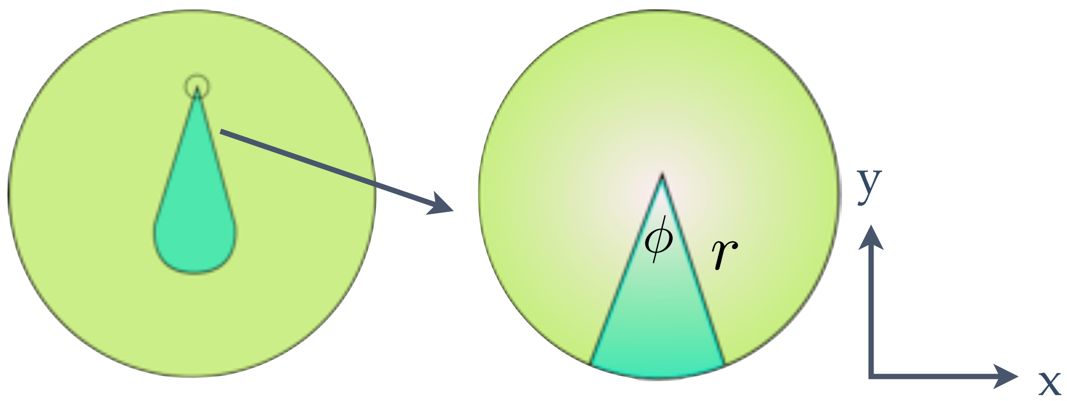

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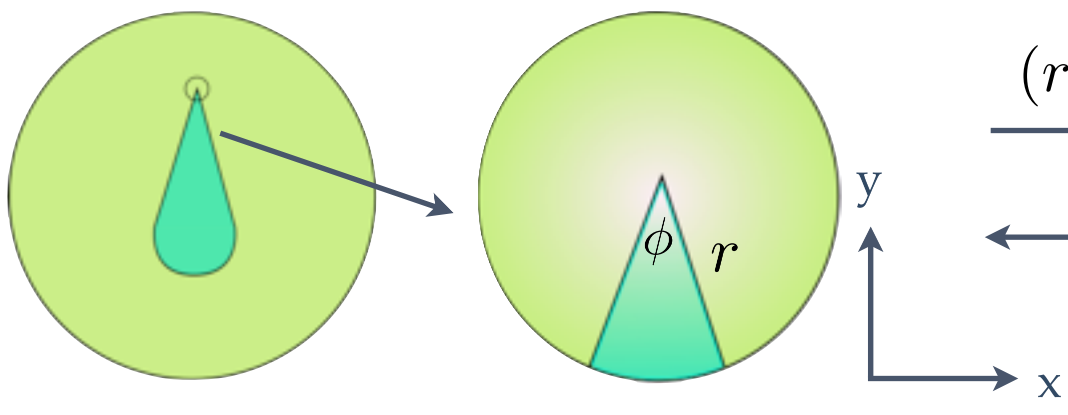

$$(r,\theta) \rightarrow (z = log(r), \theta)$$

Euler

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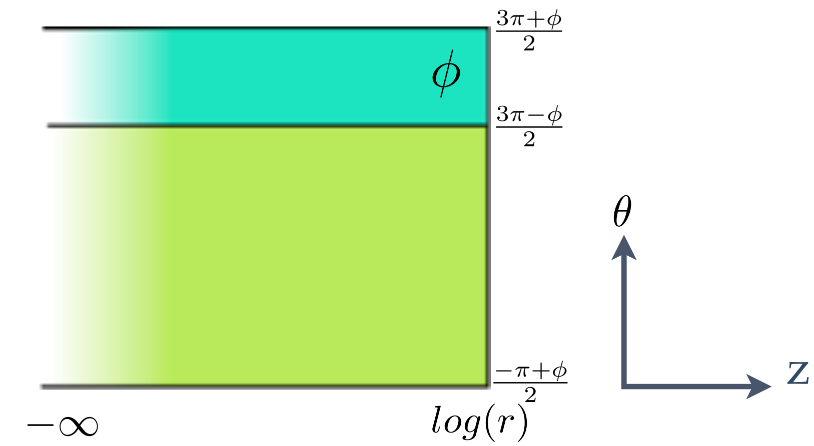

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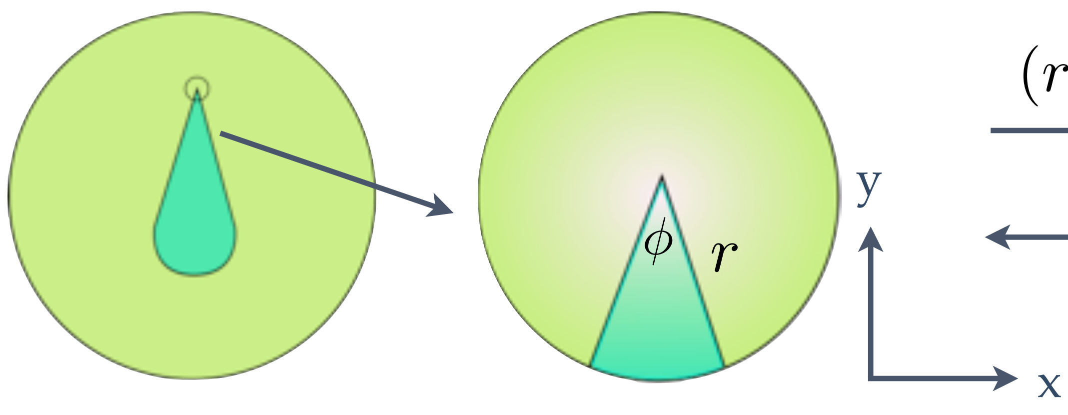

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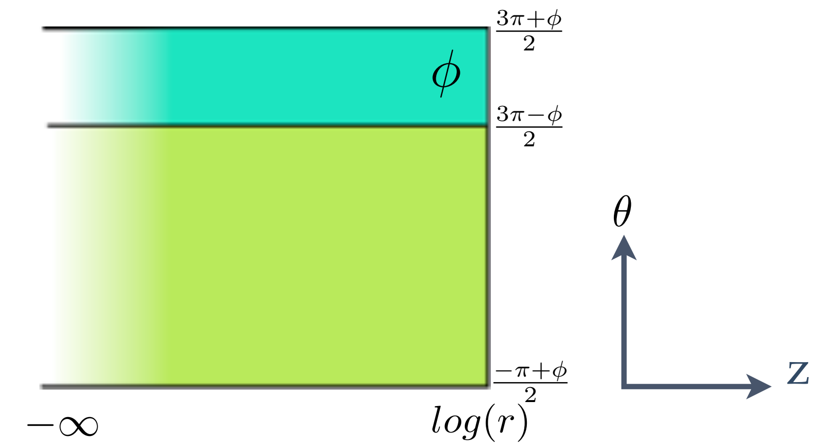

Asymptotic behaviour near the corner

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Behaviour at infinity in the waveguide

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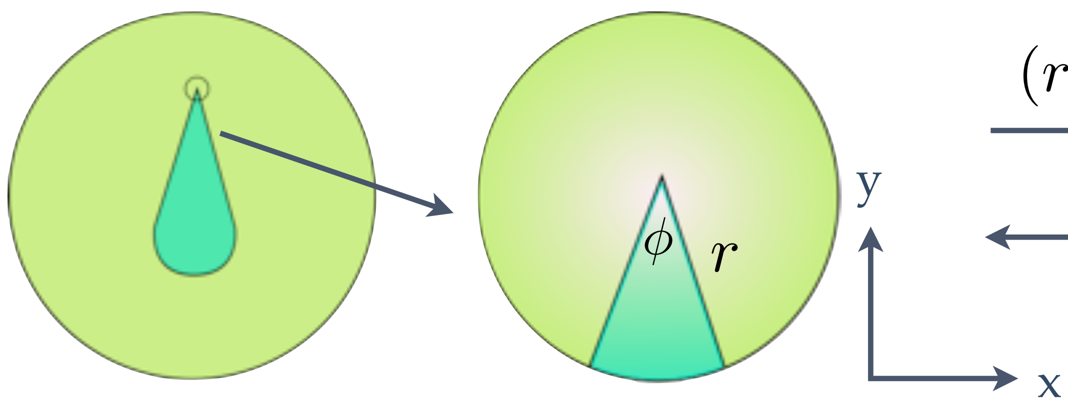

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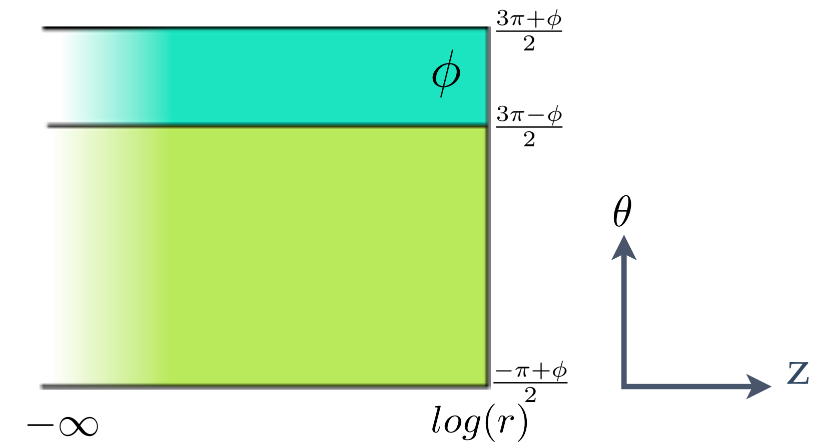

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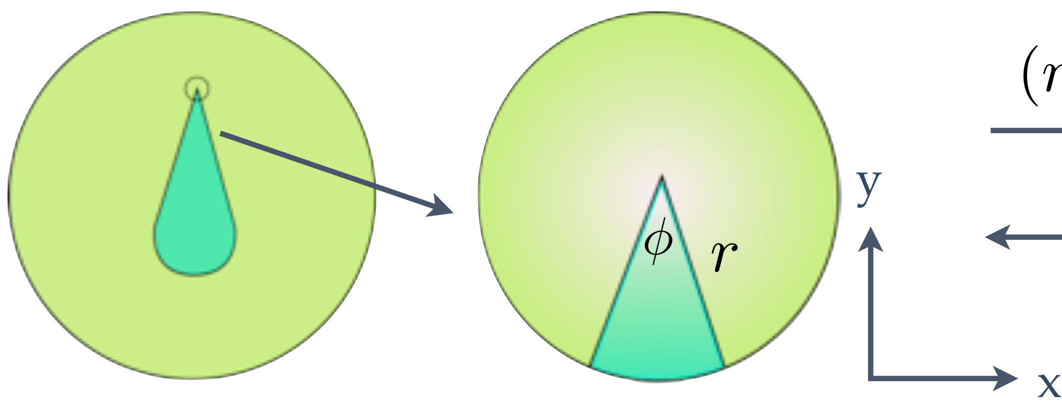

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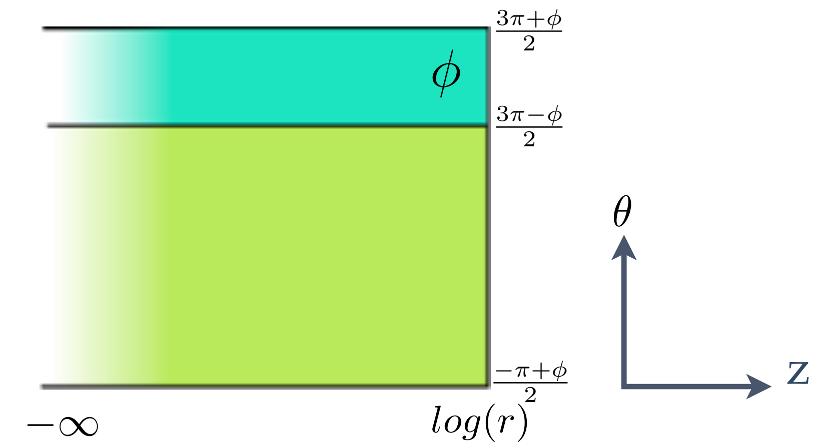

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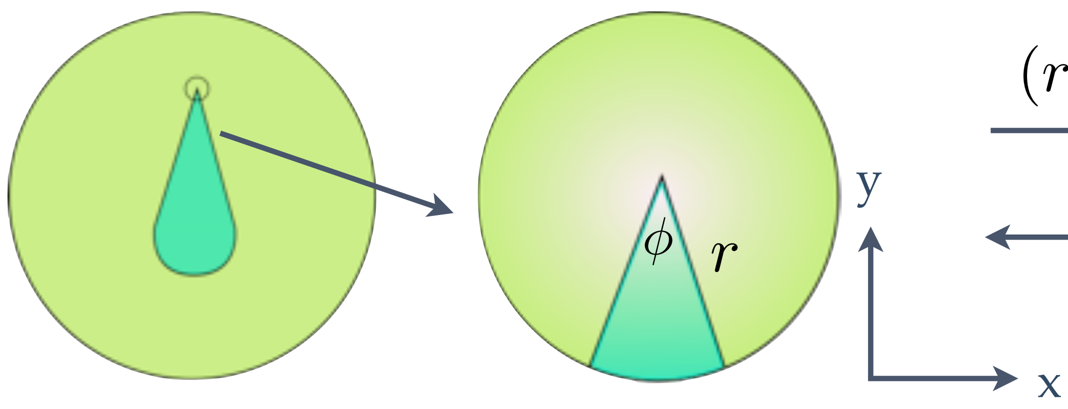

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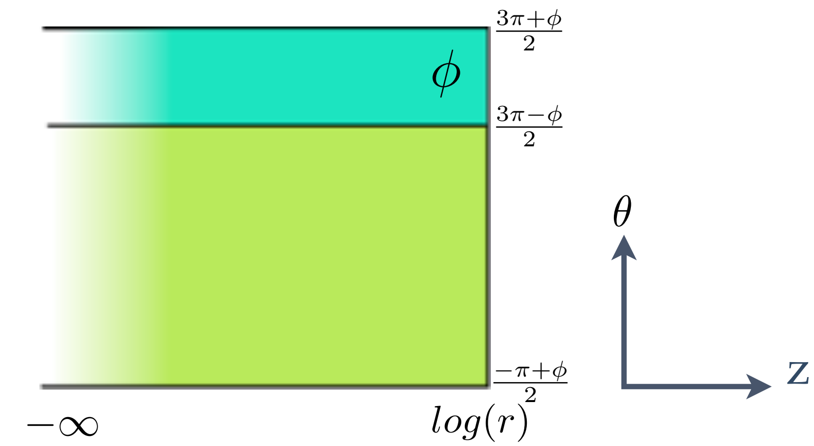

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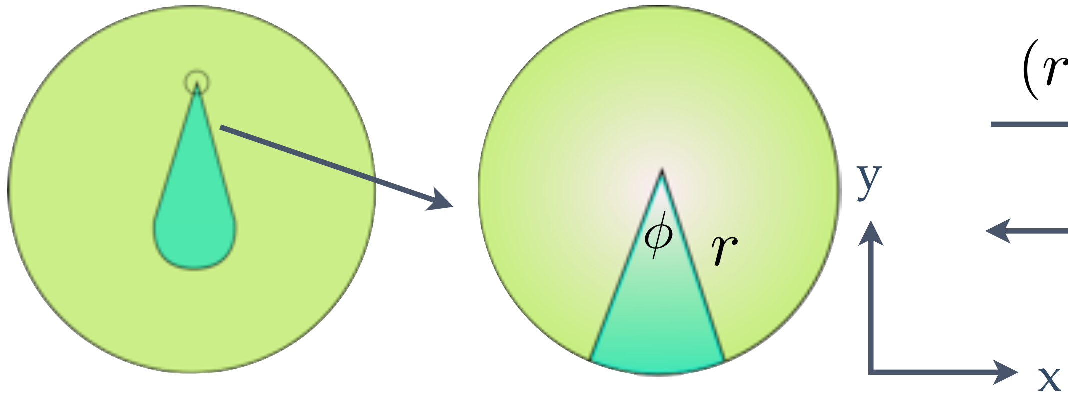

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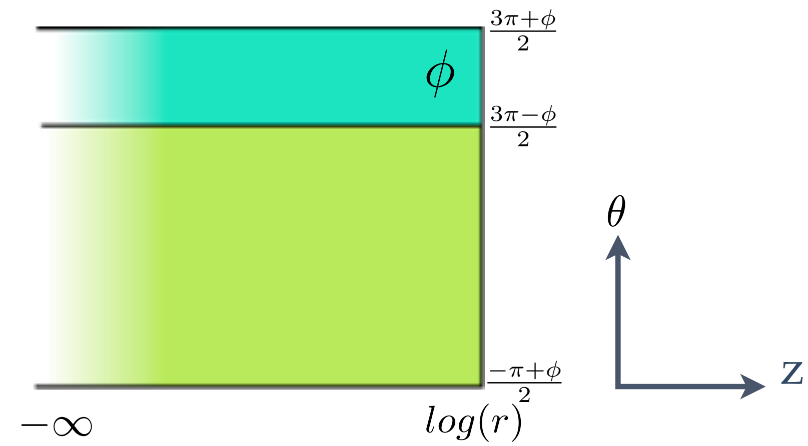

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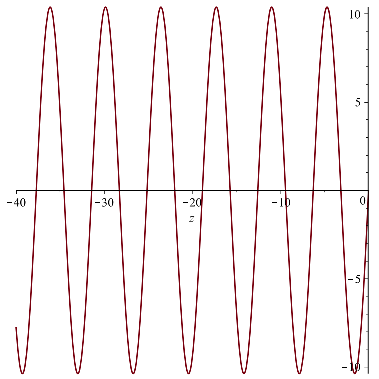

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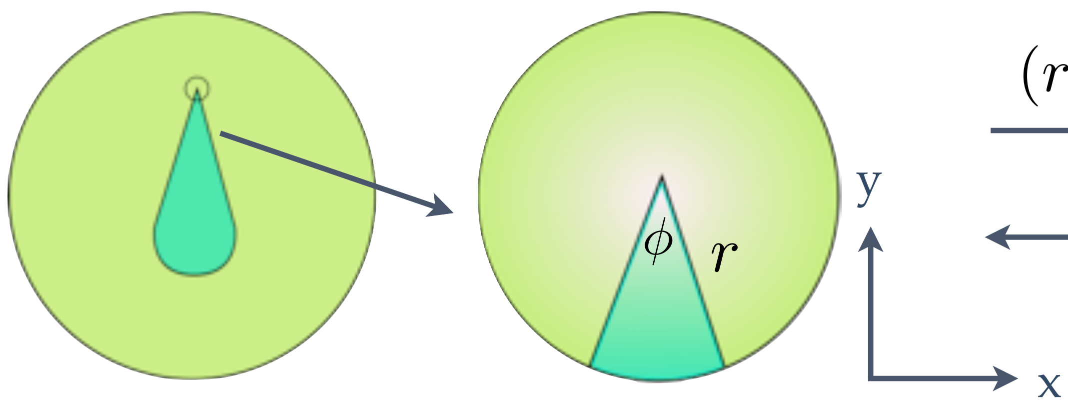

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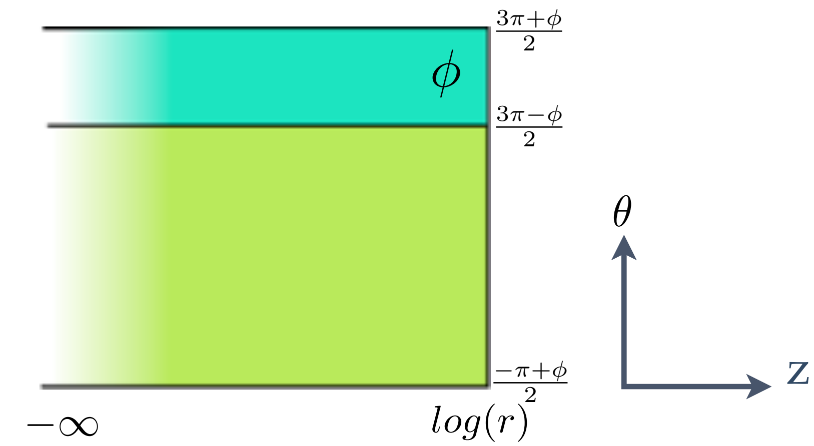

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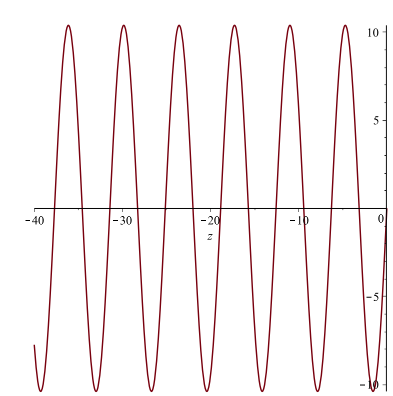

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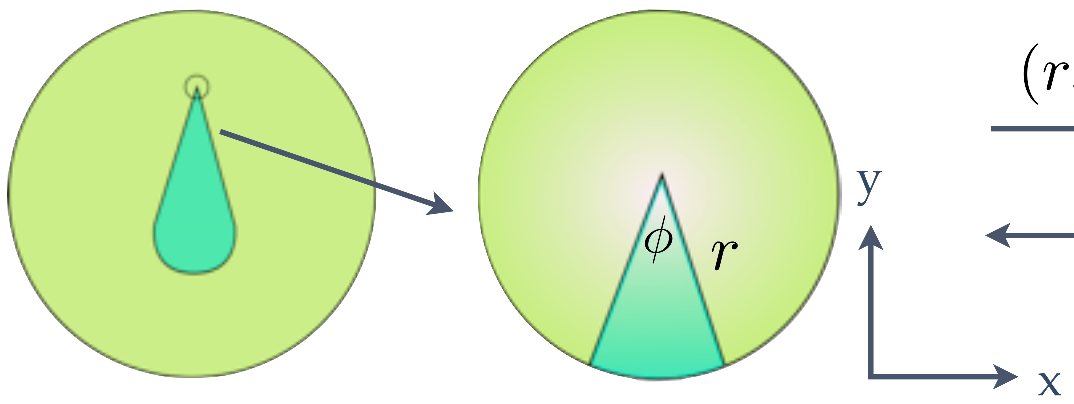

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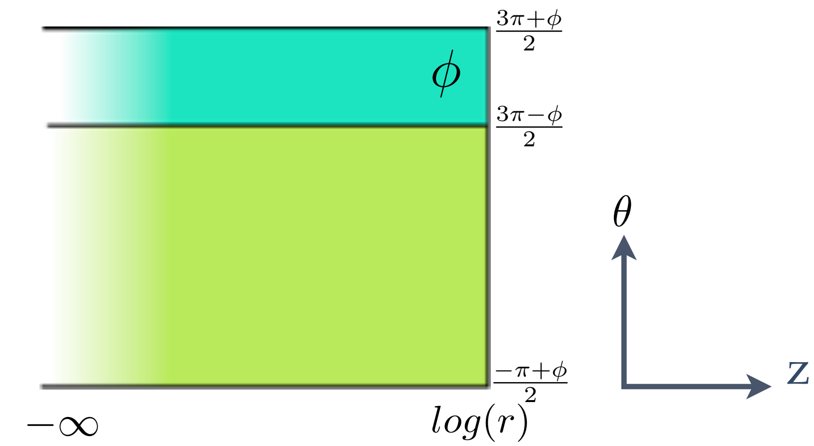

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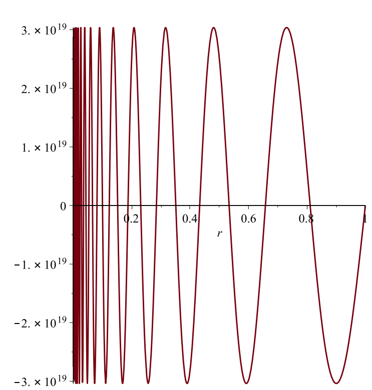

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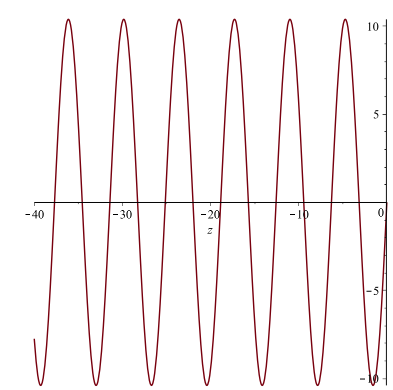

This is due to sign-changing coefficient !

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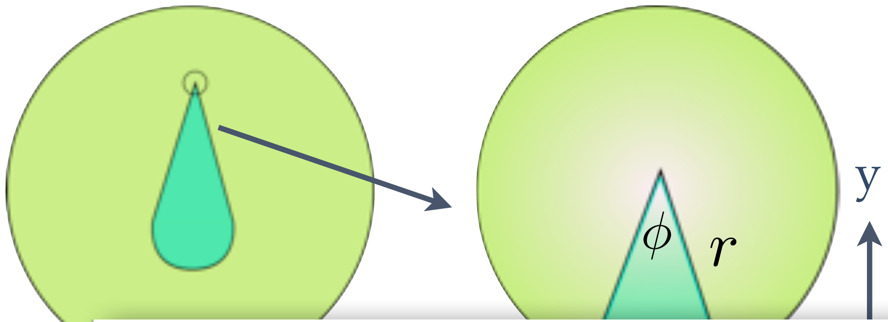

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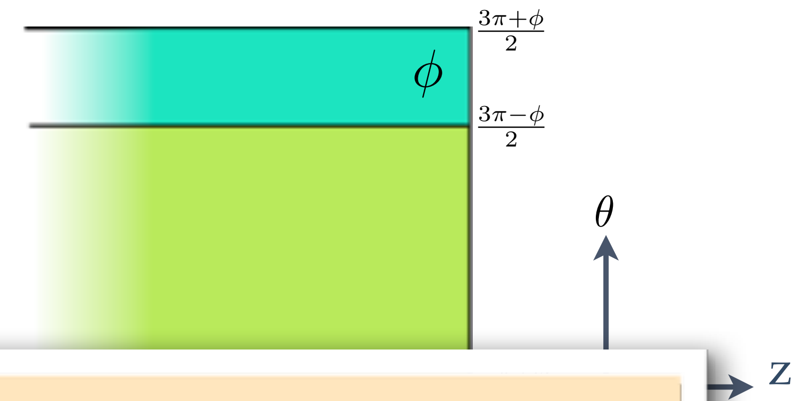
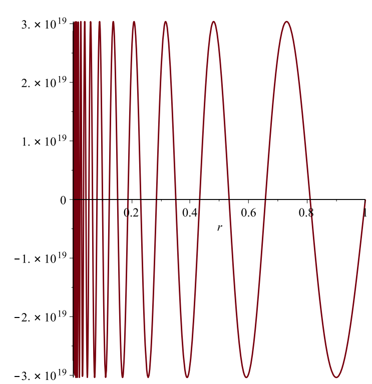


One singularity carries energy absorbed by the corner, the other brings energy emitted from the corner.

Appearance of two black-hole waves

$s^{\pm}(r,\theta) = r^{\pm i\kappa}\phi(\theta)$



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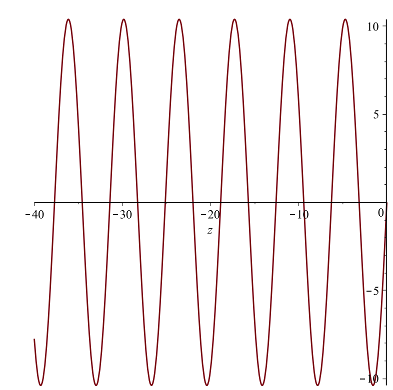
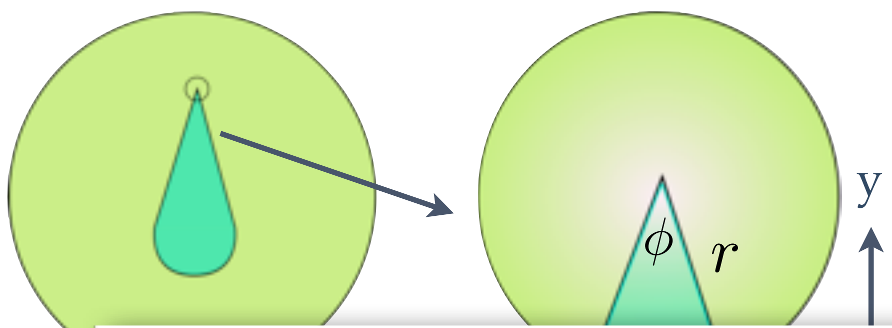


This is due to sign-changing coefficient !

Zoom at the corner

To simplify, let us consider a metallic inclusion with only one corner.



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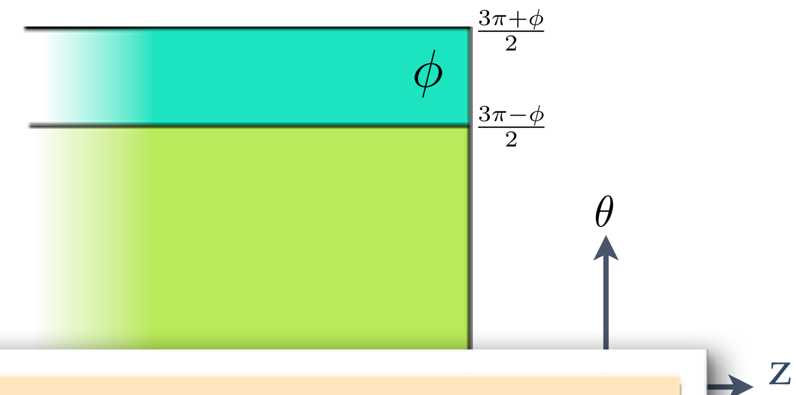

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The physical solution takes into account the one that does not add energy into the system, the outgoing solution in the waveguide setting.

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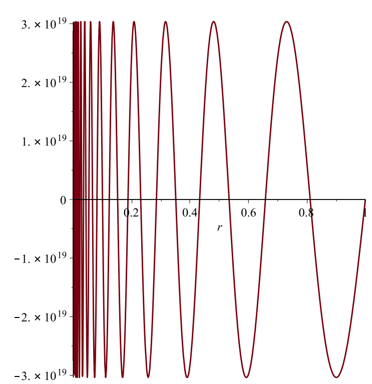

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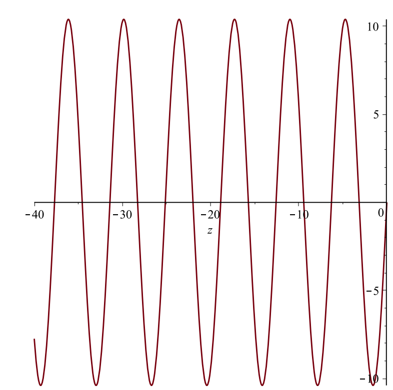

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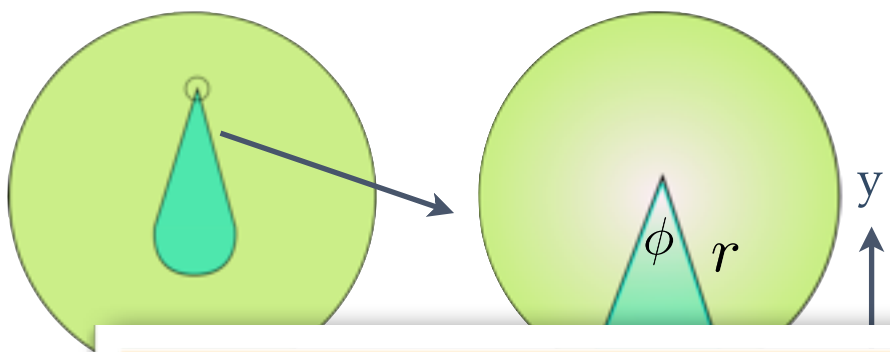

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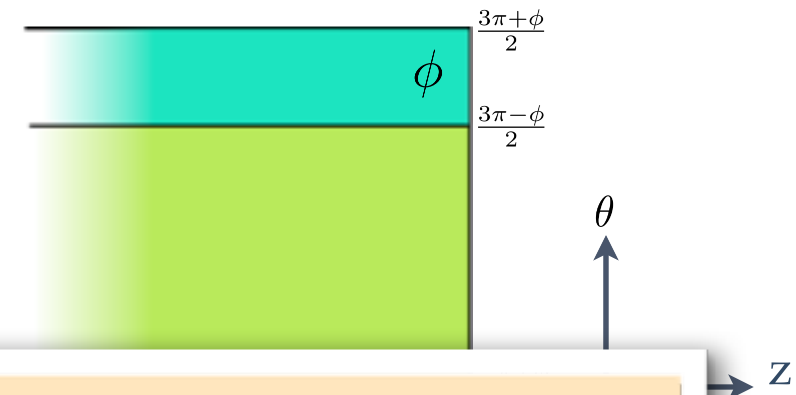

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How to proceed numerically to select the good singularity ?

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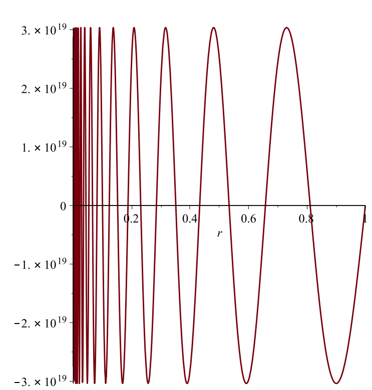

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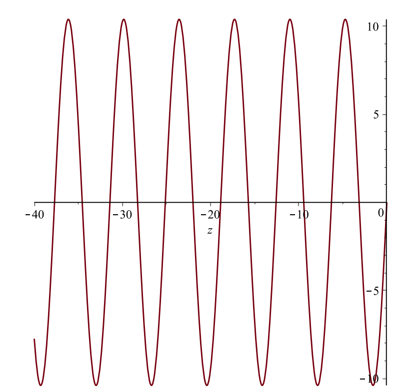

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An adapted numerical method

We put a PML in the Strip: then the propagatives modes become evanescent, and we can use FEM.

$$\frac{\partial}{\partial z} \longmapsto \alpha \frac{\partial}{\partial z} \quad \alpha \in \mathbb{C},\ 0 < arg(\alpha) < \frac{\pi}{2}$$

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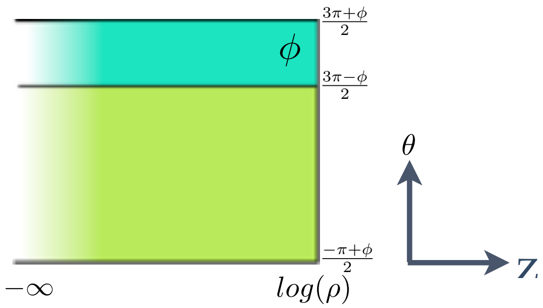

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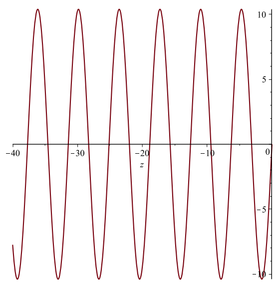

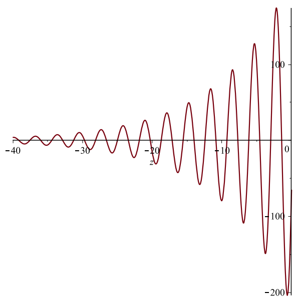

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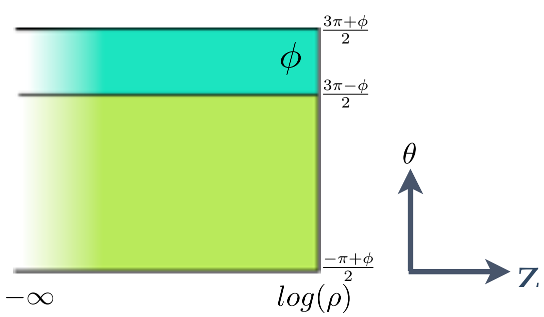

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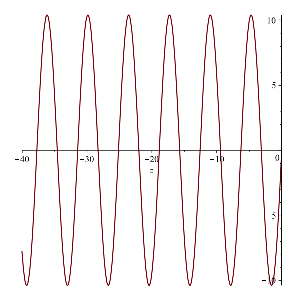

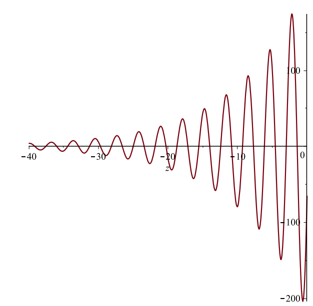

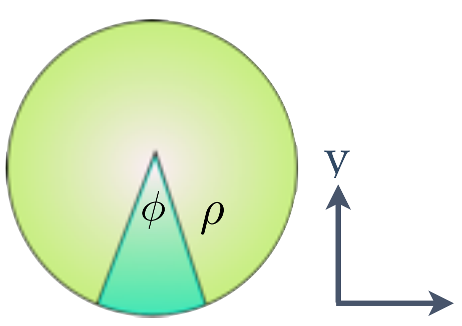

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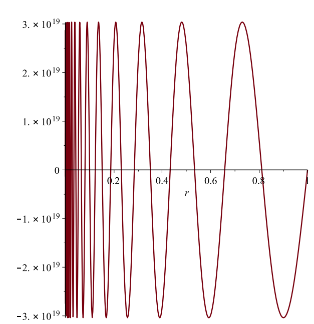

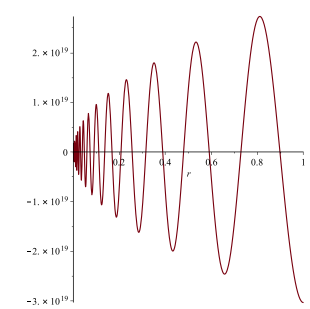

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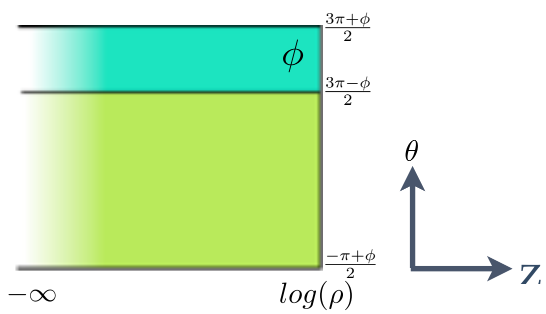

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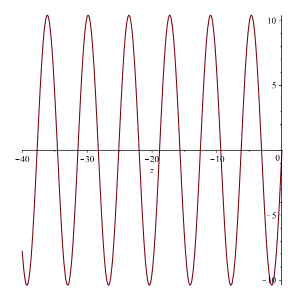

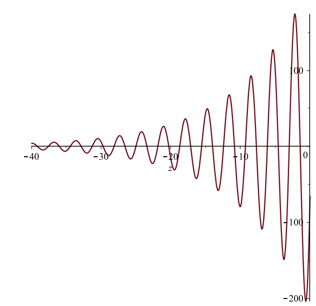

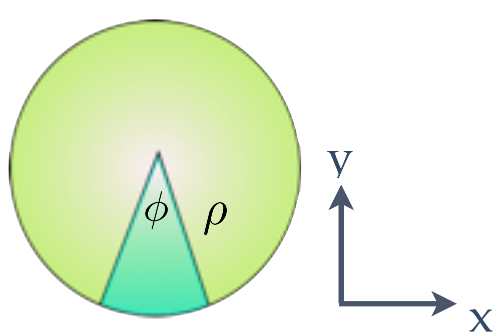

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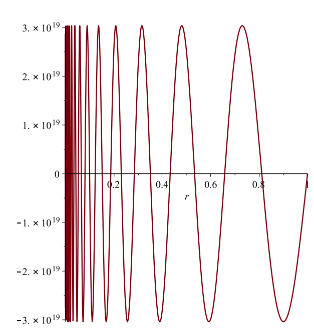
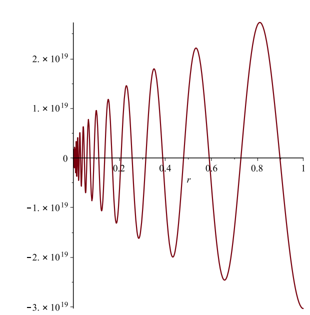
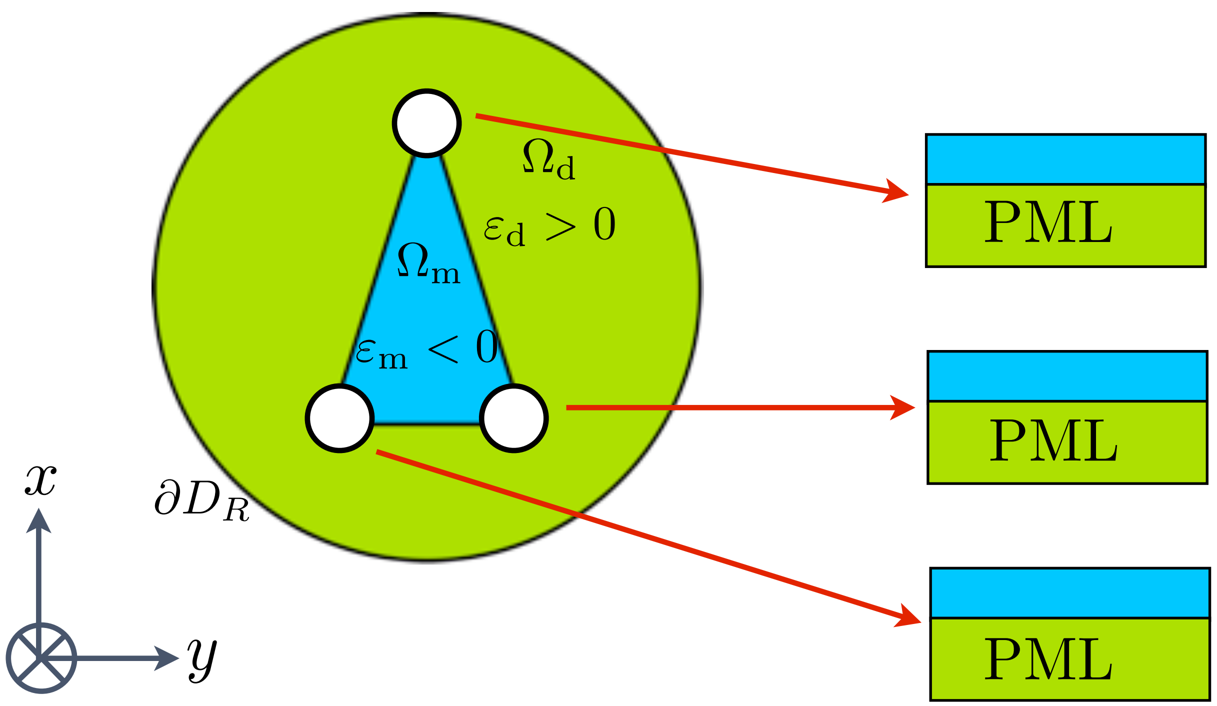




PML easier to implement in the Strip

Implementation: splitting the domain



$$\mathrm{div}\left(\frac{1}{\epsilon}\nabla u\right) + \omega^2 c^{-2}\mu u = 0 \quad D_R \setminus \cup\ \mathrm{PML}$$

$$\partial_n u - iku = \partial_n u^{\mathrm{inc}} - iku^{\mathrm{inc}} \quad \partial D_R$$

+ PML matching conditions +

$$\frac{\alpha}{\epsilon}\partial_{zz}u + \frac{1}{\alpha}\partial_\theta \frac{1}{\epsilon}\partial_\theta u + \frac{\omega^2}{\alpha c^2}\mu e^{\frac{2z}{\alpha}} u = 0 \quad \mathrm{PML}$$

$$\partial_z u(-L, \cdot) = 0$$

+ periodic conditions

Resolution using Lagrange FE of order 2 with a Matlab code.

Numerical results

$\kappa_\varepsilon \in I_c \quad \Longleftrightarrow \quad \omega \in [3.839 \text{ PHz}; 12.733 \text{ PHz}].$ $\omega_{\text{sp}} = 9.42$ PHz. Results for $\omega = 9$ PHz.

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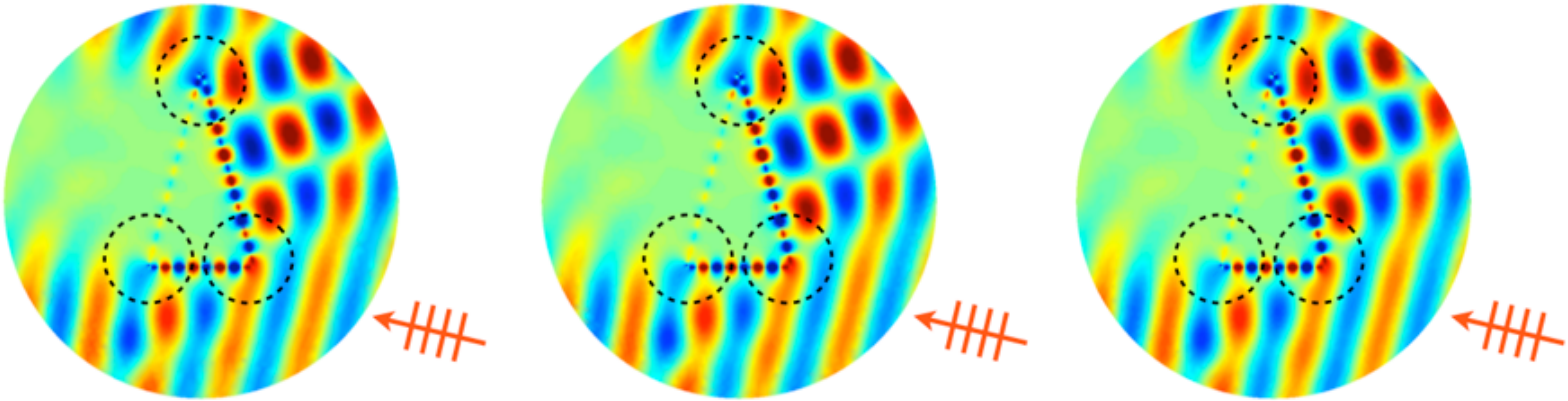

coarse mesh intermediate mesh refined mesh

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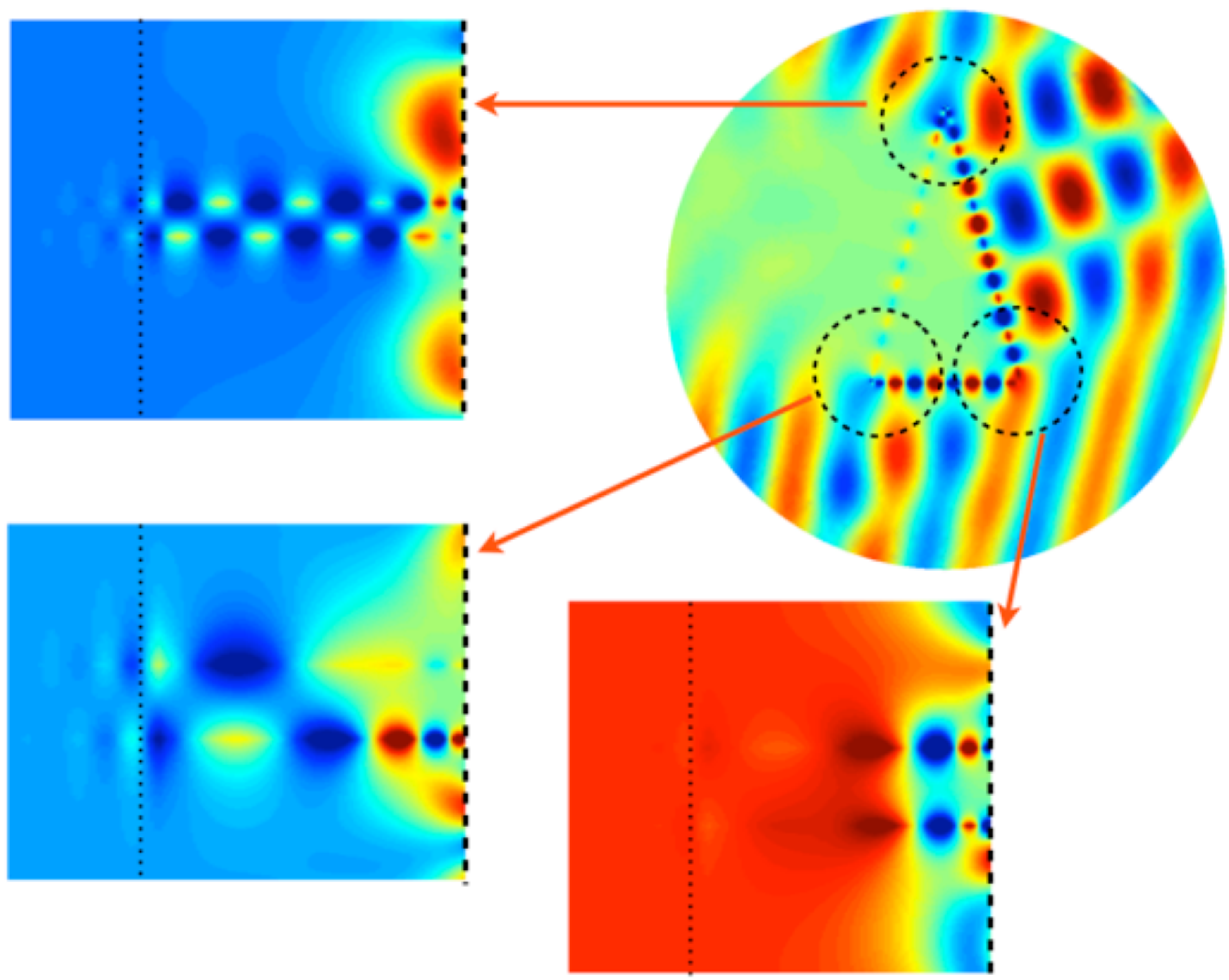

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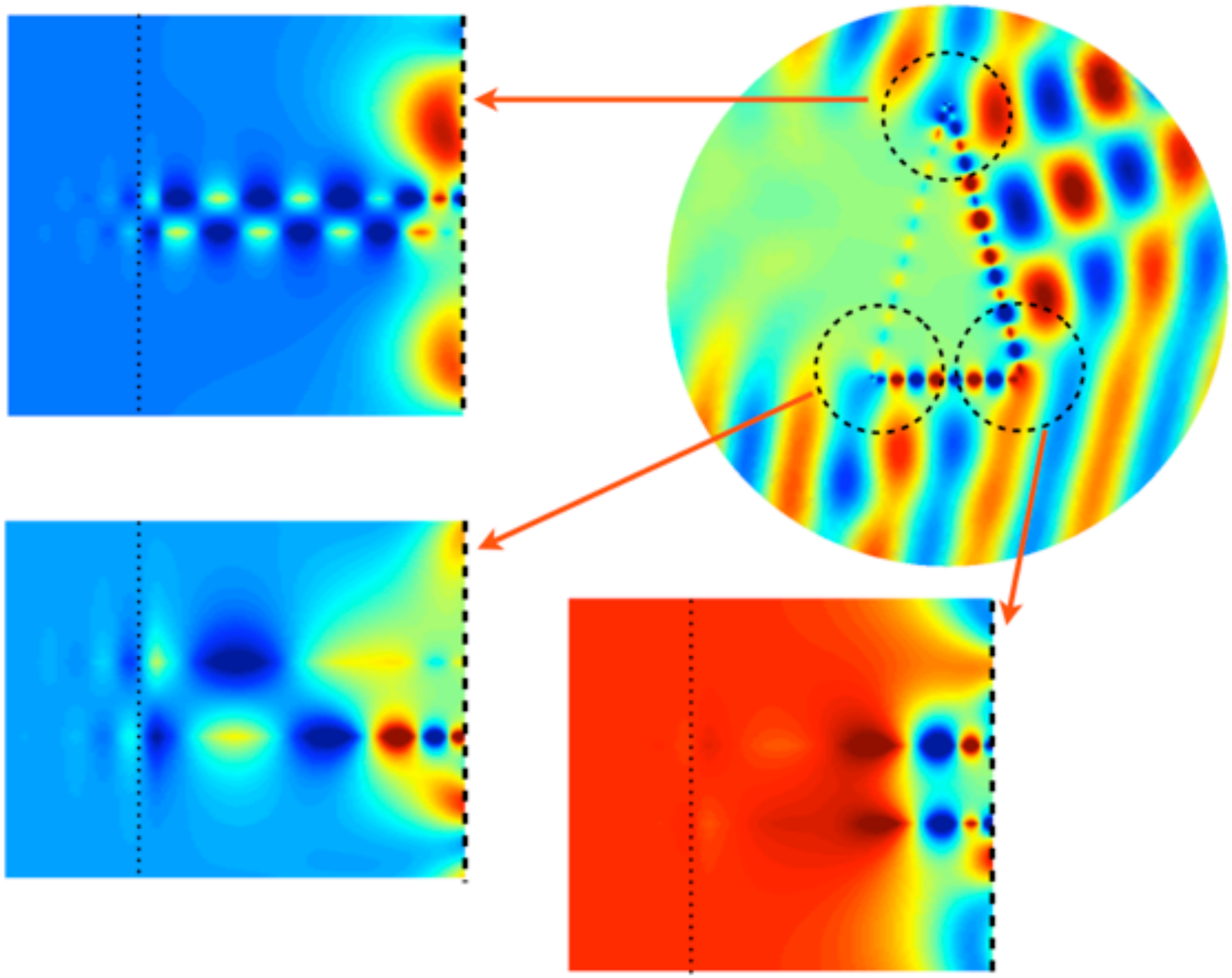

The numerical method with PMLs is stable. Let us go back to the dissipative problem.

Back to dissipative medium

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Considering losses in the metal, then the problem is well-posed.

The selected outgoing singularity becomes of finite energy. If dissipation is small, it requires meshes sufficiently refined at the corners to capture the oscillations.

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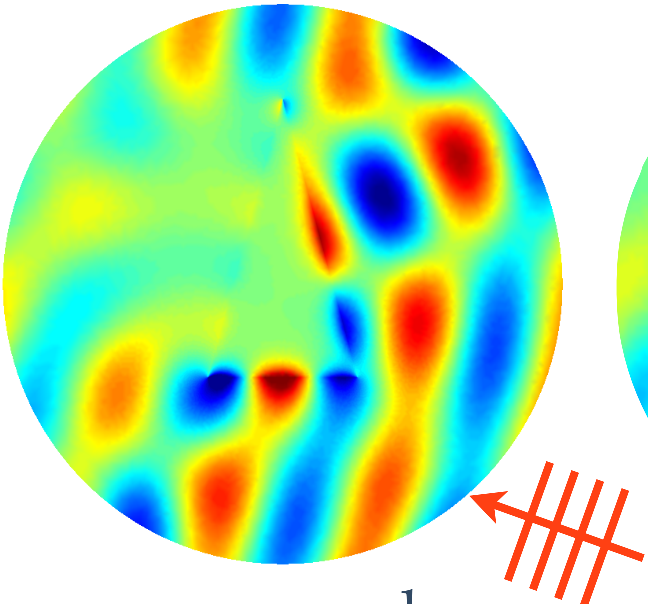
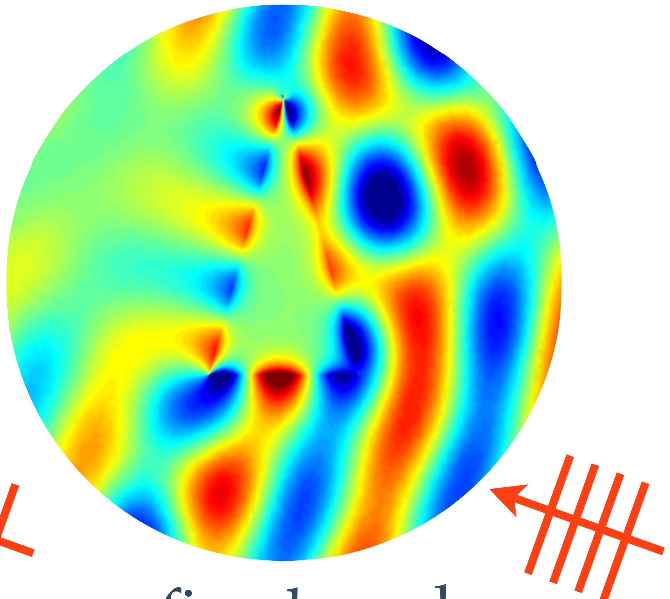


coarse mesh



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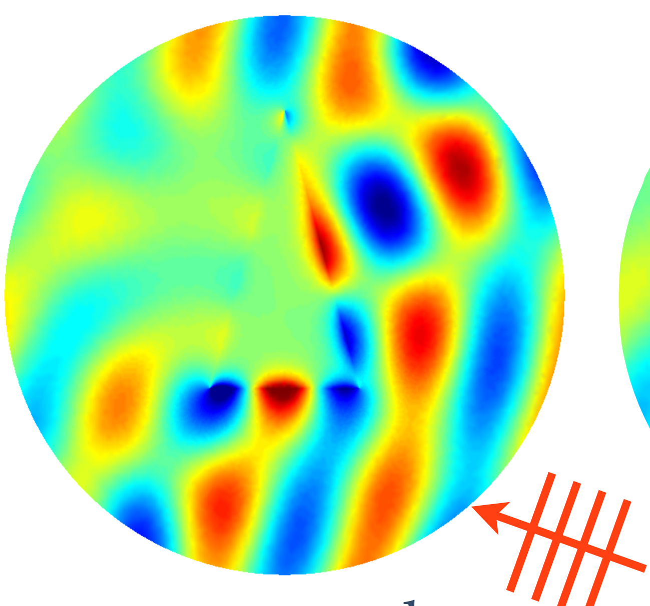

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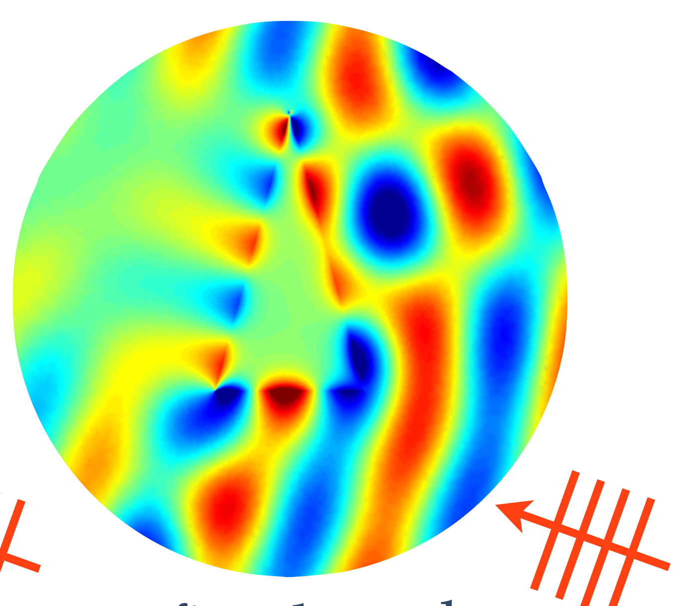

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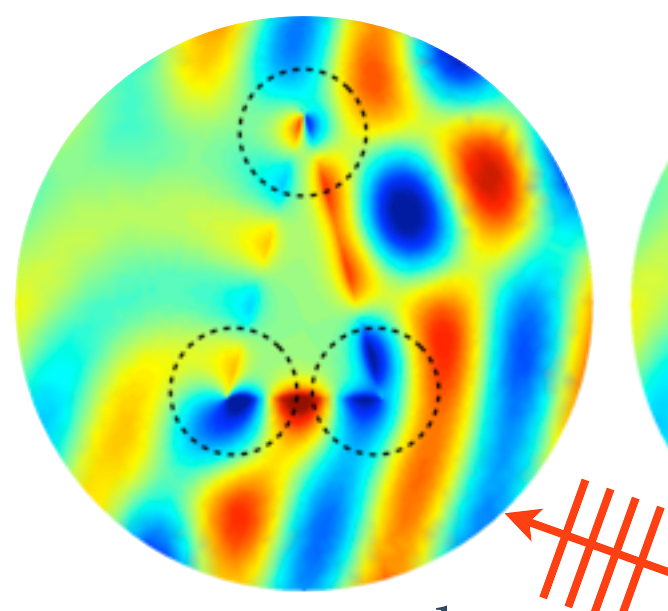

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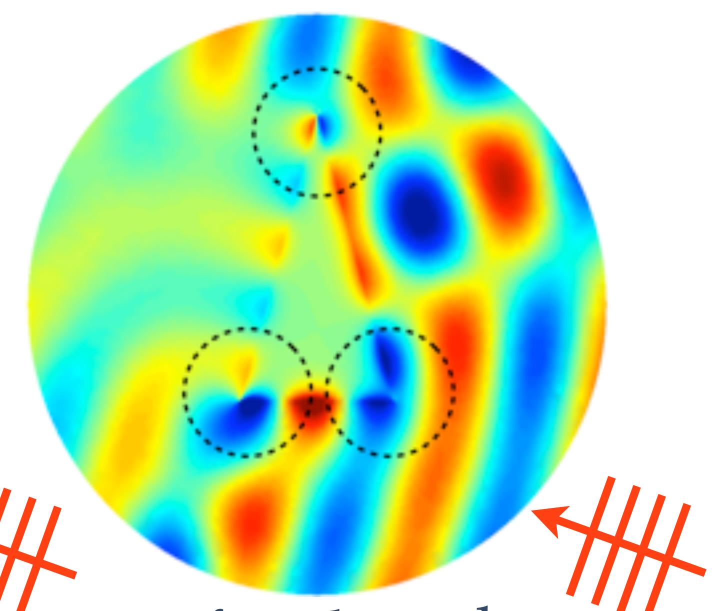

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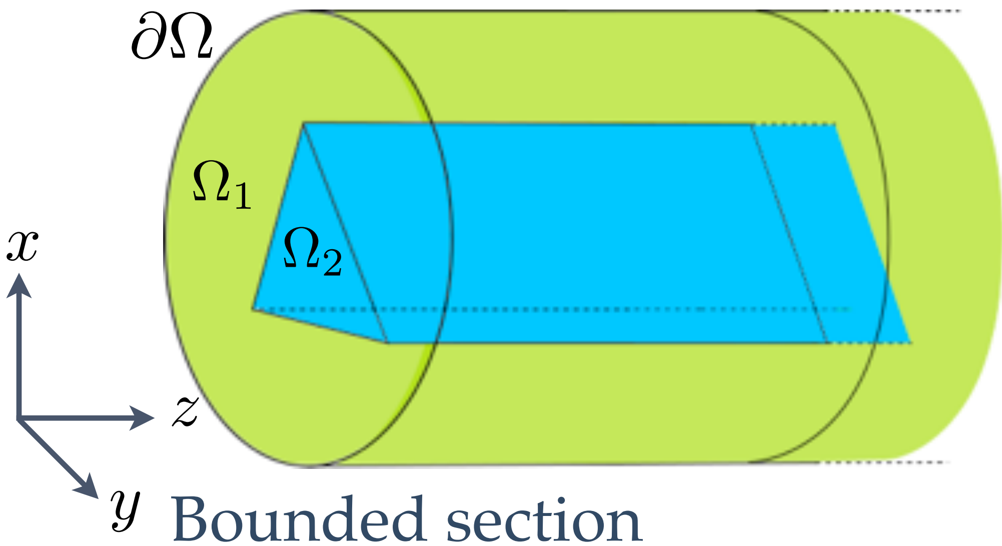
This work is the object of an article (submitted very soon). The case of dispersive media is the object of discussions with the Fresnel Institute (Marseille, France).

Outline

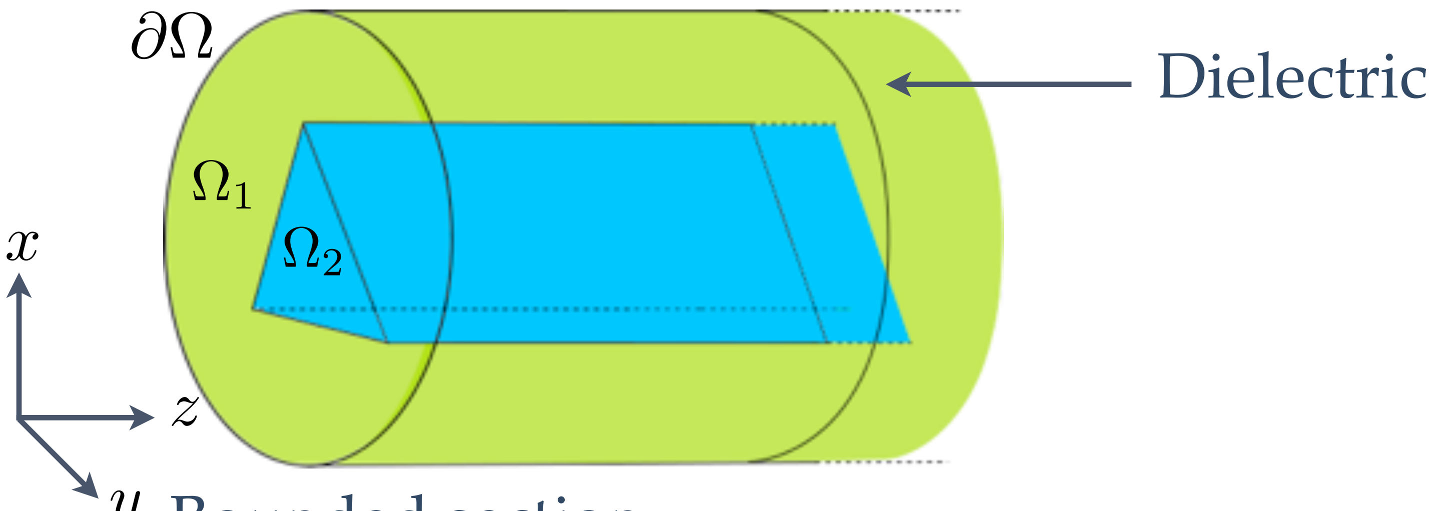
- Introduction
- Scattering problem with sign-changing coefficients
- **Guided modes in a plasmonic waveguide**

Guided modes in a plasmonic waveguide



Bounded section

Guided modes in a plasmonic waveguide



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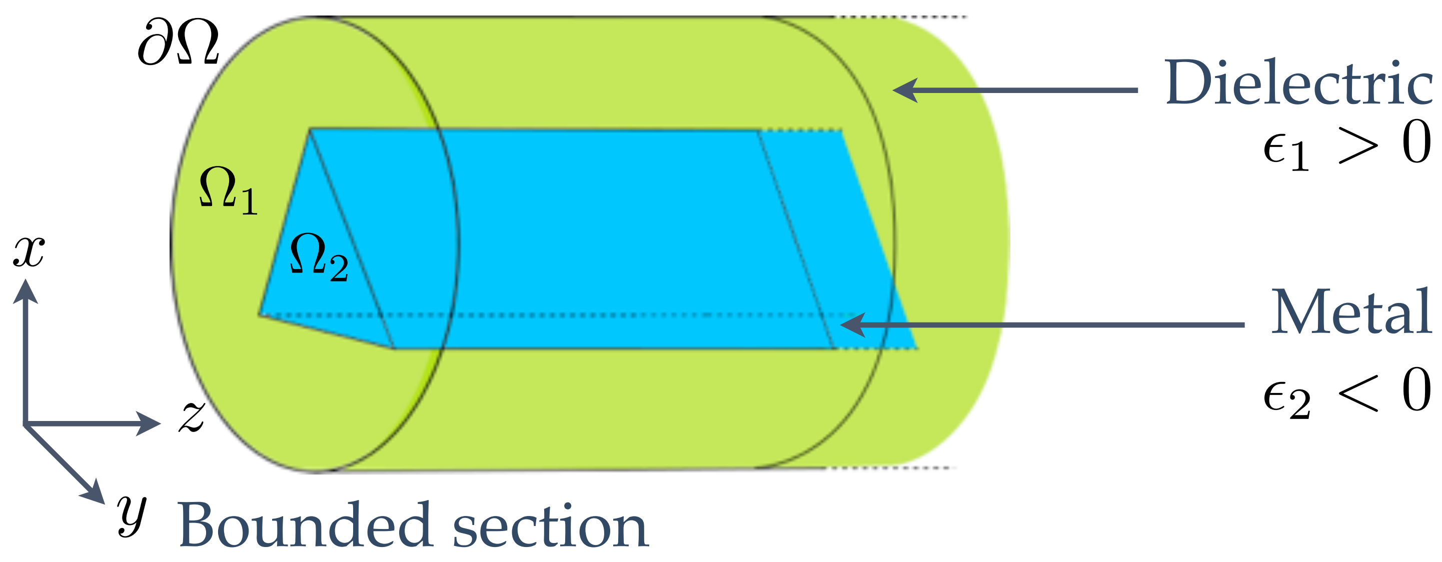

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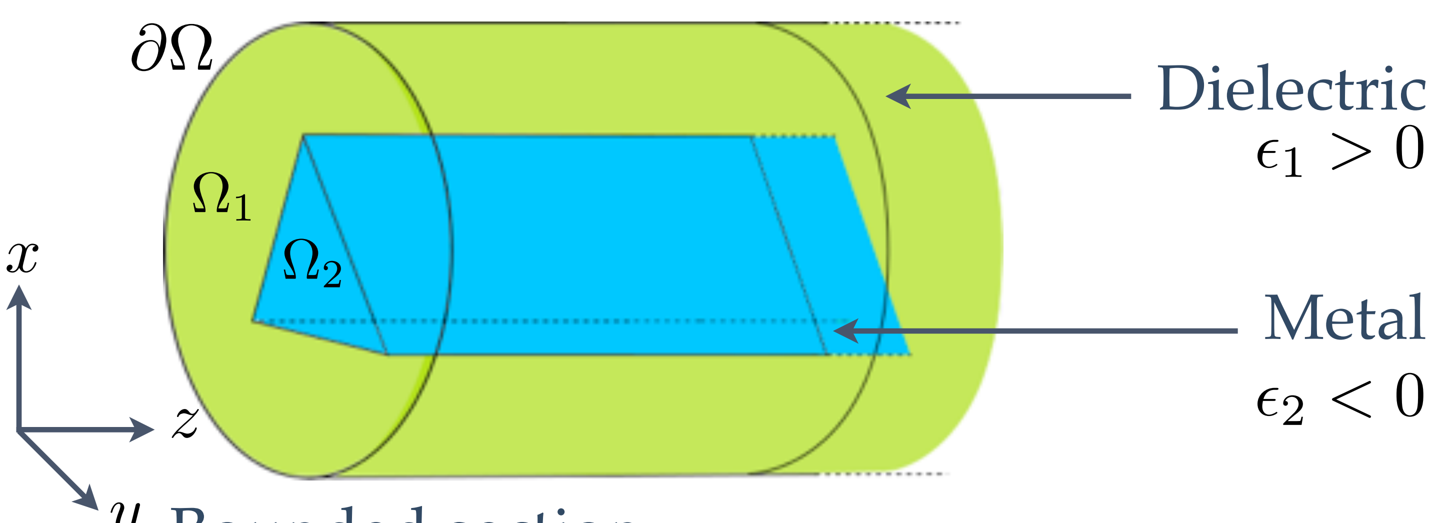

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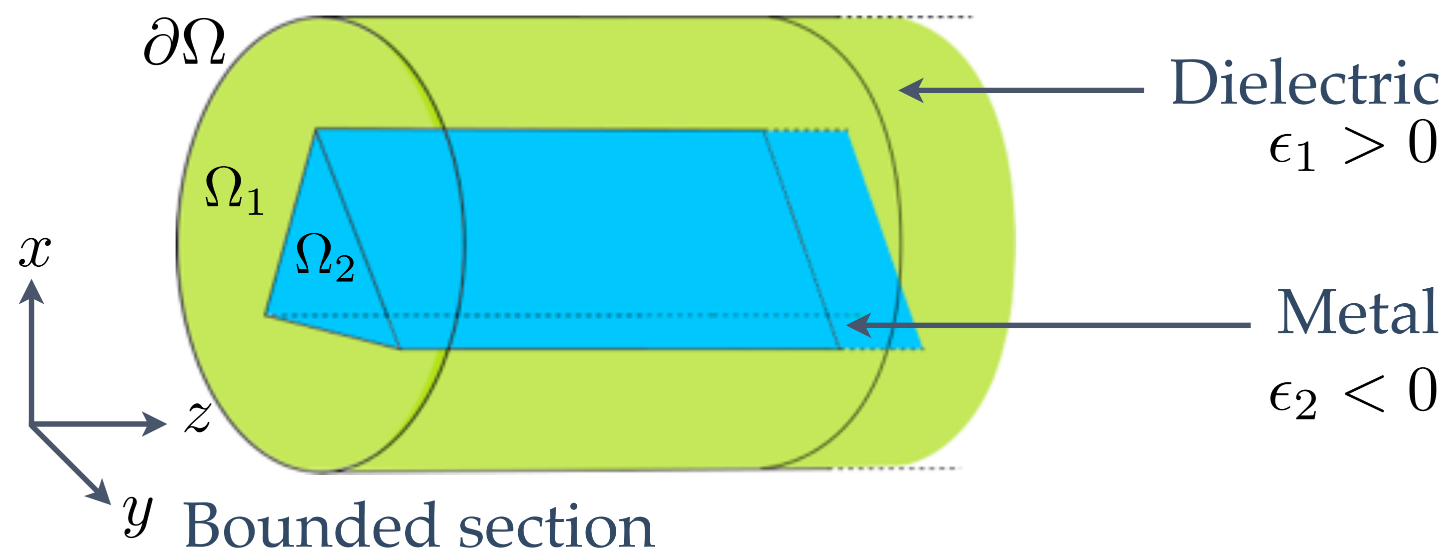
Metal permittivity modeled by the dissipationless Drude's model

$$\epsilon(\omega) = \epsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2}\right)$$

Guided modes in a plasmonic waveguide



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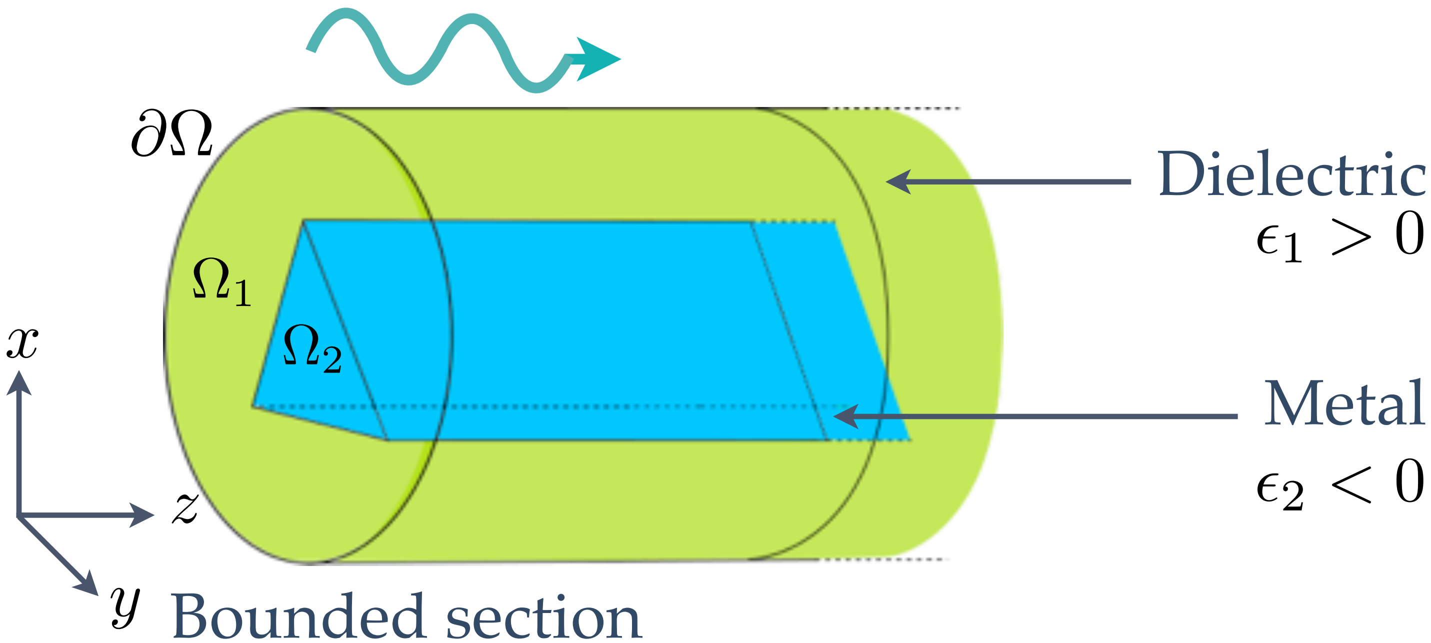

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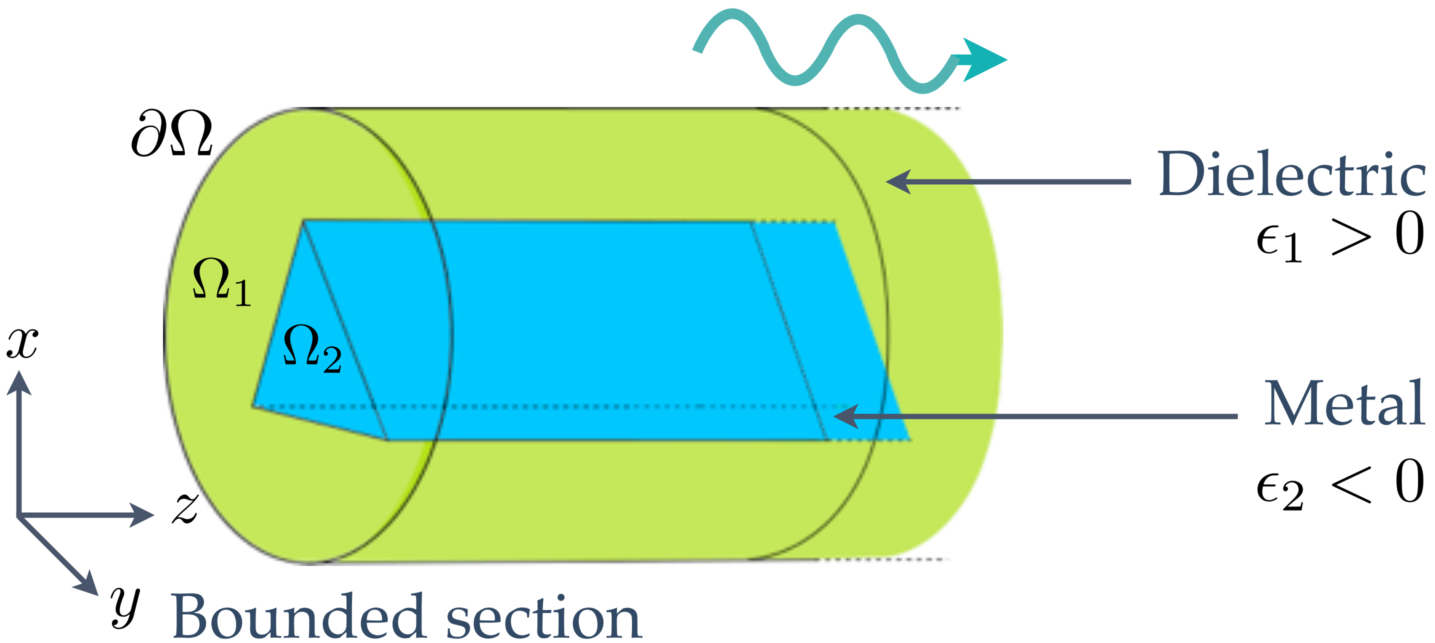

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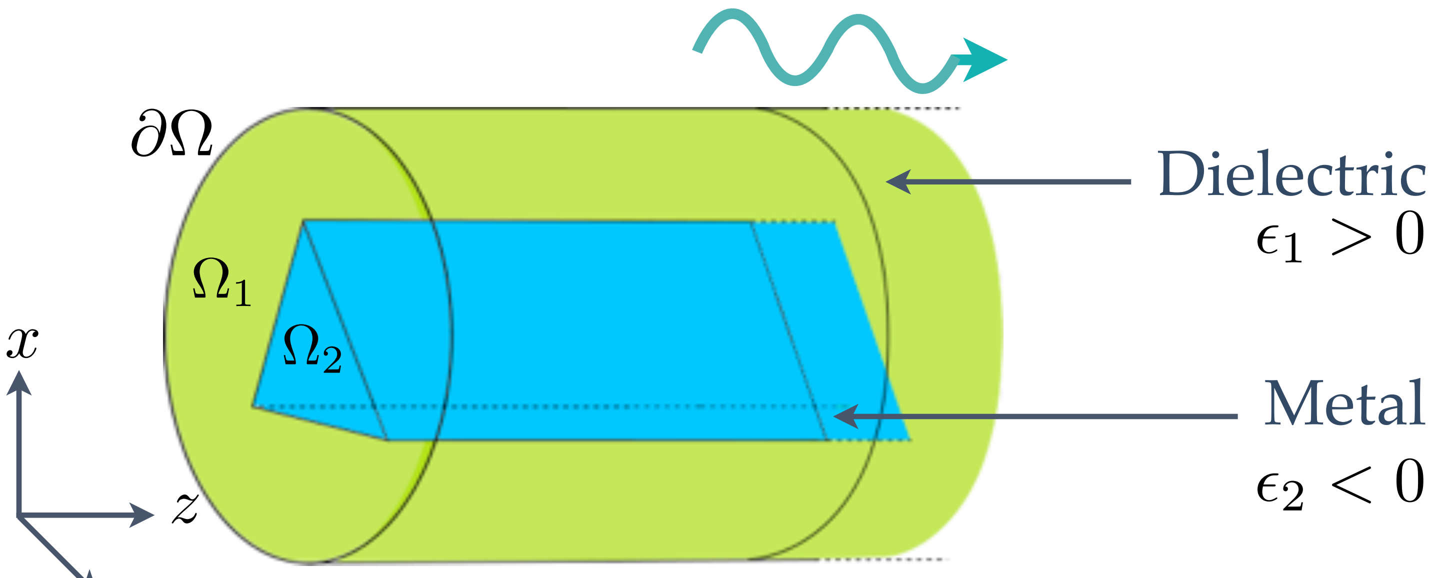

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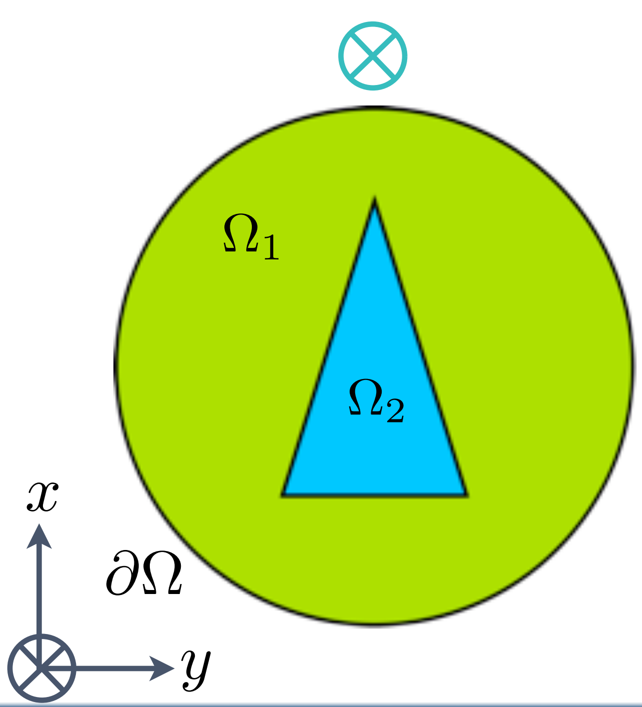
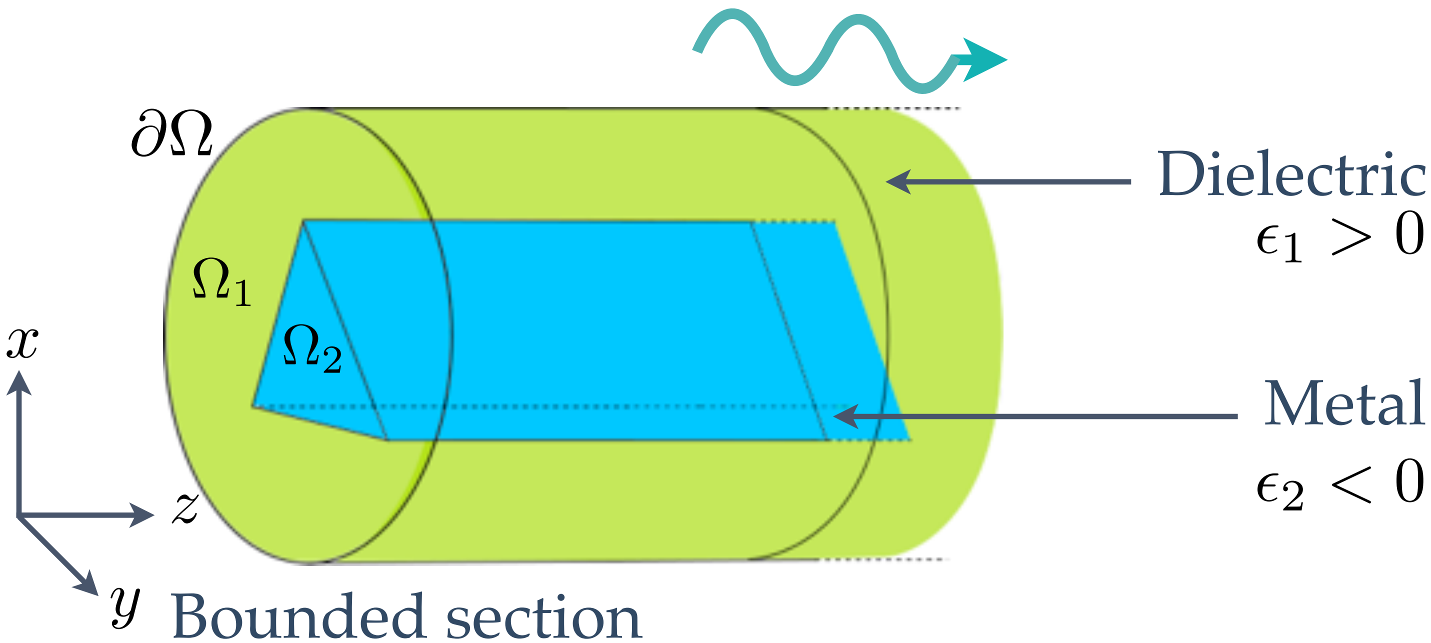
Reduction to a 2D Eigenproblem $\boxed{A(\beta)\widetilde{u} = \omega^2 \widetilde{u}}$



Guided modes in a plasmonic waveguide



Metal permittivity modeled by the dissipationless Drude's model

$$\epsilon(\omega) = \epsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2}\right)$$

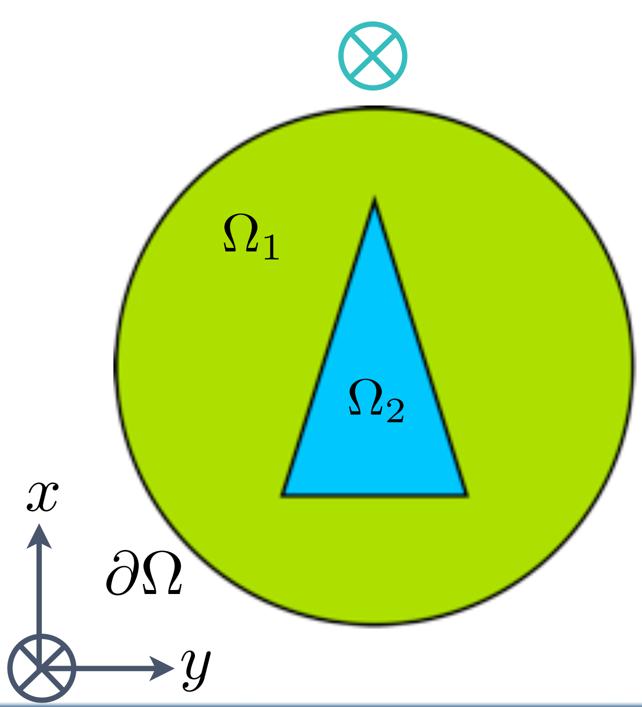
Bounded section

We consider the time-harmonic scalar model of Maxwell's equations (simplified model).

Looking for propagative waves along z : $u(x,y,z,t) = \widetilde{u}(x,y)e^{i(\beta z - \omega t)}$ $\quad \beta,\ \omega \in \mathbb{R}$

Reduction to a 2D Eigenproblem $\boxed{A(\beta)\widetilde{u} = \omega^2 \widetilde{u}}$

$$\boxed{\operatorname{div}\left(\frac{1}{\epsilon}\nabla\widetilde{u}\right) - \frac{\beta^2}{\epsilon}\widetilde{u} + \omega^2\mu\widetilde{u} = 0 \quad \Omega \qquad \mu > 0}$$

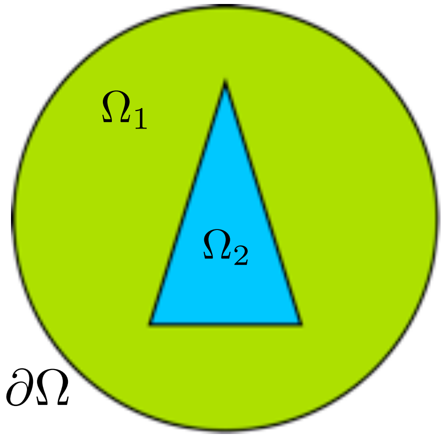


-linearized eigenproblem

-sign-changing coefficient

-corners

Some numerical experiments (1)



$$\left|\begin{array}{l}\text{For } \beta \in \mathbb{R}, \text{ Find } \widetilde{u} \in V_0 \setminus \{0\}, \omega \in \mathbb{C} \text{ s.t.} \\ A(\beta)\widetilde{u} = \omega^2 \widetilde{u}\end{array}\right.$$

Numerical illustrations with FE

Parameters $\epsilon_1 = 1 \quad \epsilon_2 = -\frac{10}{7} \quad \beta = 1$

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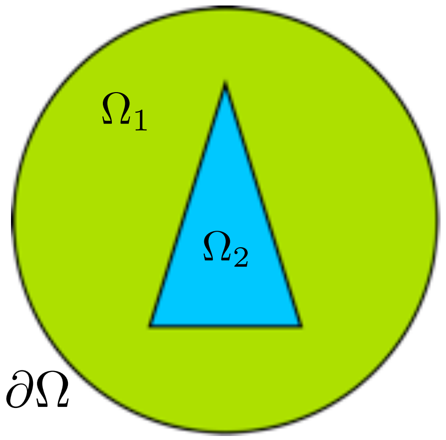

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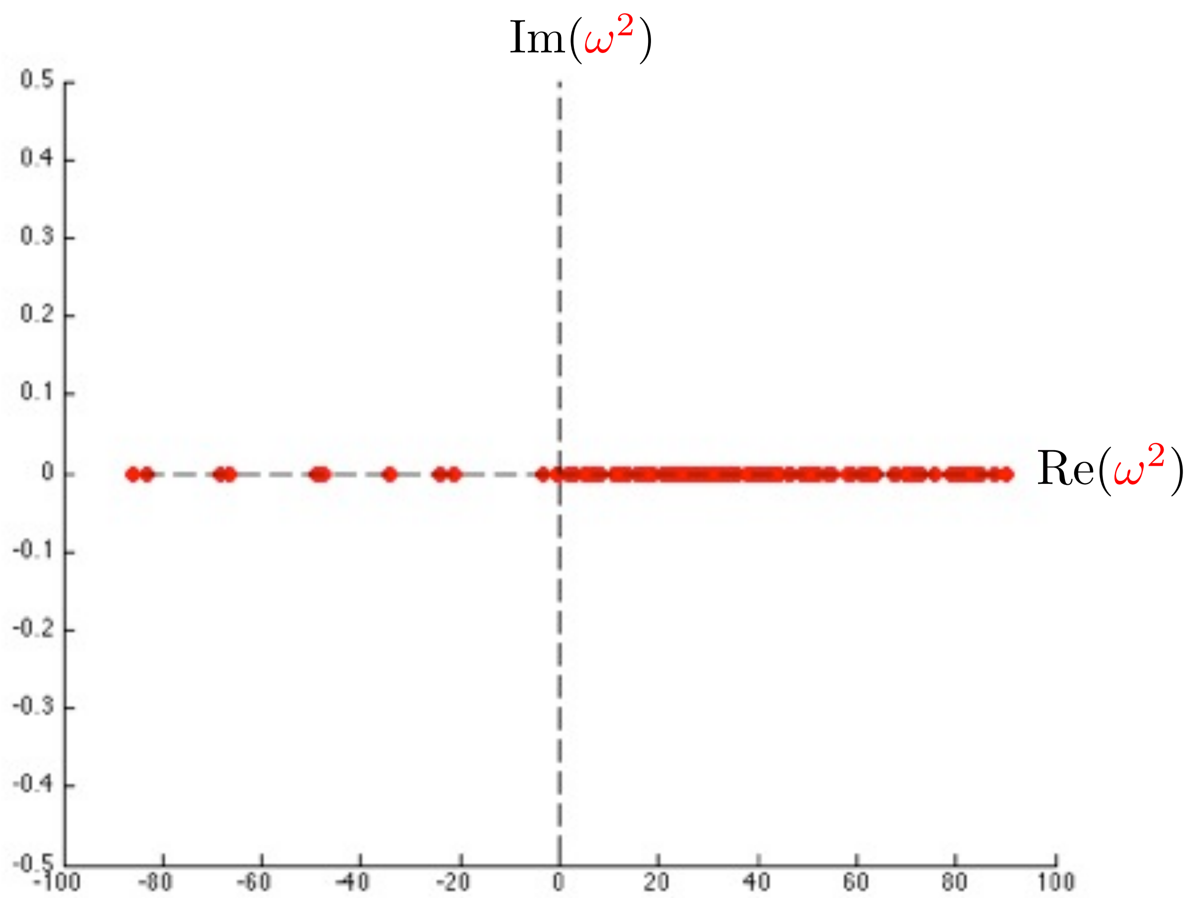

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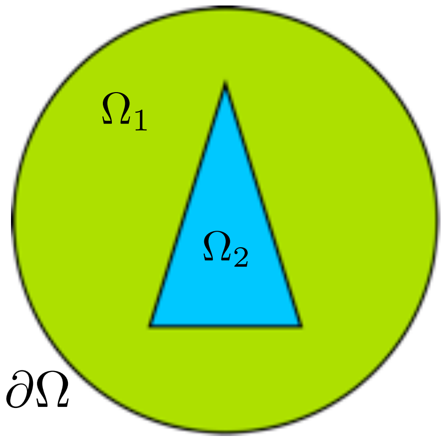

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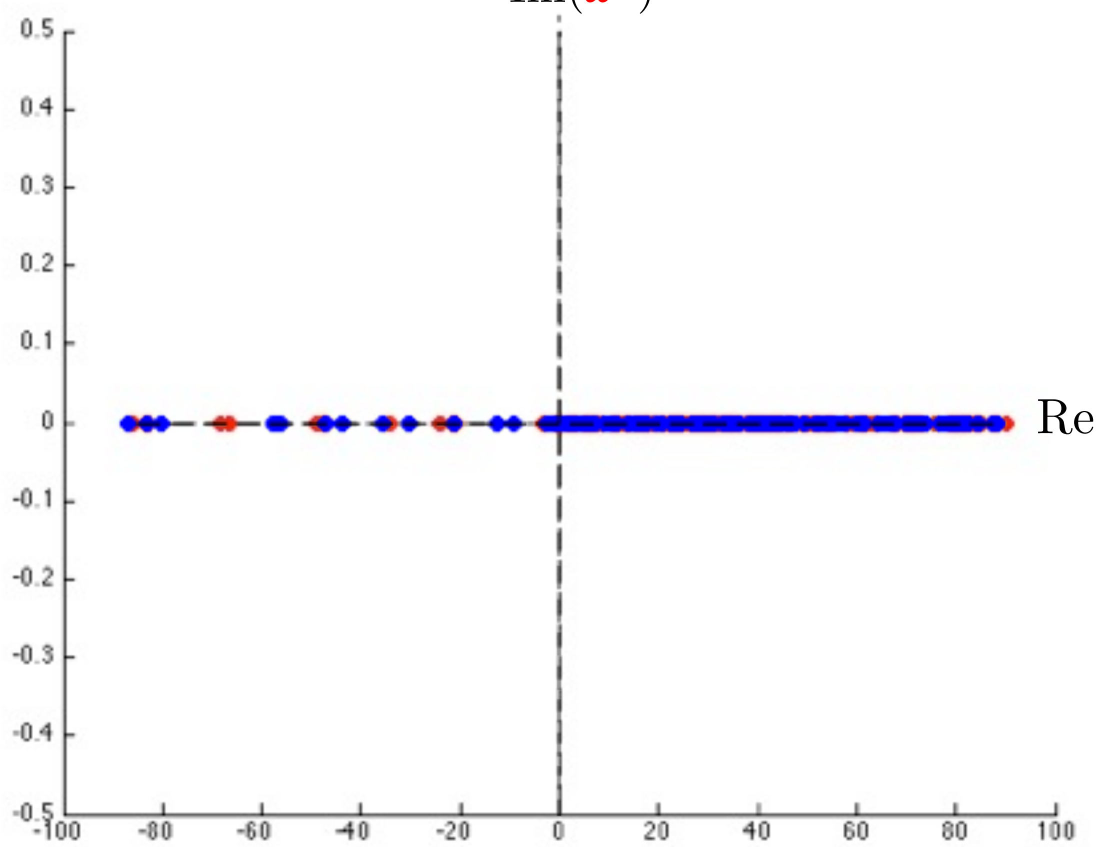

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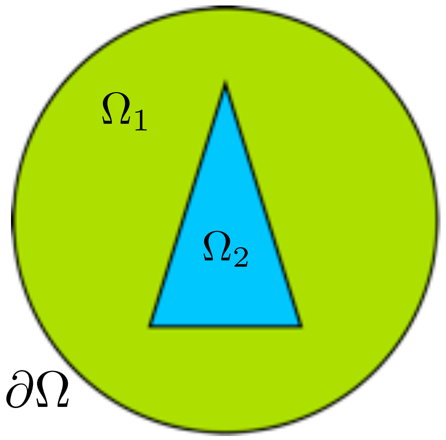

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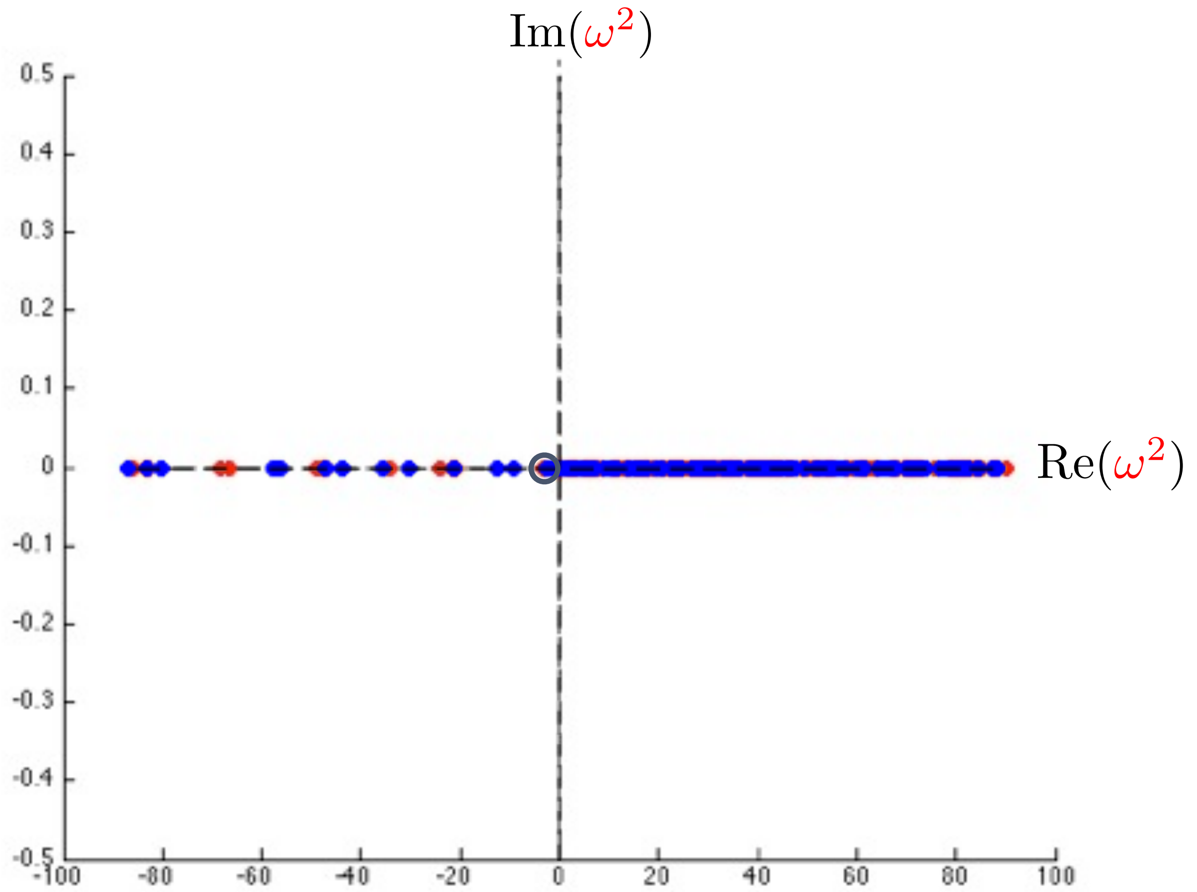

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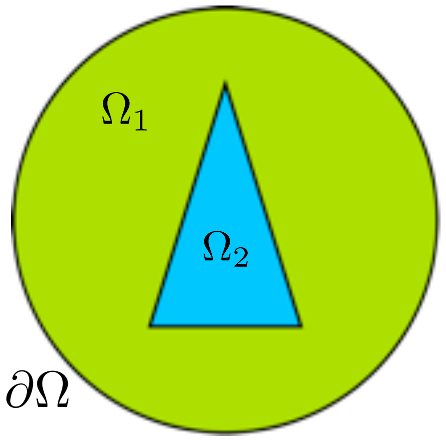

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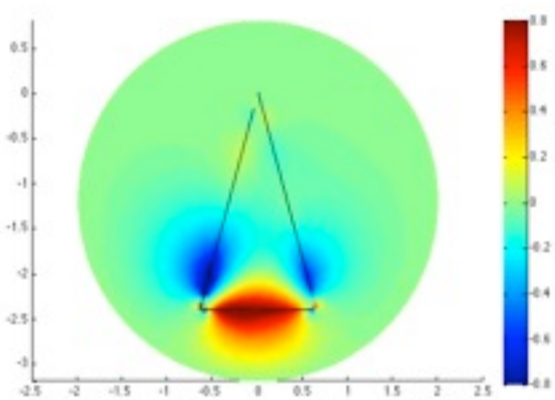

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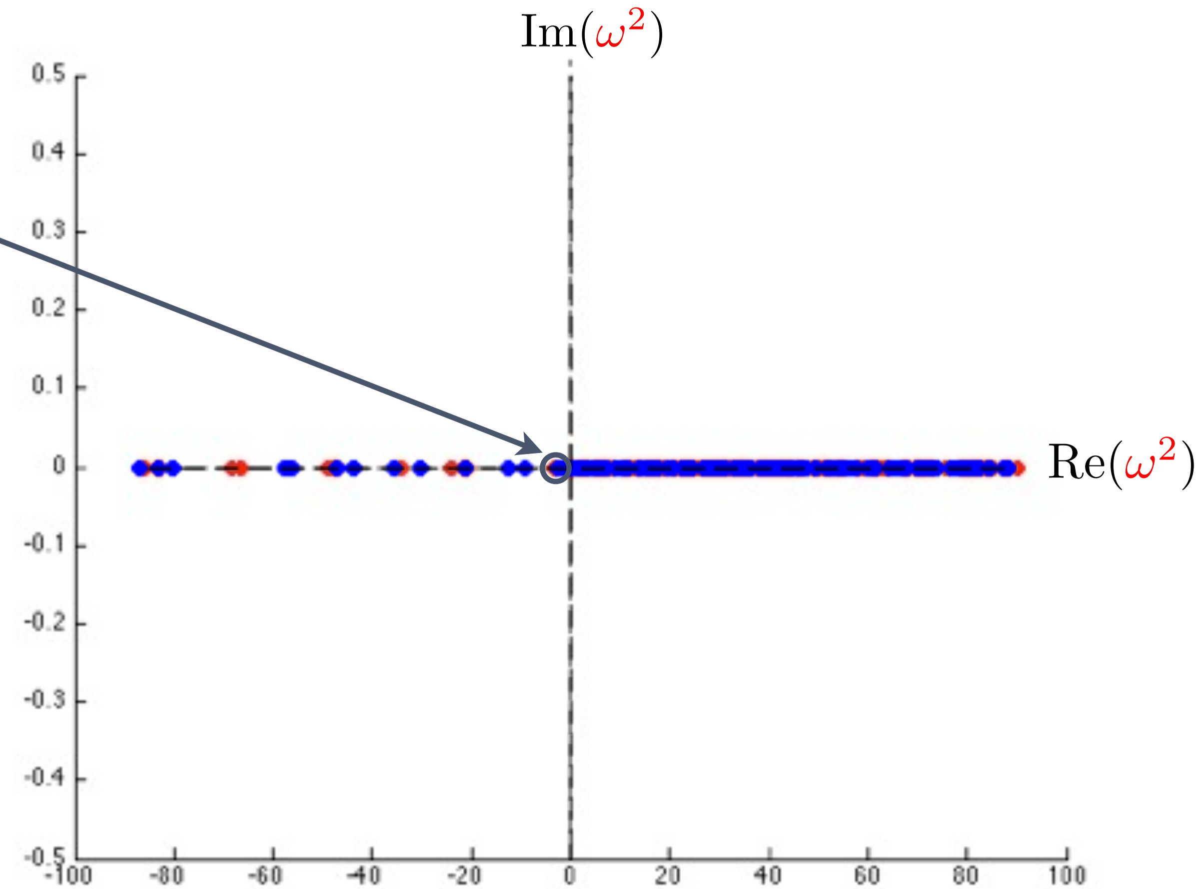

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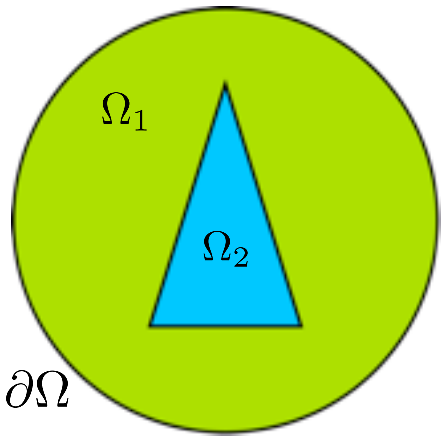

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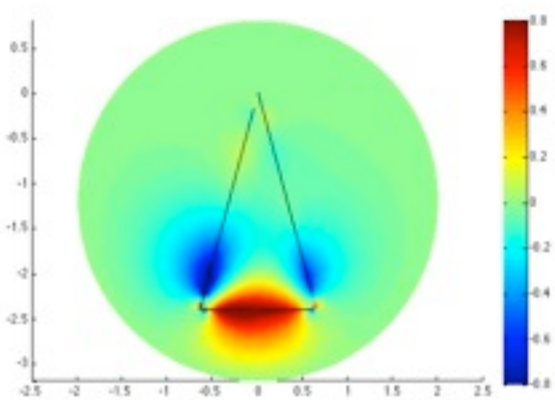

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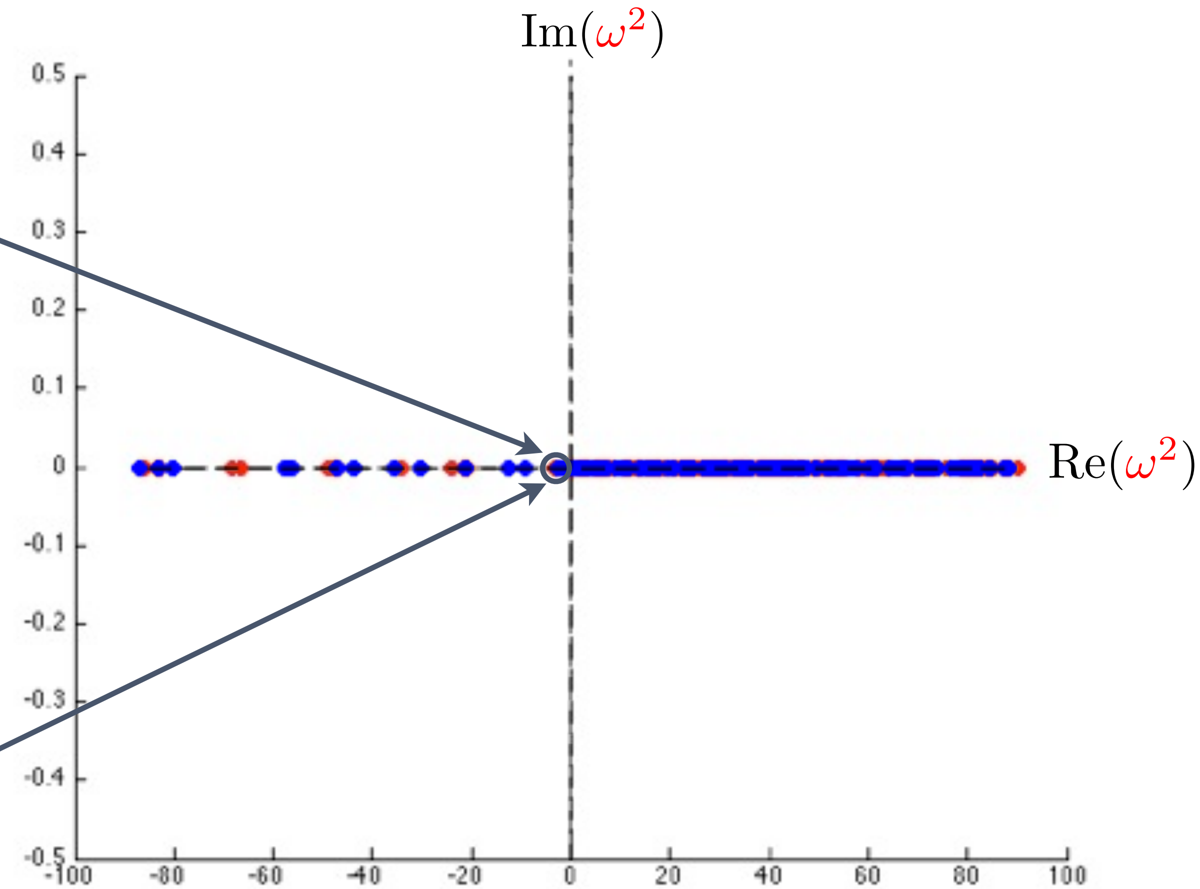
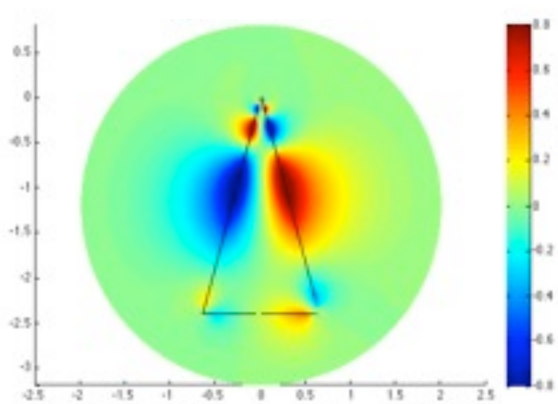
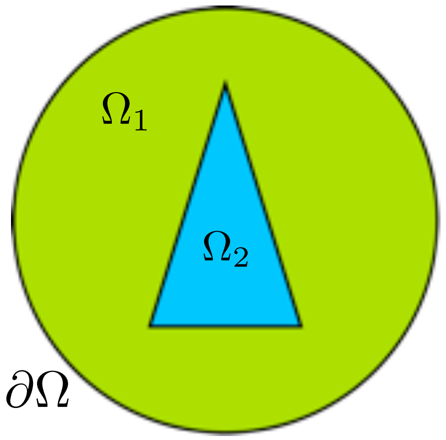




For a fine mesh

No convergence due to black-hole waves

Some numerical experiments (1)



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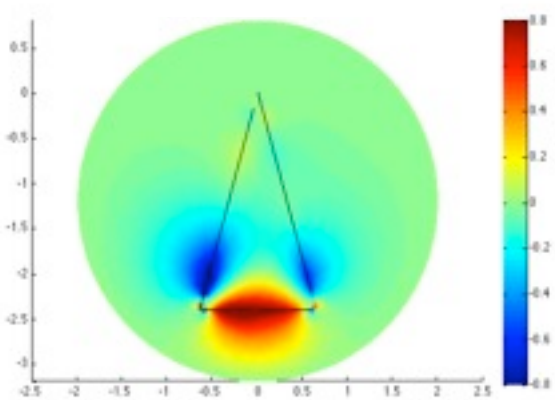

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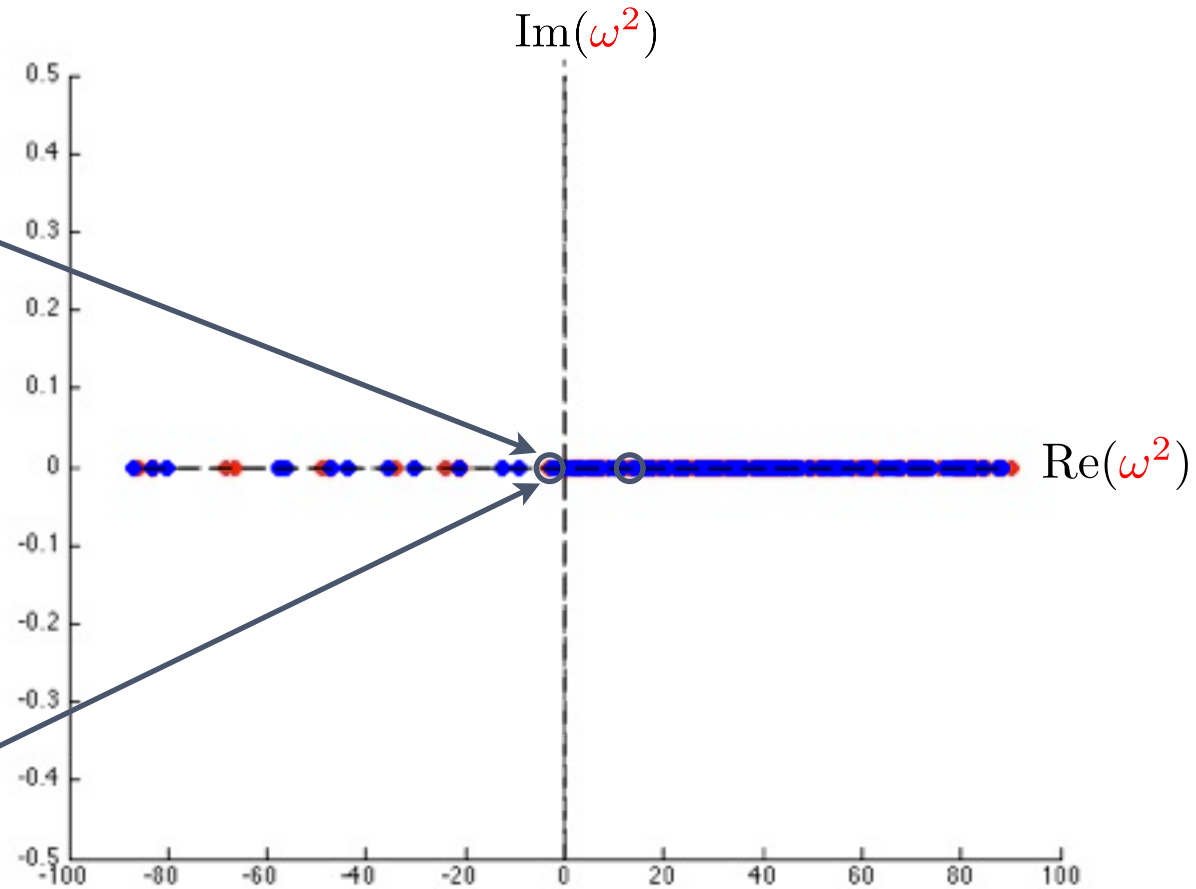

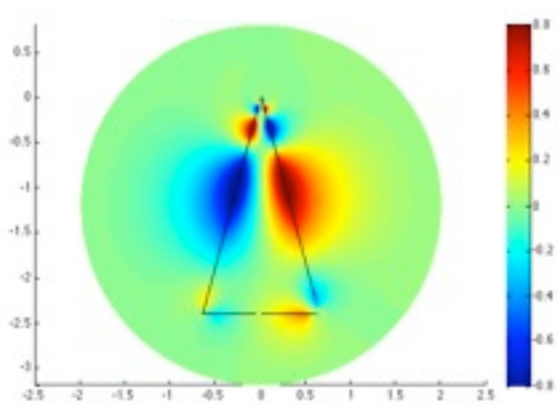

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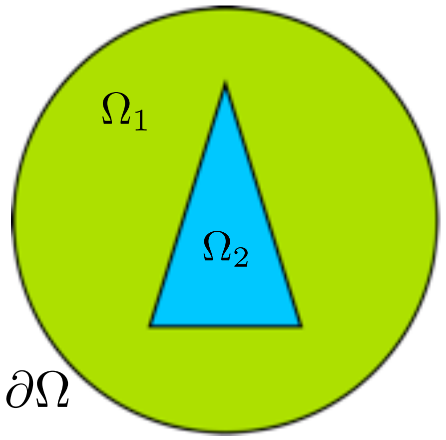

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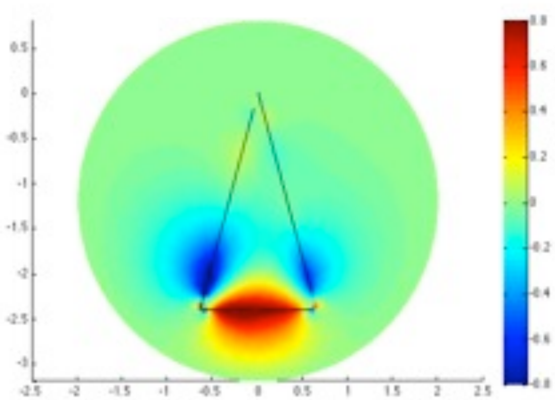

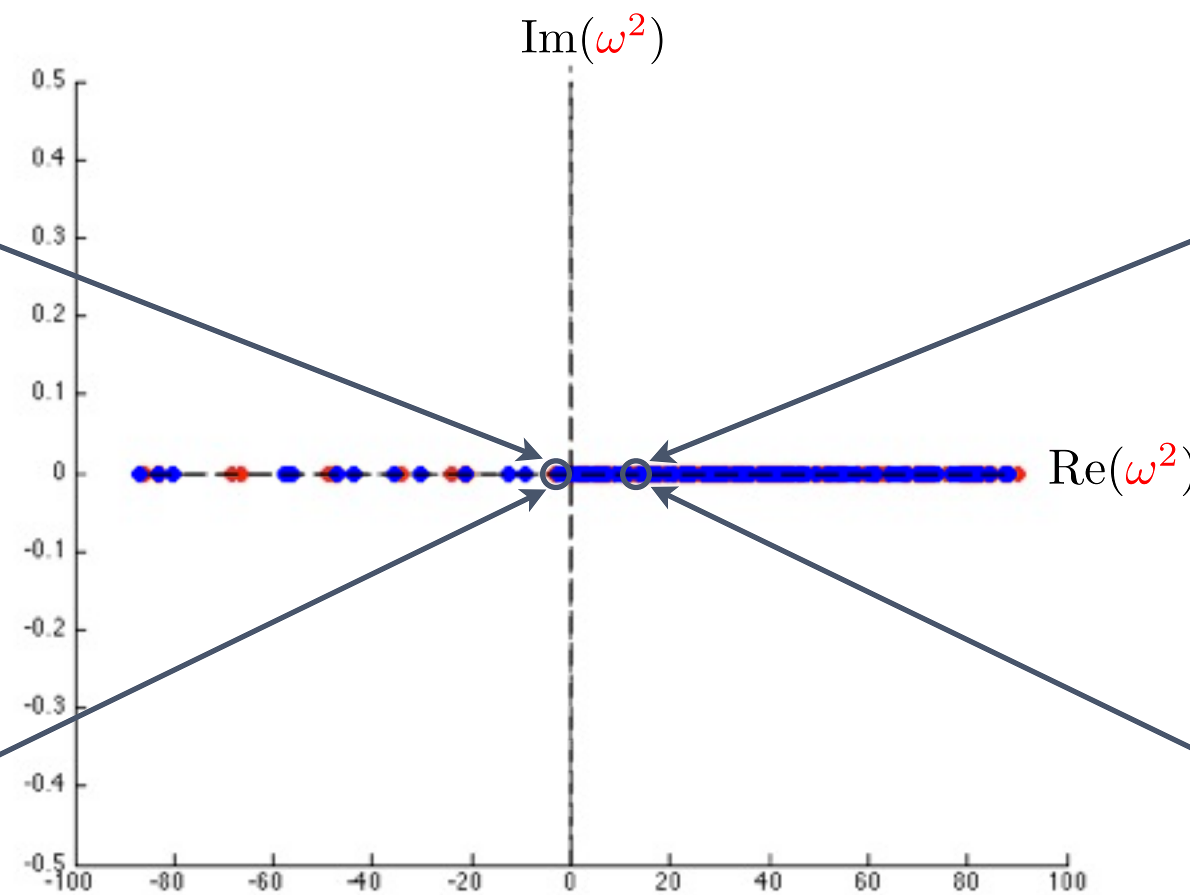

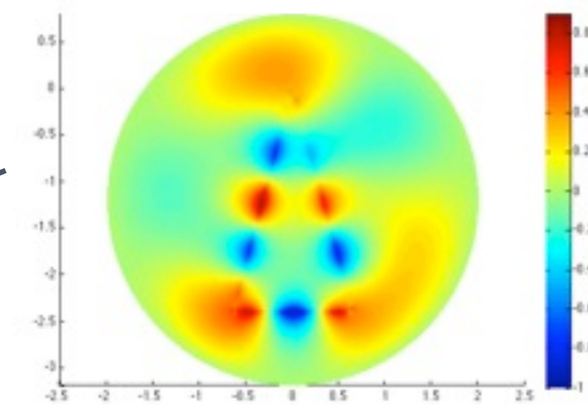

For a coarse mesh

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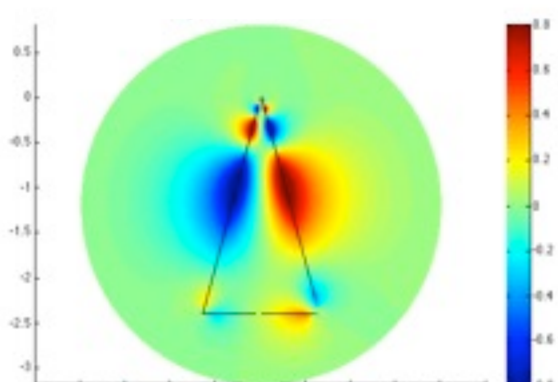

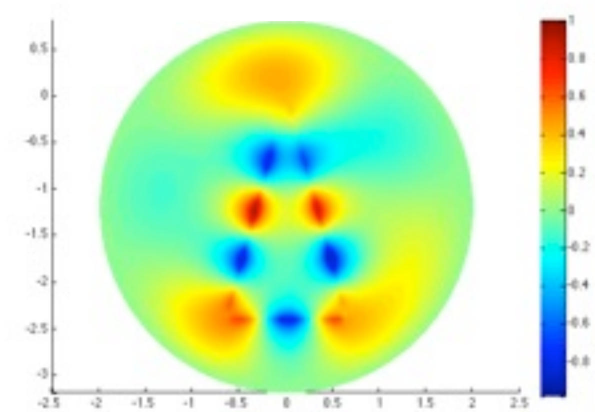

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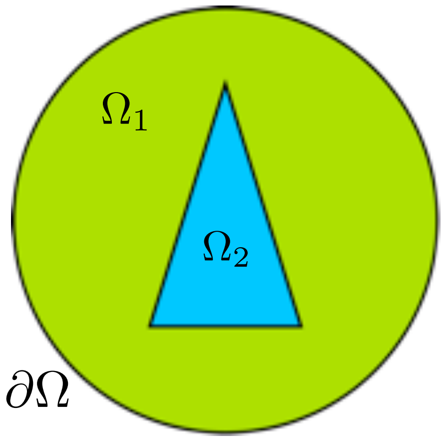

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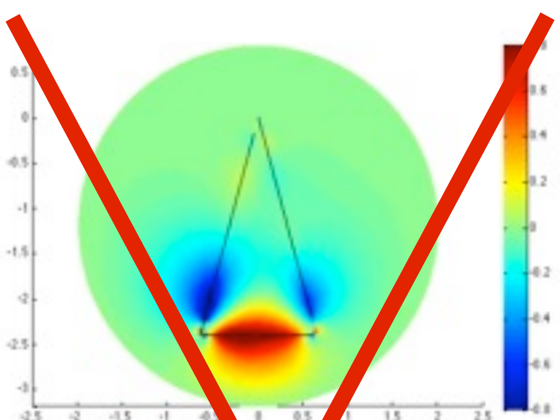

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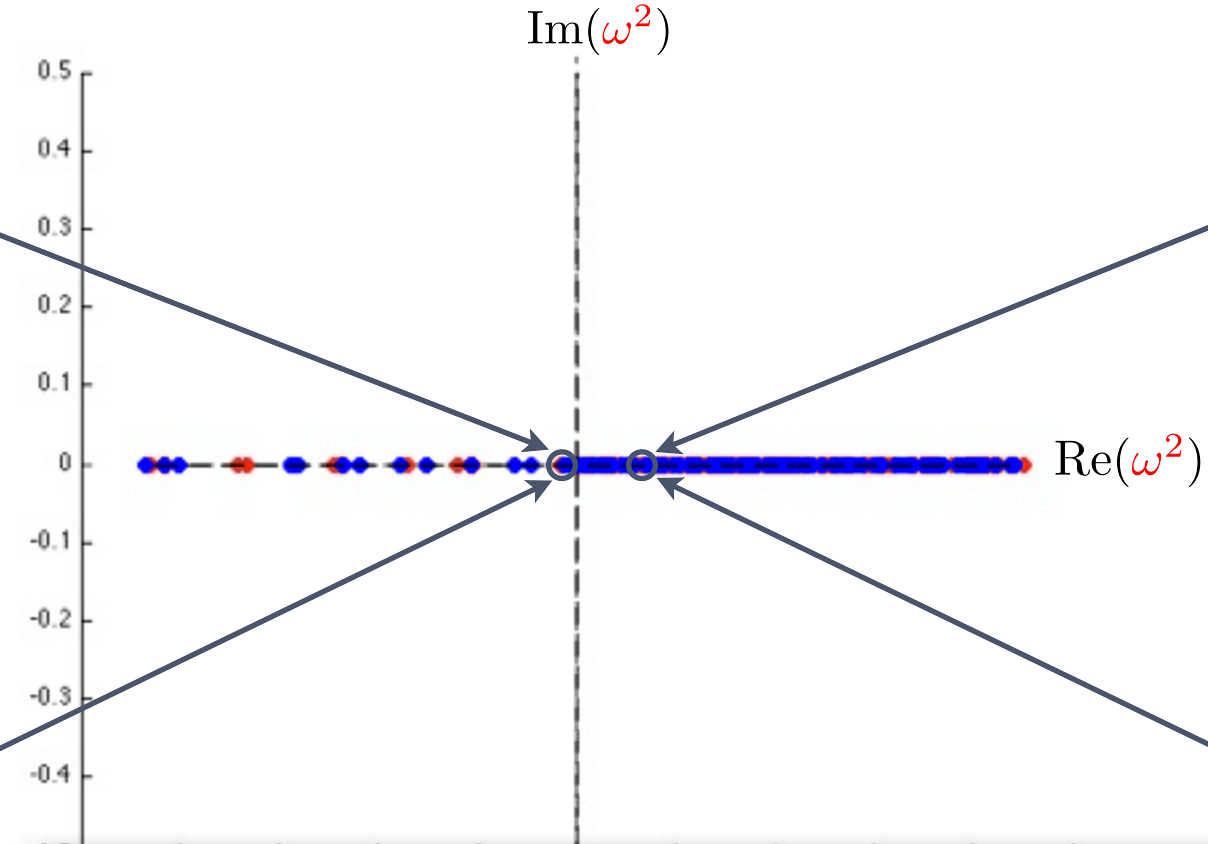

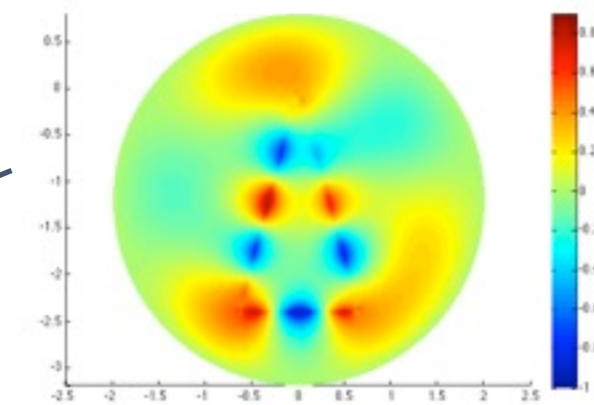

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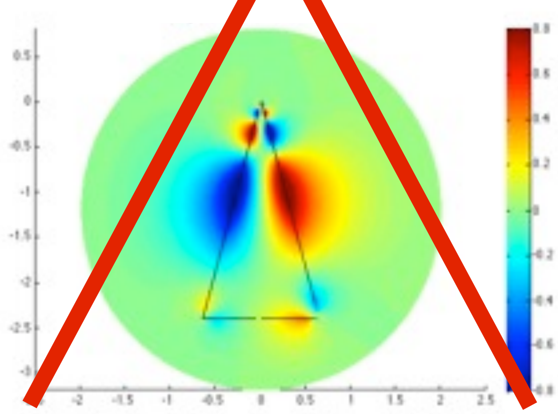
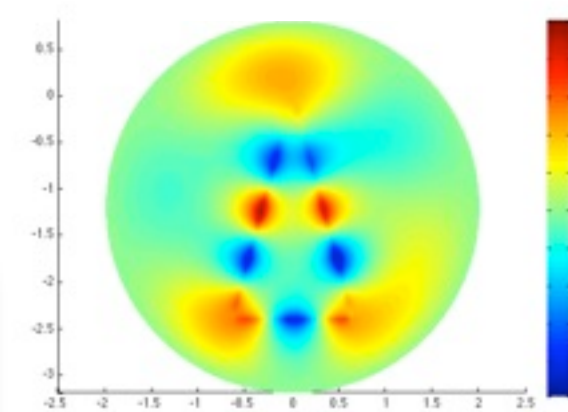


For a fine mesh

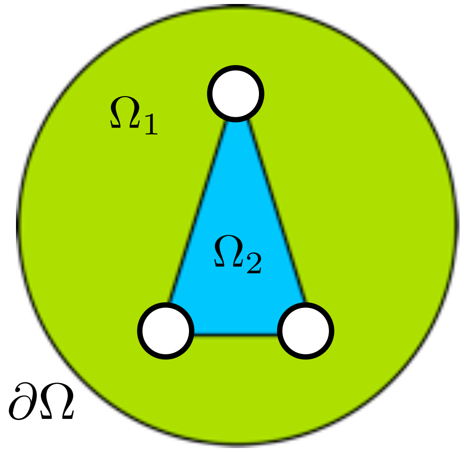
No convergence due to

No FEM convergence but some modes seem stable: guided modes are hidden in this spectrum !



For a fine mesh

Some numerical experiments (2)



For $\beta \in \mathbb{R}$, Find $\widetilde{u} \in V_0 \setminus \{0\}$, $\omega \in \mathbb{C}$ s.t.

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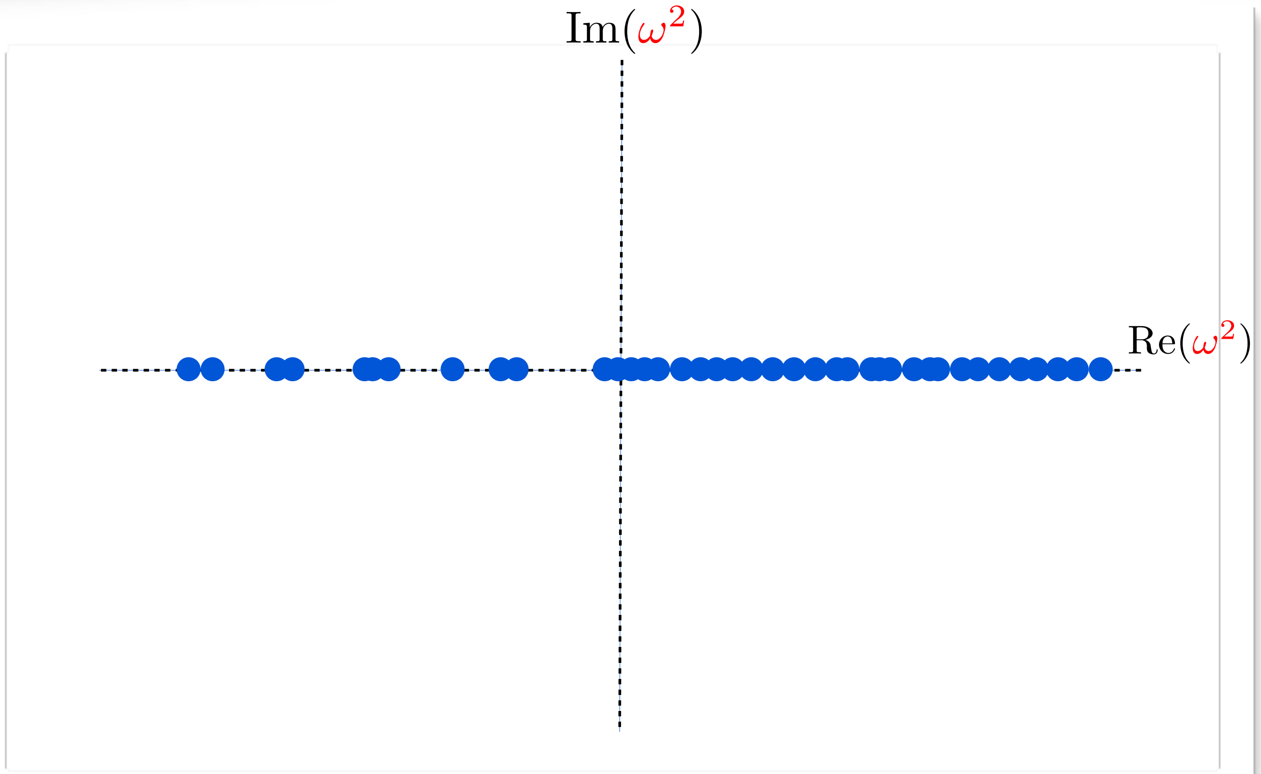
New numerical method which is stable, sorts the modes and reveals the guided modes.



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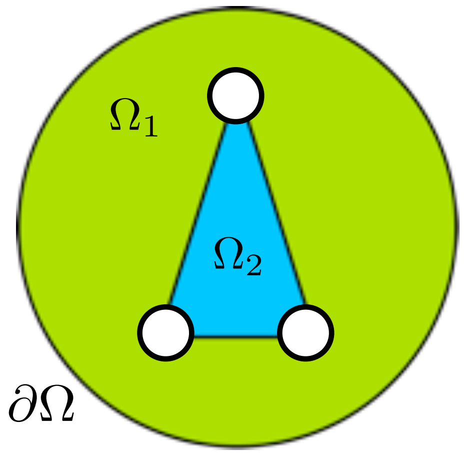

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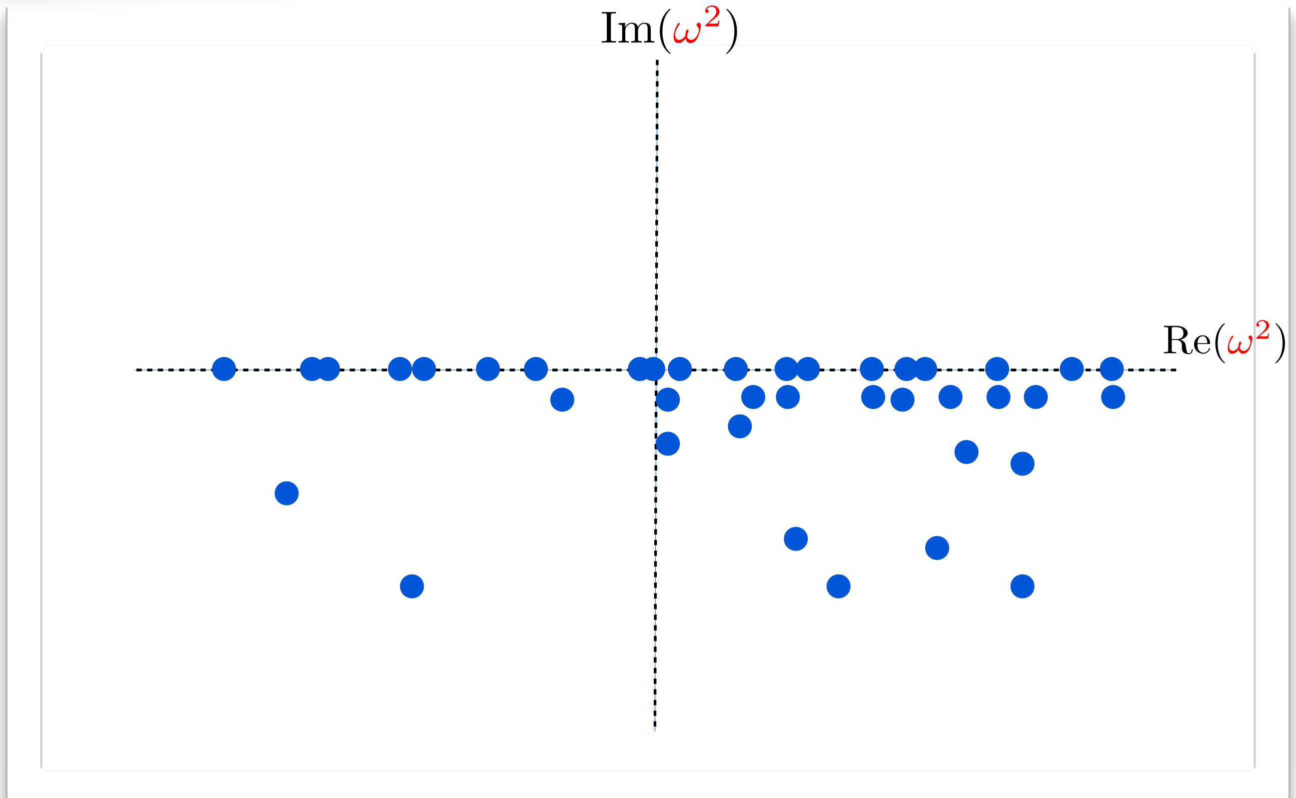

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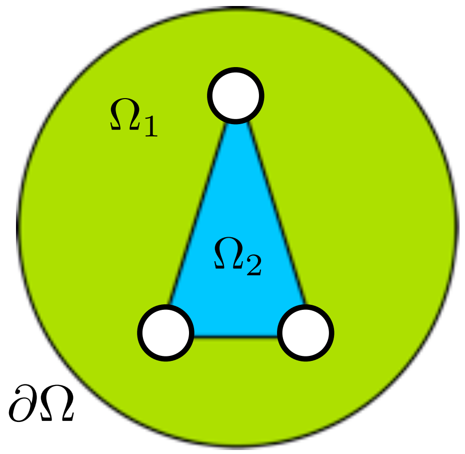

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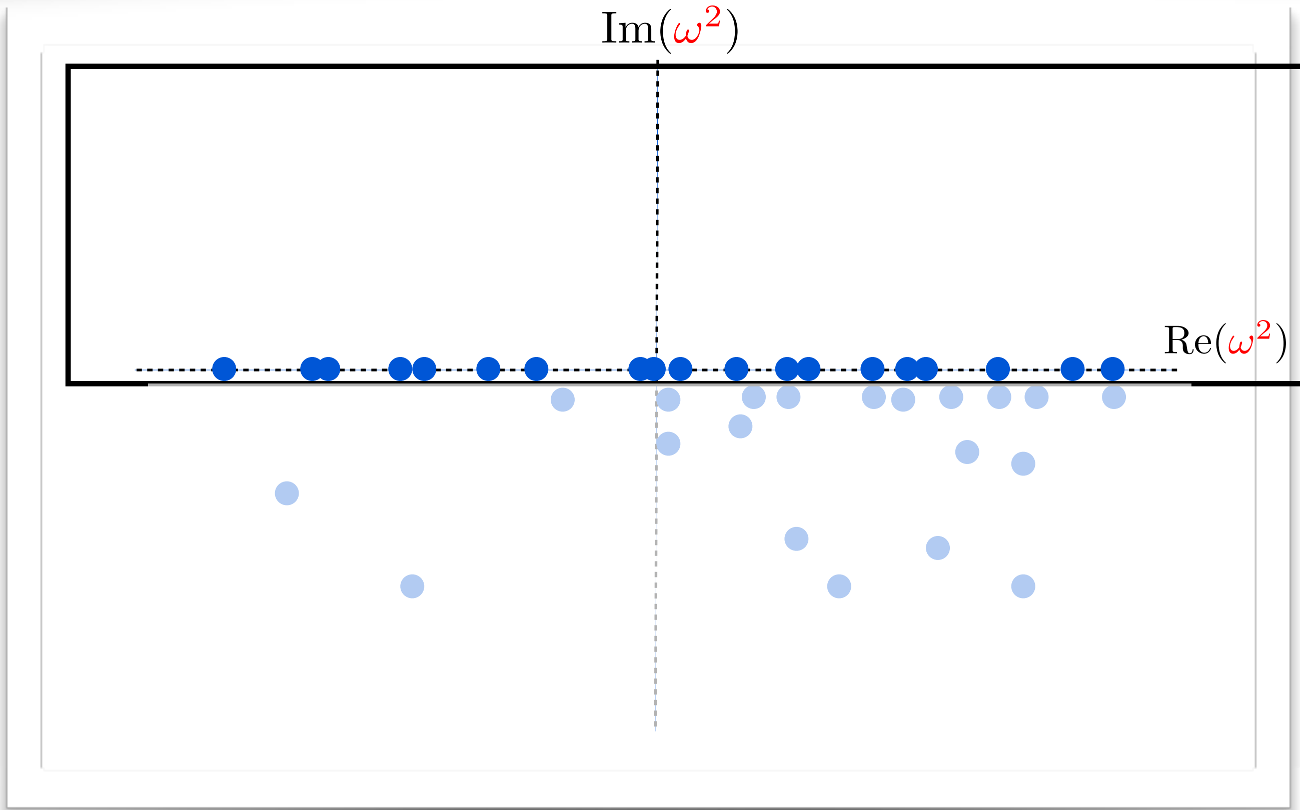

$\omega^2 \in \mathbb{R}$
guided / evanescent modes

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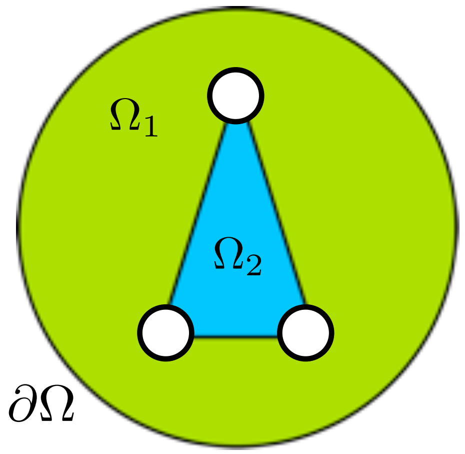

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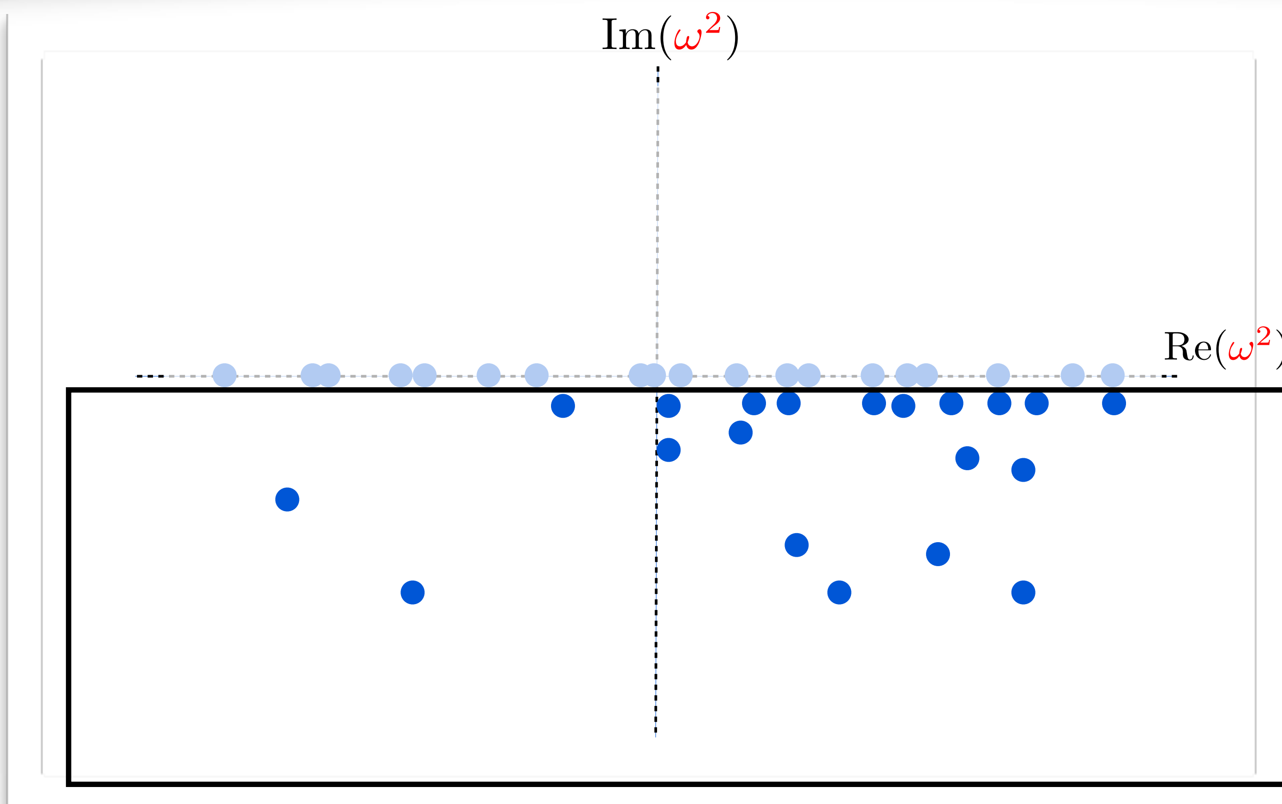

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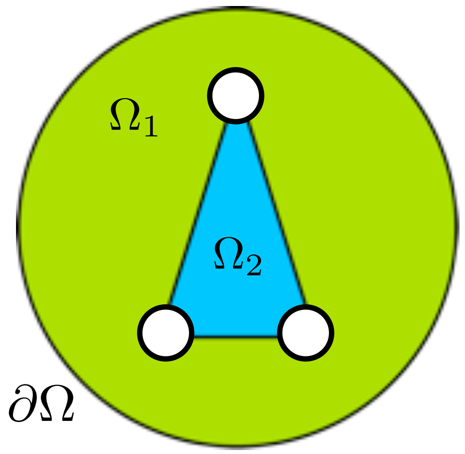

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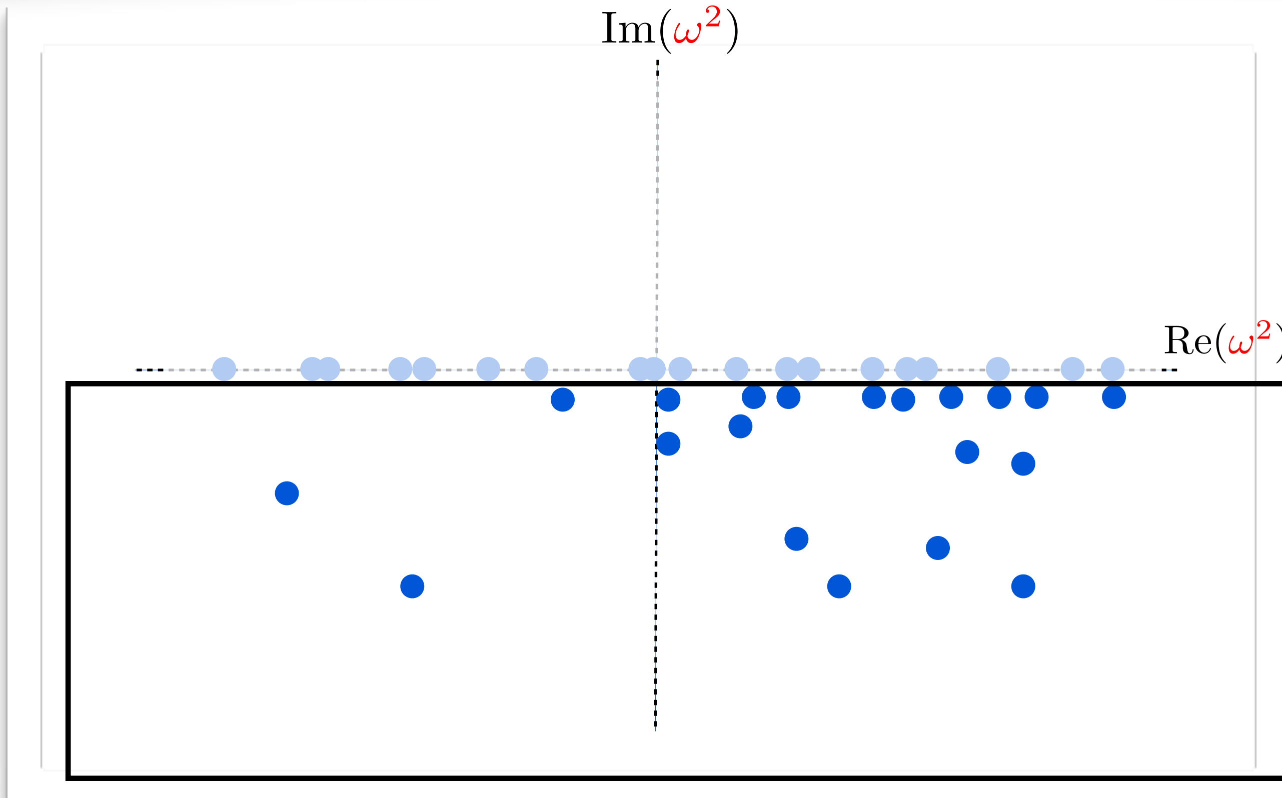

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Explanation via energy technique

Ongoing work

- Numerical analysis requires some conditions on the mesh
- Extensions to Maxwell's equations are currently in progress.
- Non linear eigenproblem (dissipationless Drude's model).
- What's happening when metamaterials ?
- Open plasmonic waveguides.

Publications and communications

- 3 articles in preparation
- Several international communications: WAVES 13, PIERS 13, KOZVAWES 14, OWTNM 14, Leaky Days 15, WAVES 15.

Thank you for your attention.