Numerical methods for light scattering in plasmonic structures with corners

Camille Carvalho

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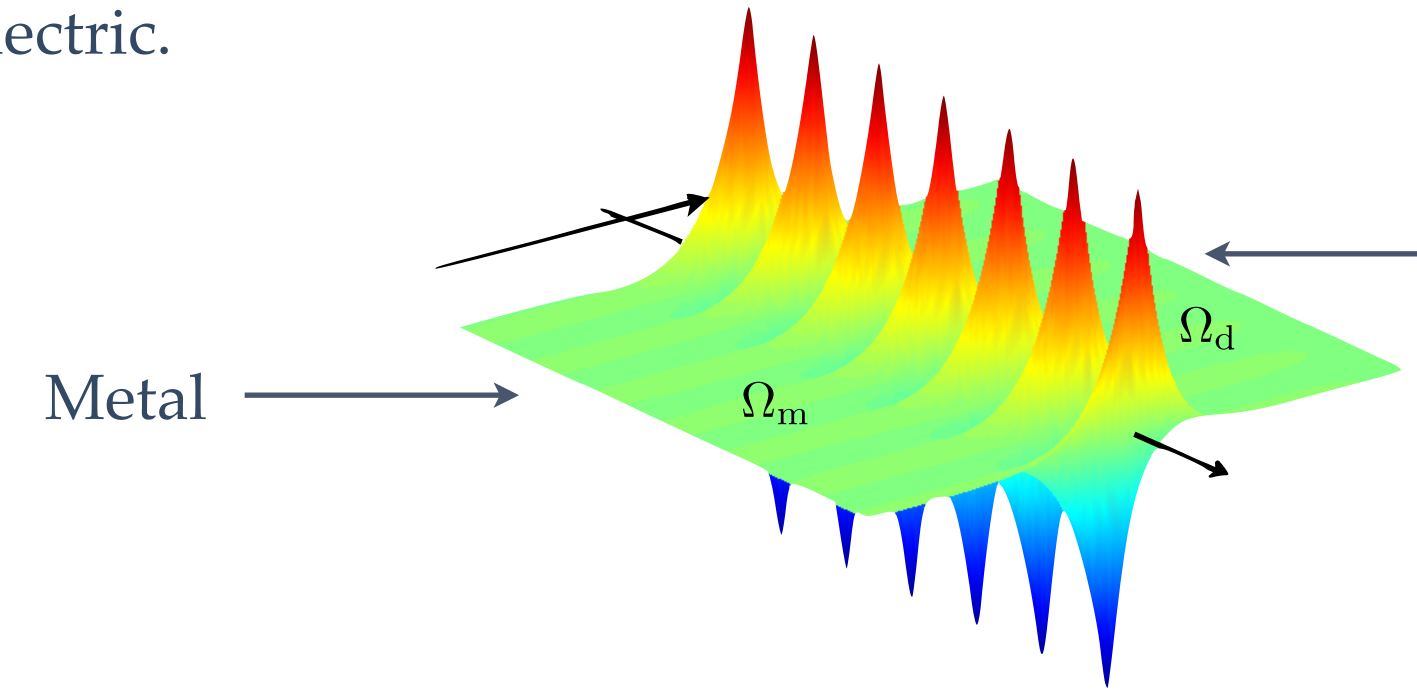

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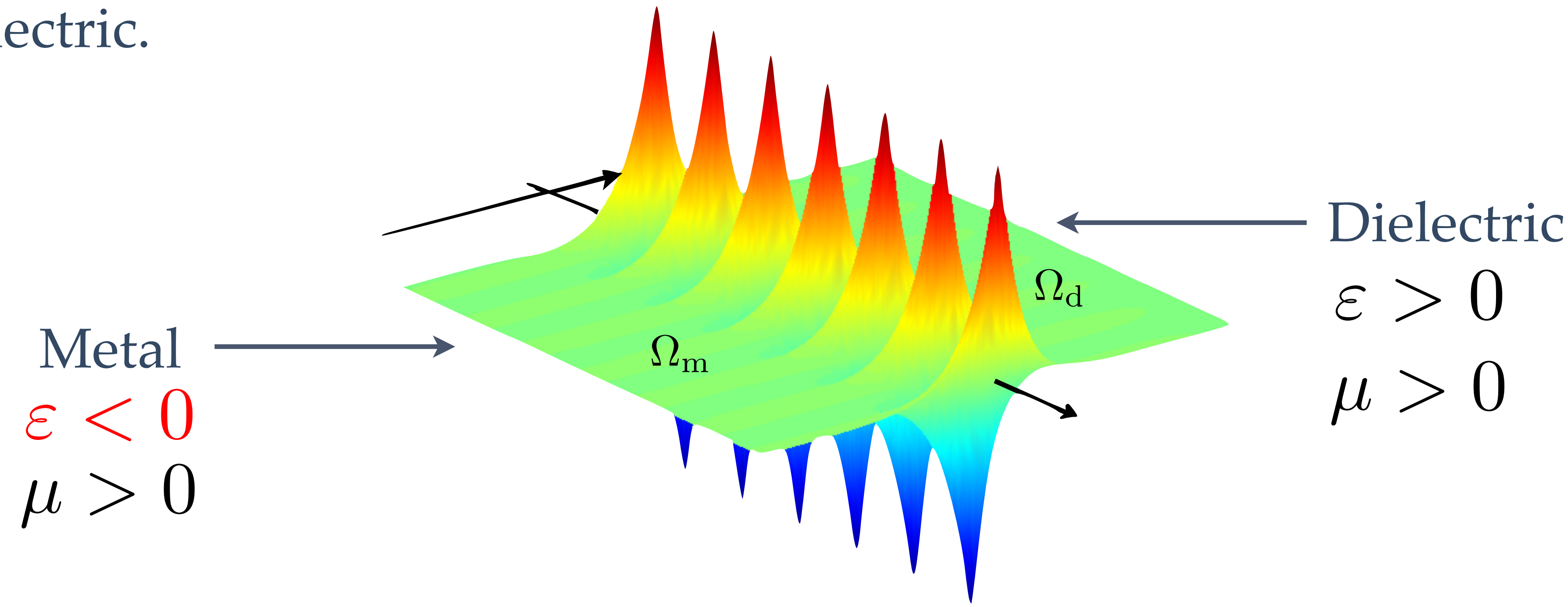

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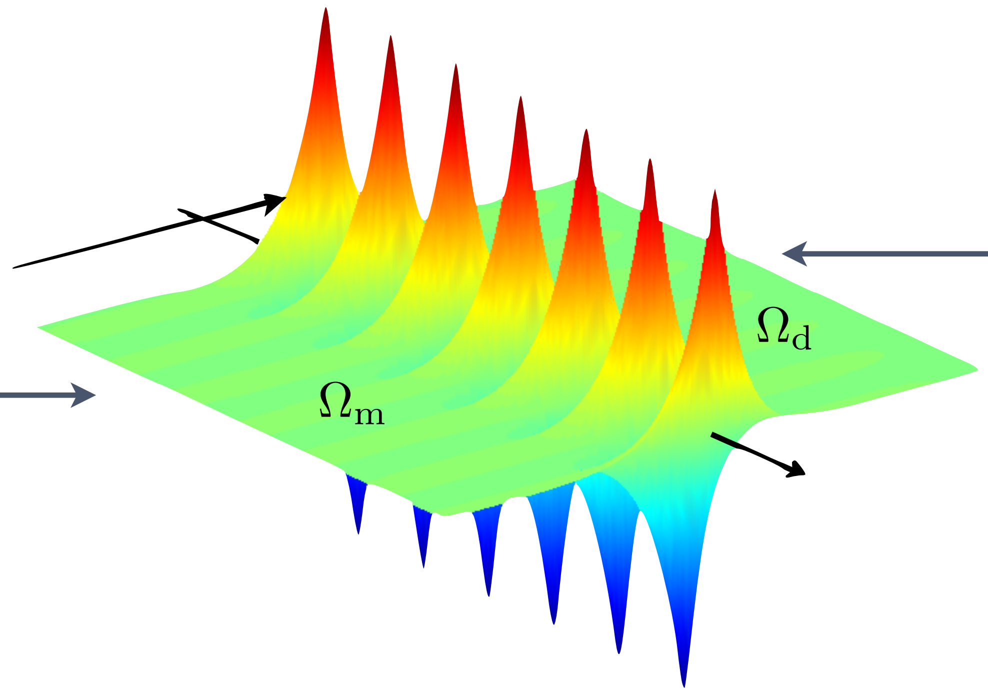

Metal
$\varepsilon < 0$
$\mu > 0$

Dielectric
$\varepsilon > 0$
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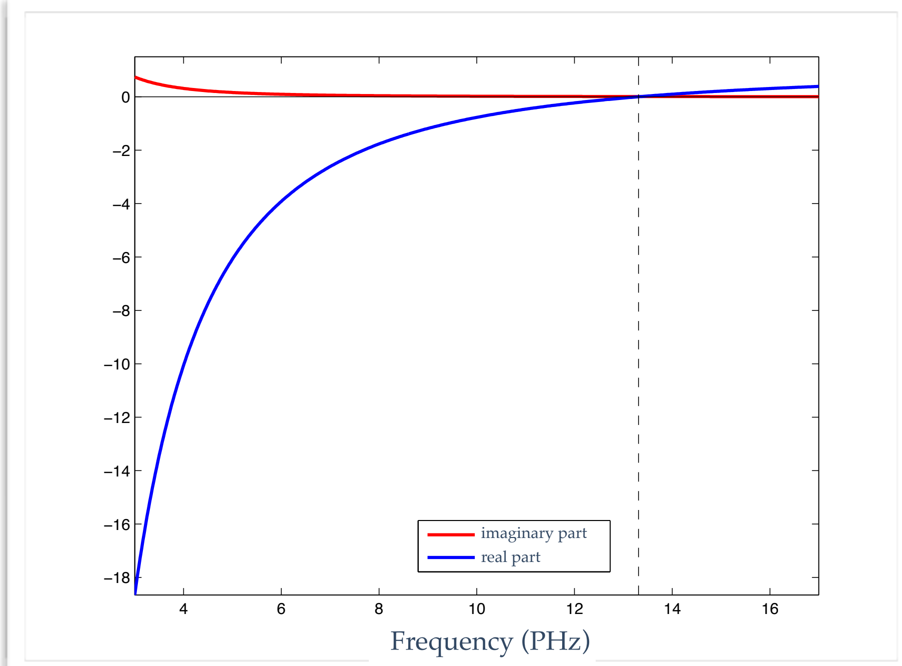

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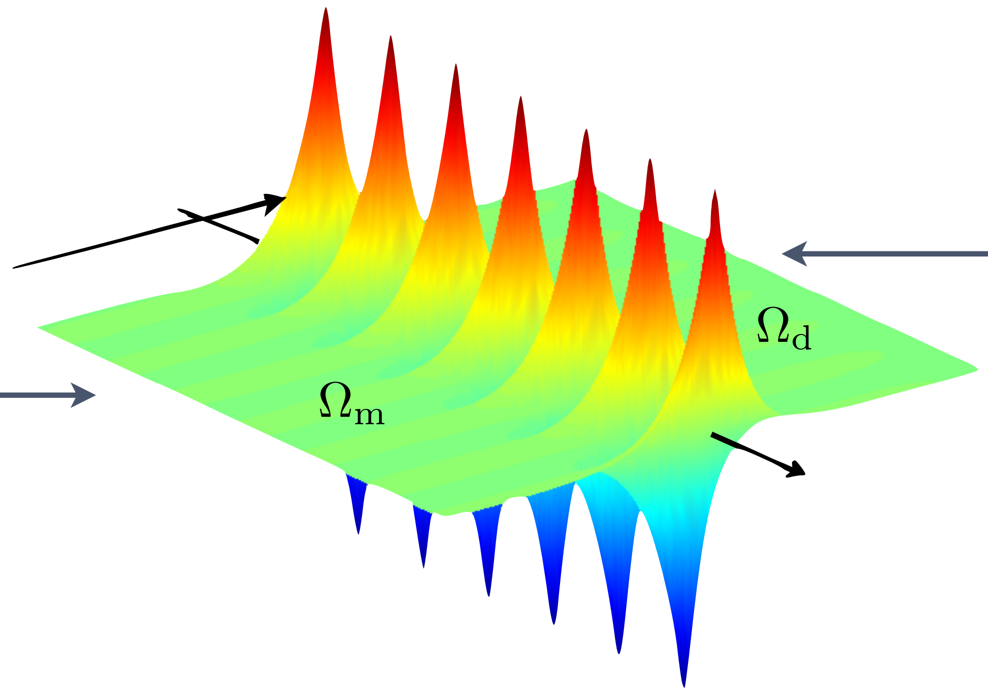

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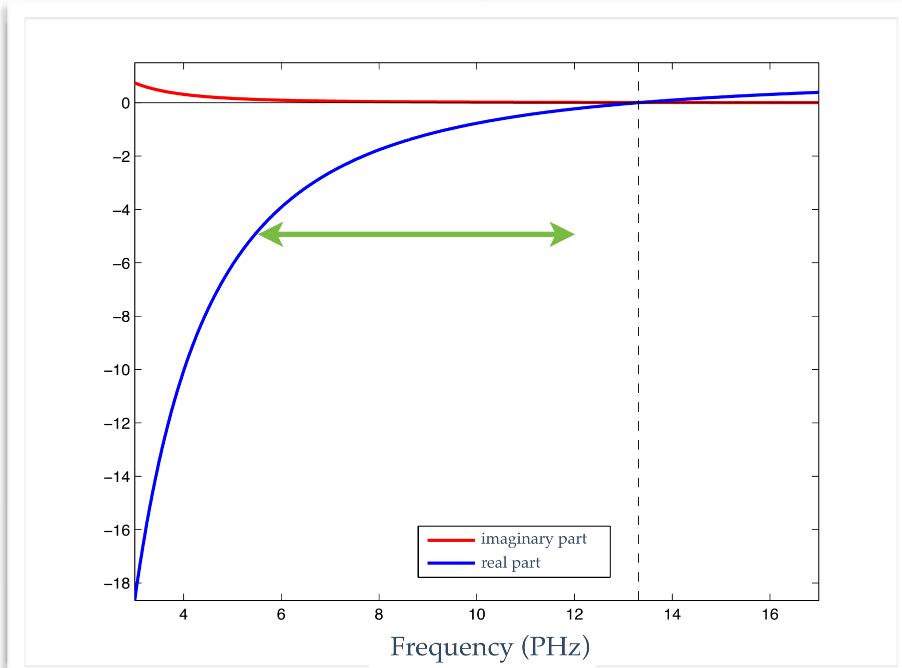
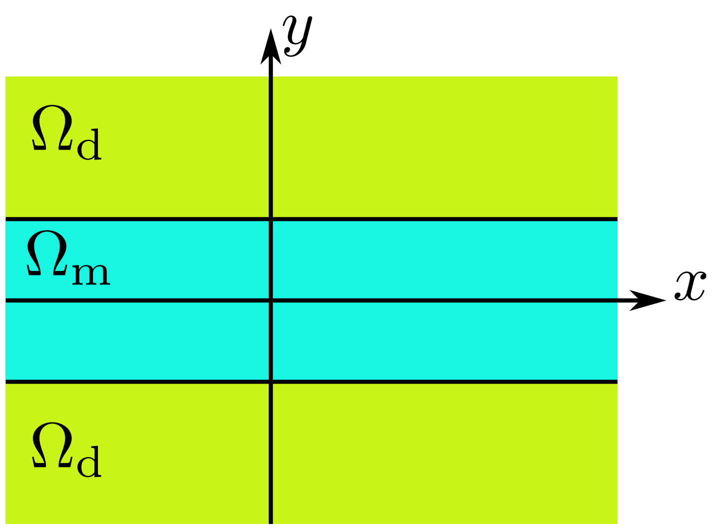
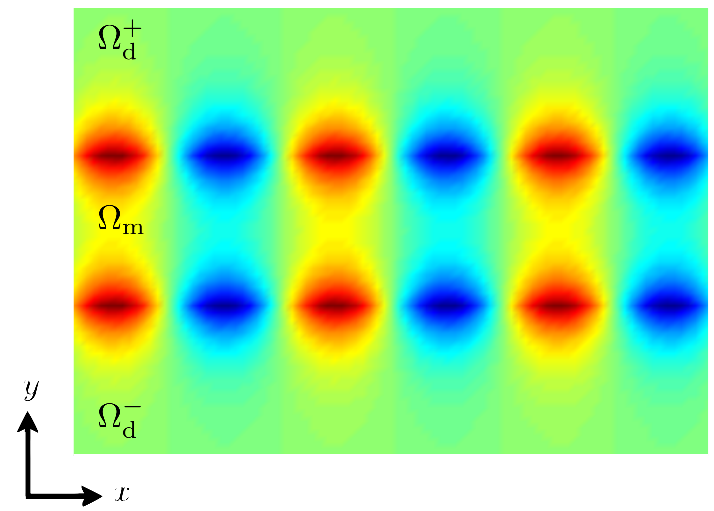


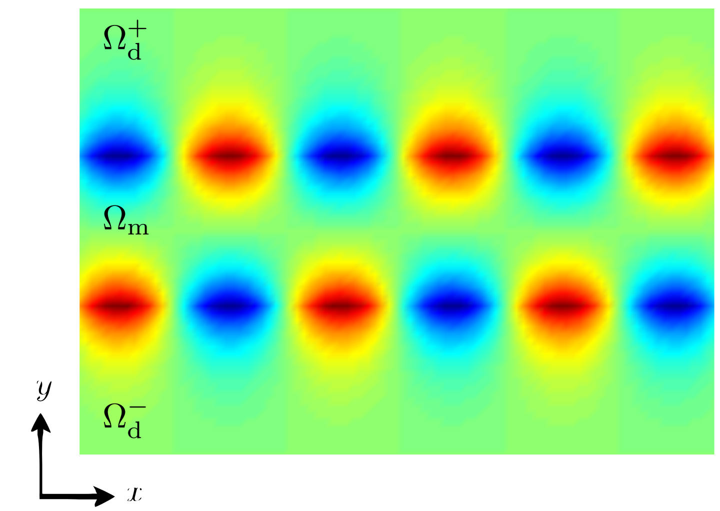
At optical frequencies ($\gamma \ll \omega < \omega_p$), ε has a negative real part and a neglectable imaginary part.

Surface plasmons and geometries

For simple geometries, one can get the expression of surface plasmons (use of separation of variables and deal with ODEs).







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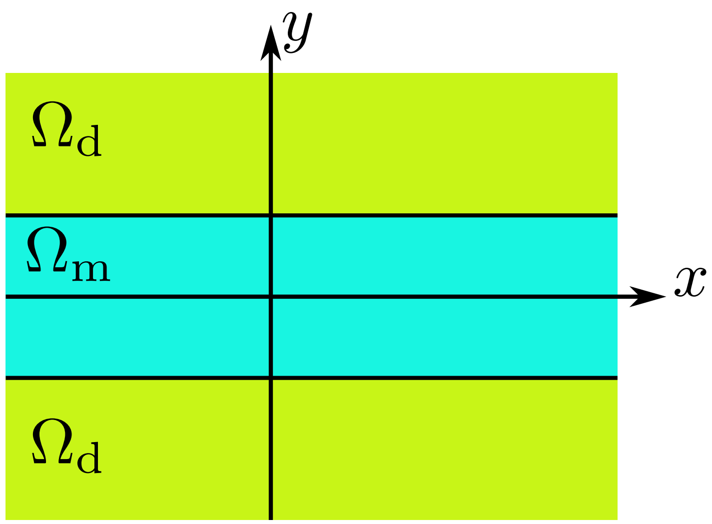

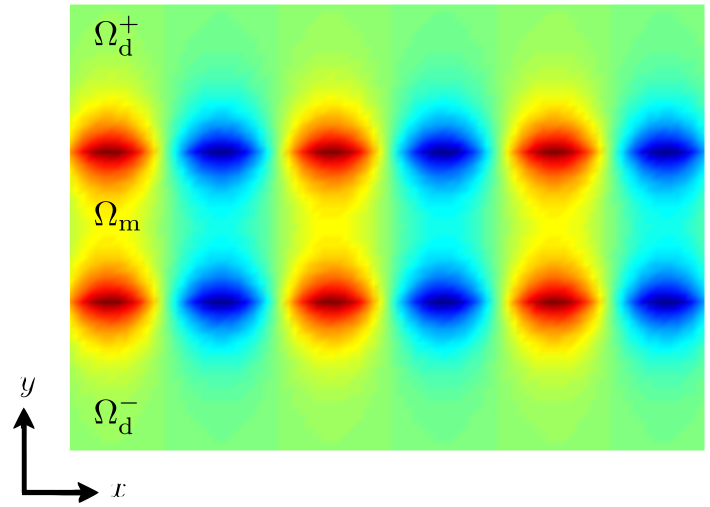

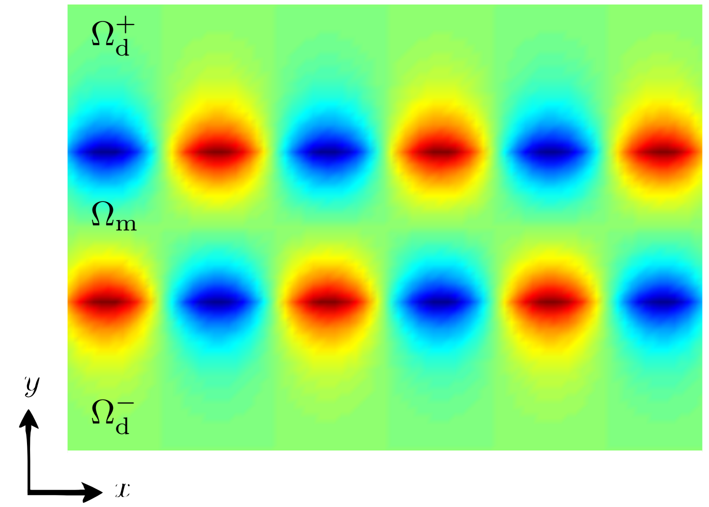

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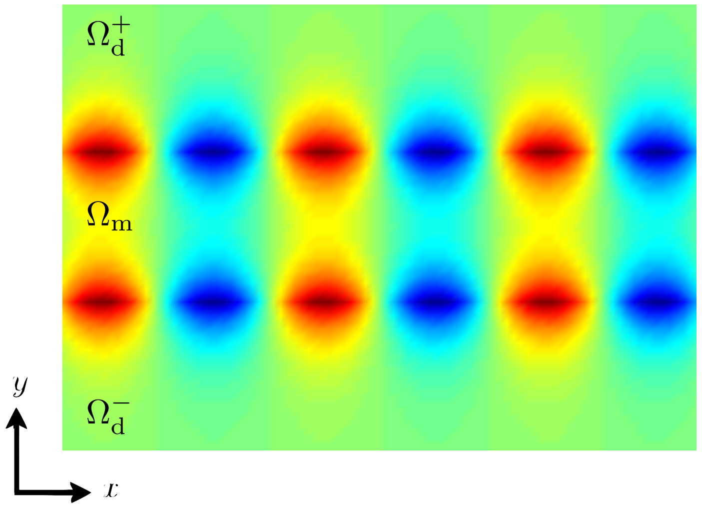

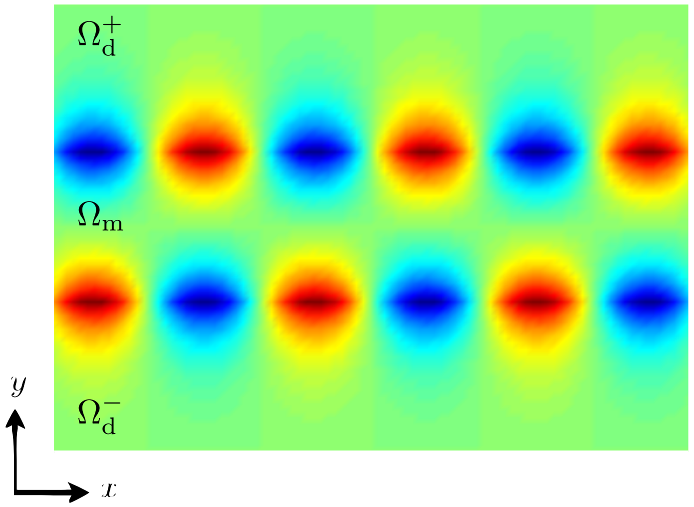

In more complex geometries:

-one has to solve PDEs with sign-changing coefficients (mathematical challenges)
-for non regular geometry singular behaviors appear
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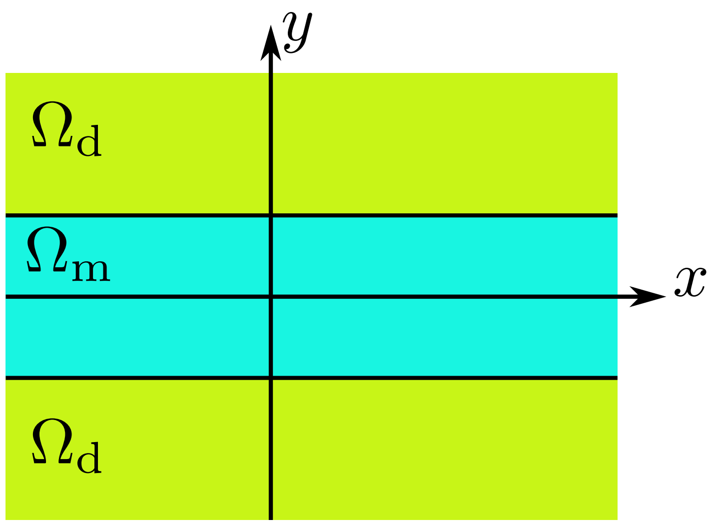

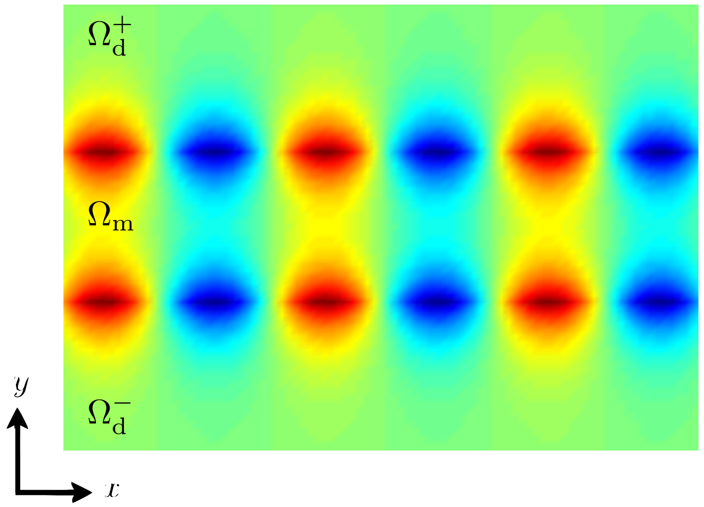

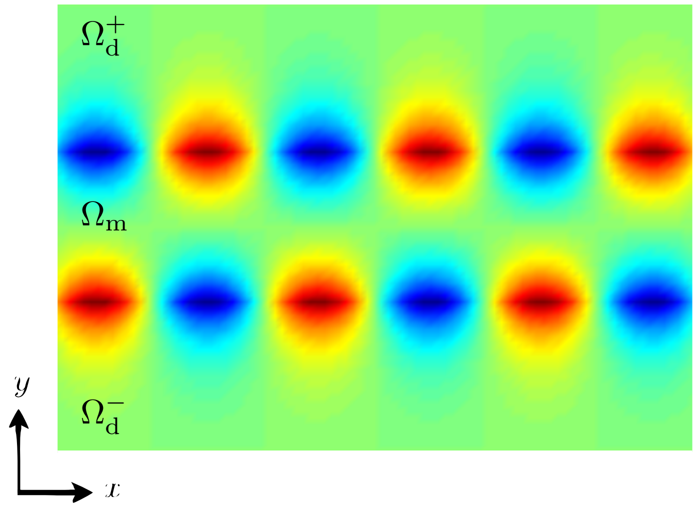

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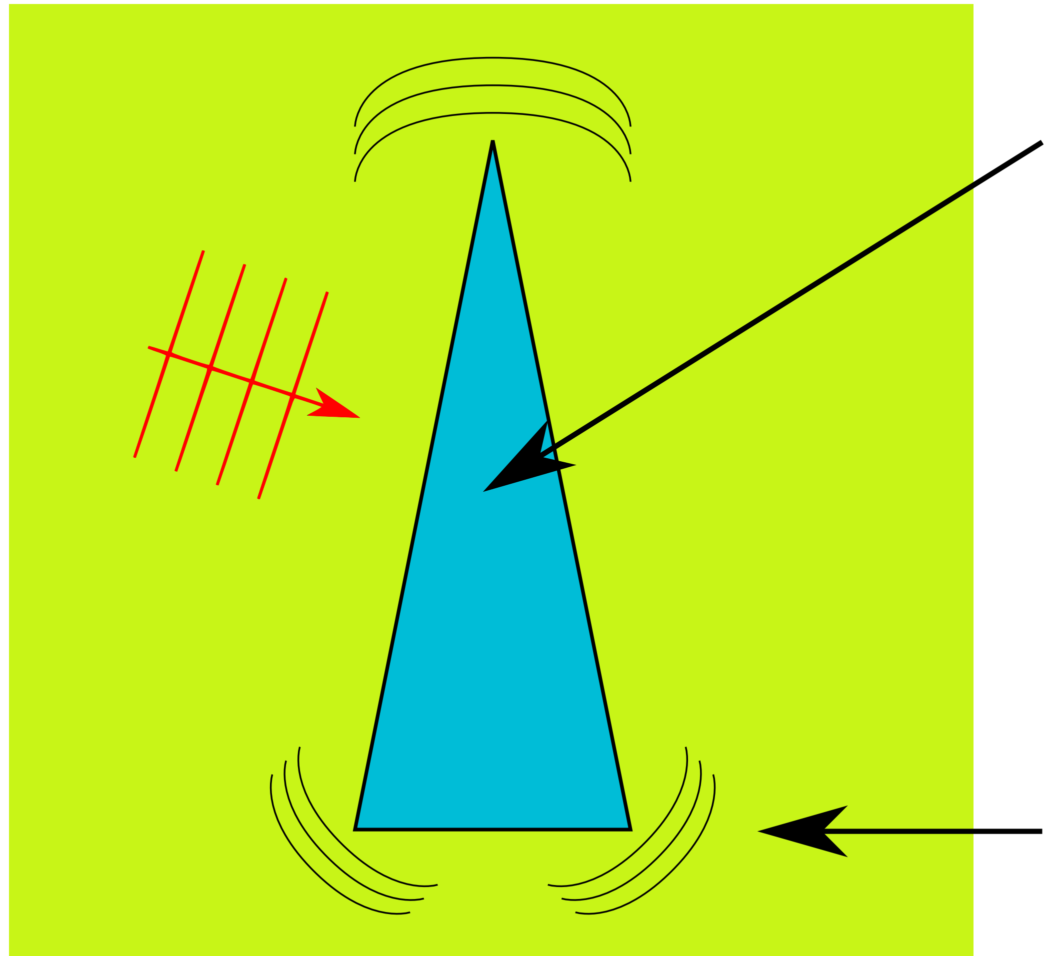
Goal: develop accurate methods that take into account the multiple scales inherent.

The plasmonic scattering problem

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

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



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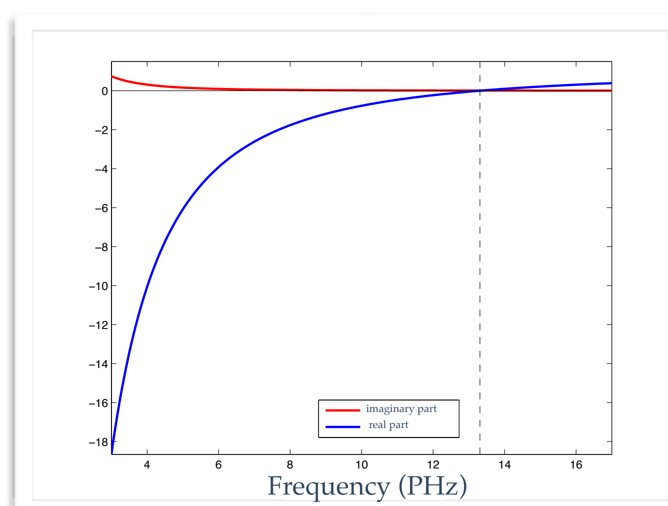
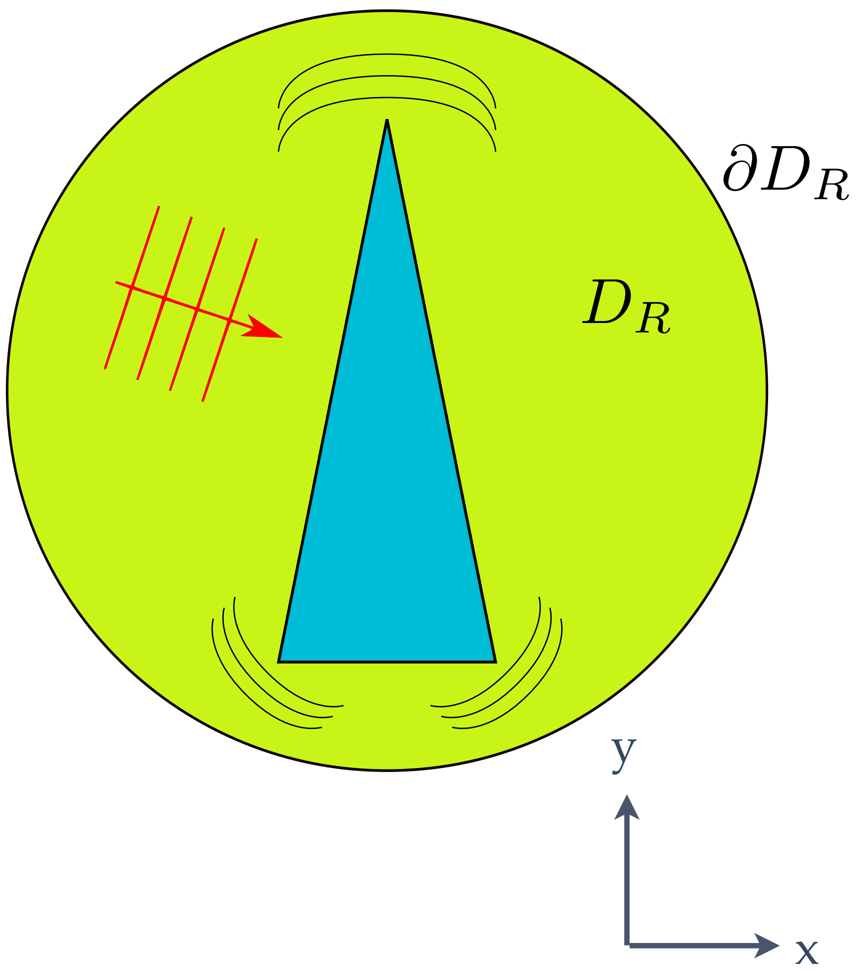


Time-harmonic equations for the TM polarization

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

$$\begin{cases} \mathrm{div}\left(\frac{1}{\varepsilon(\omega)}\nabla H_z\right) + \frac{\omega^2}{c^2}\mu H_z = 0 \text{ in } D_R \\ \partial_n H_z - ikH_z = \partial_n u^{\mathrm{inc}} - iku^{\mathrm{inc}} \text{ on } \partial D_R \end{cases}$$

- Radiation condition at finite distance



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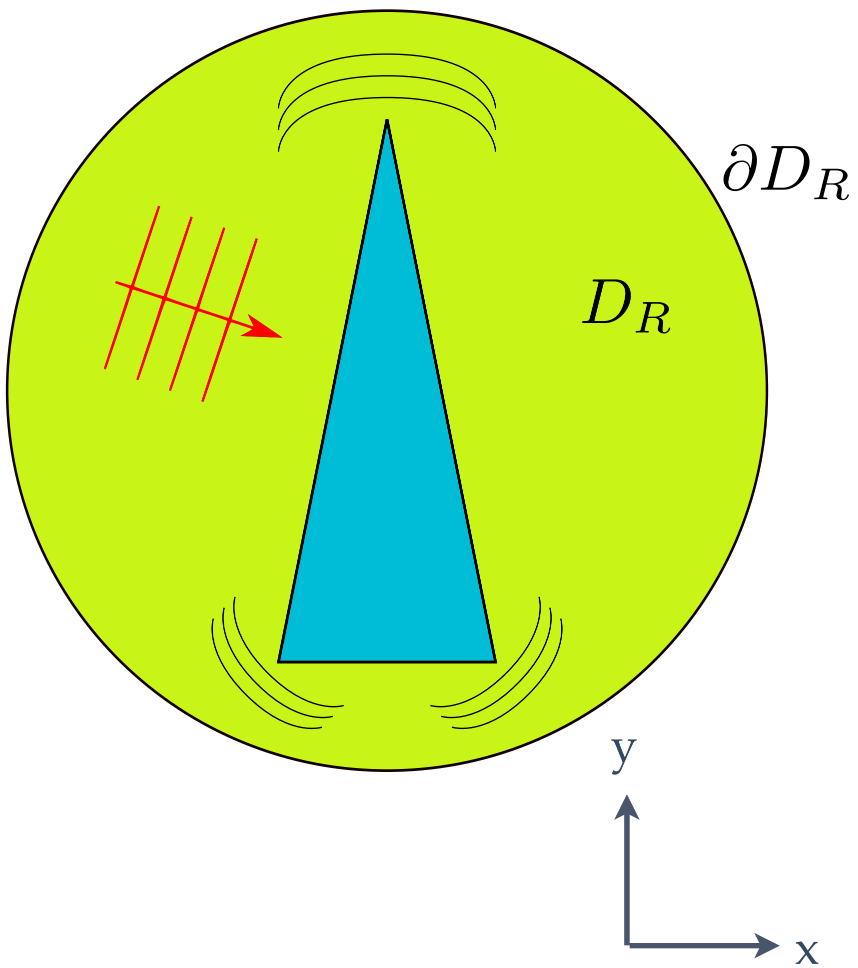

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Mathematically:
-due to the dissipation, the problem has a unique solution
(Variational formulation + Fredholm theory)
-one can approximate the solution with Finite Elements Methods

Numerical illustrations

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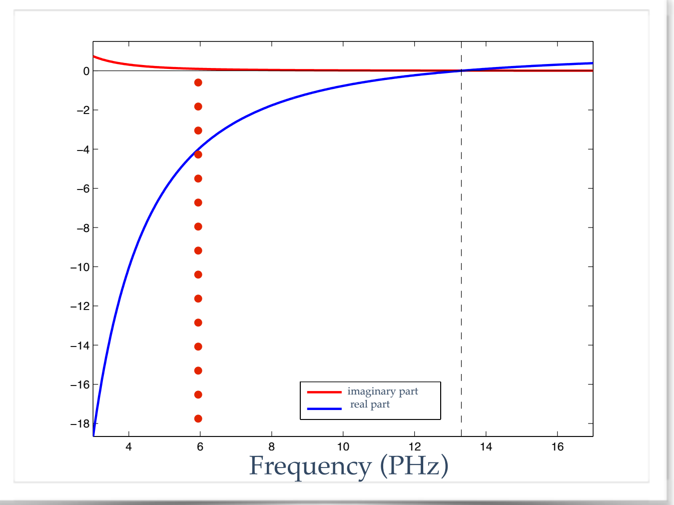
$$\varepsilon_{\mathrm{m}}(\omega) = -3.9193 + 0.0926i \qquad \varepsilon_{\mathrm{d}} = \mu_{\mathrm{d}} = \mu_{\mathrm{m}} = 1$$



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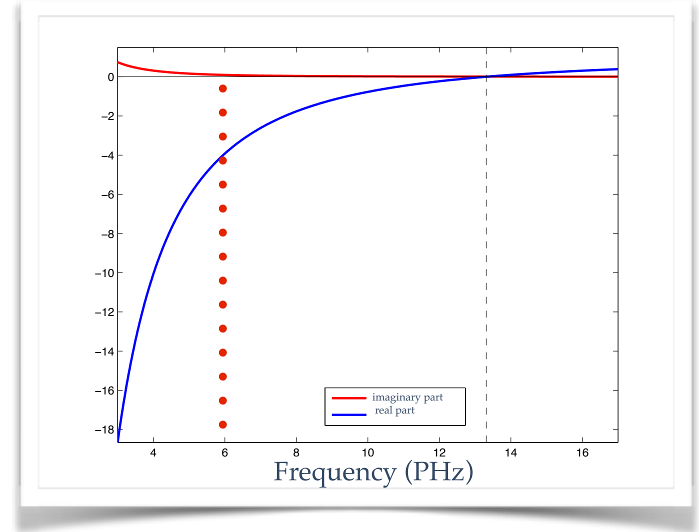

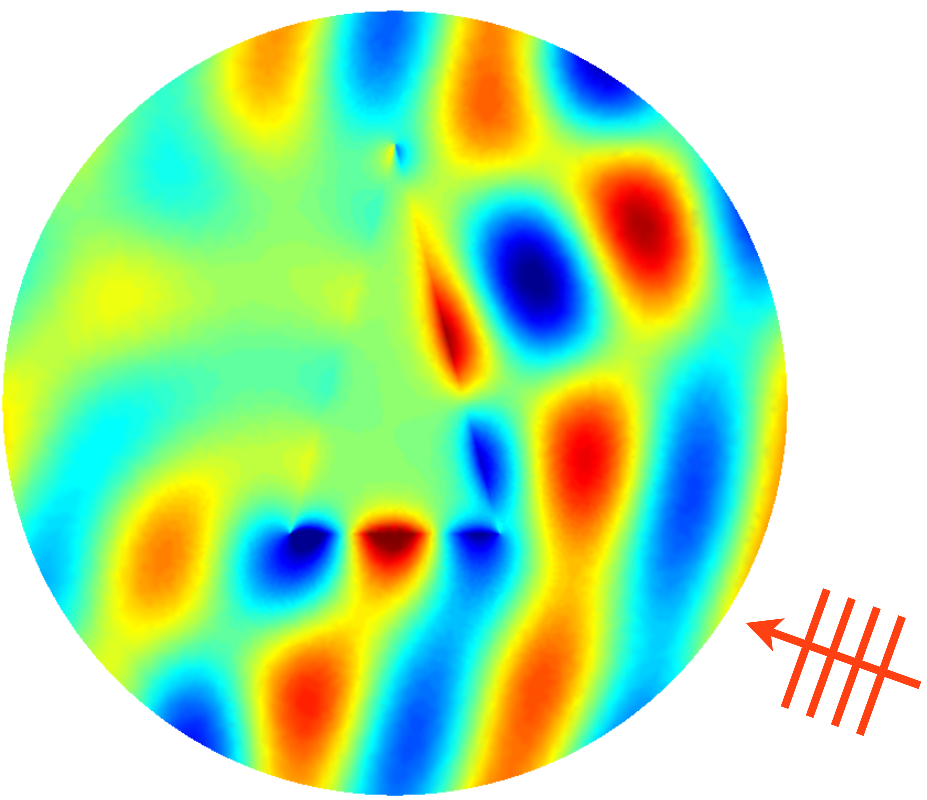

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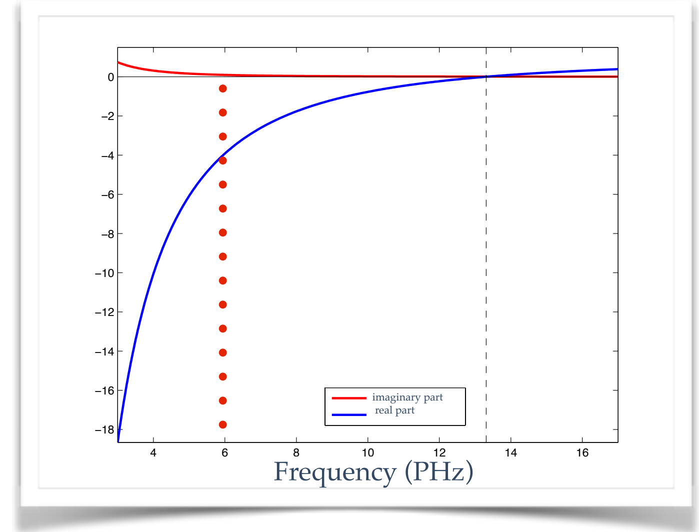

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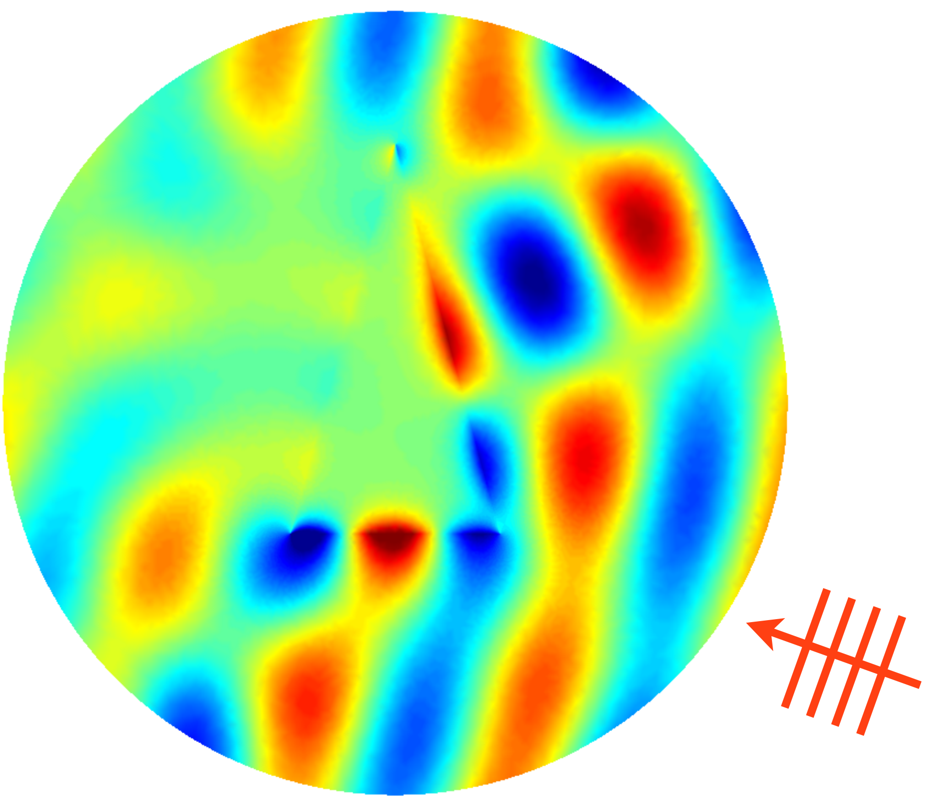

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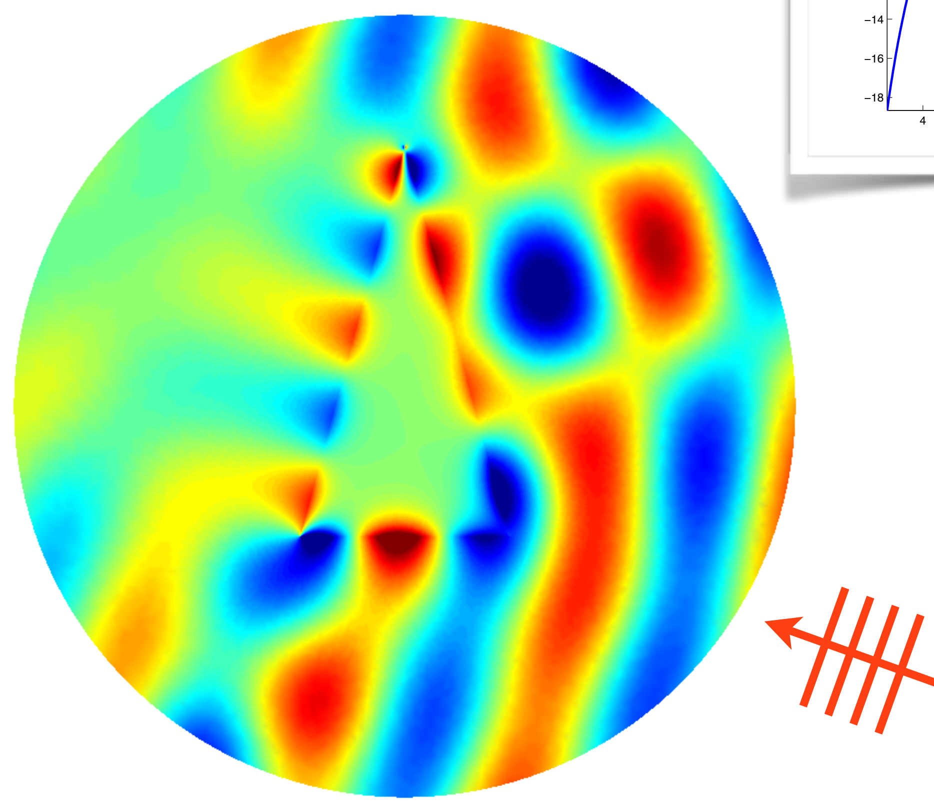

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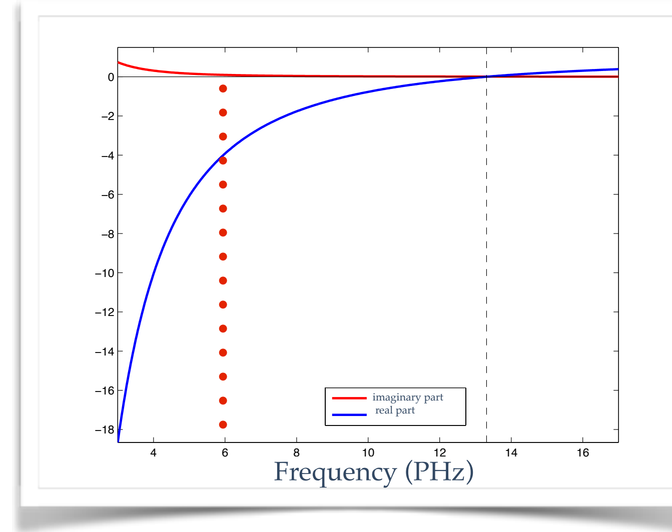

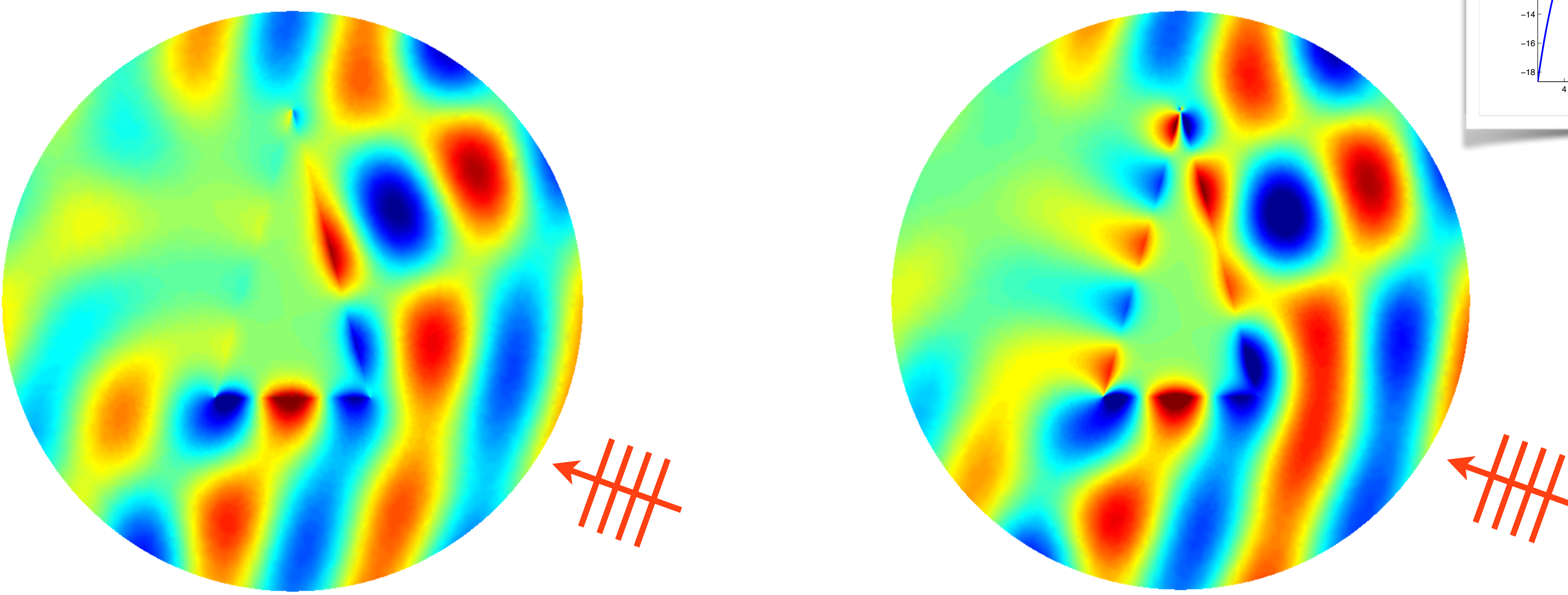

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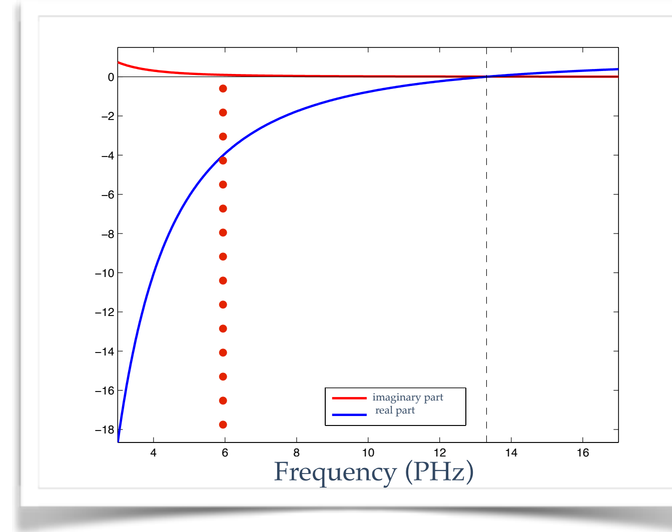

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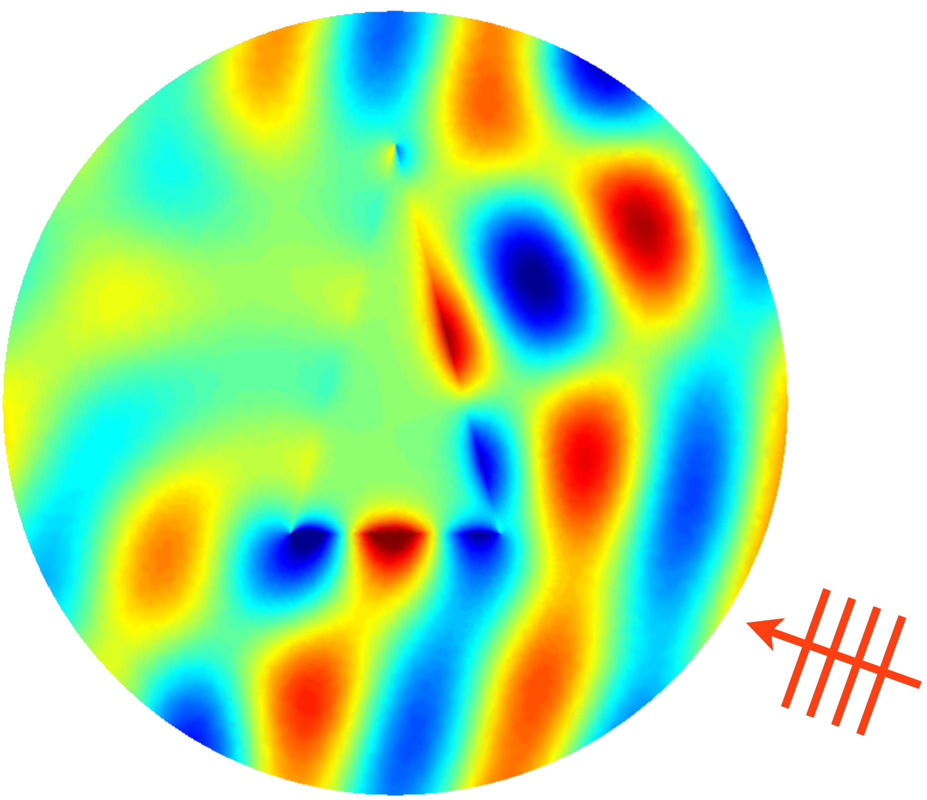

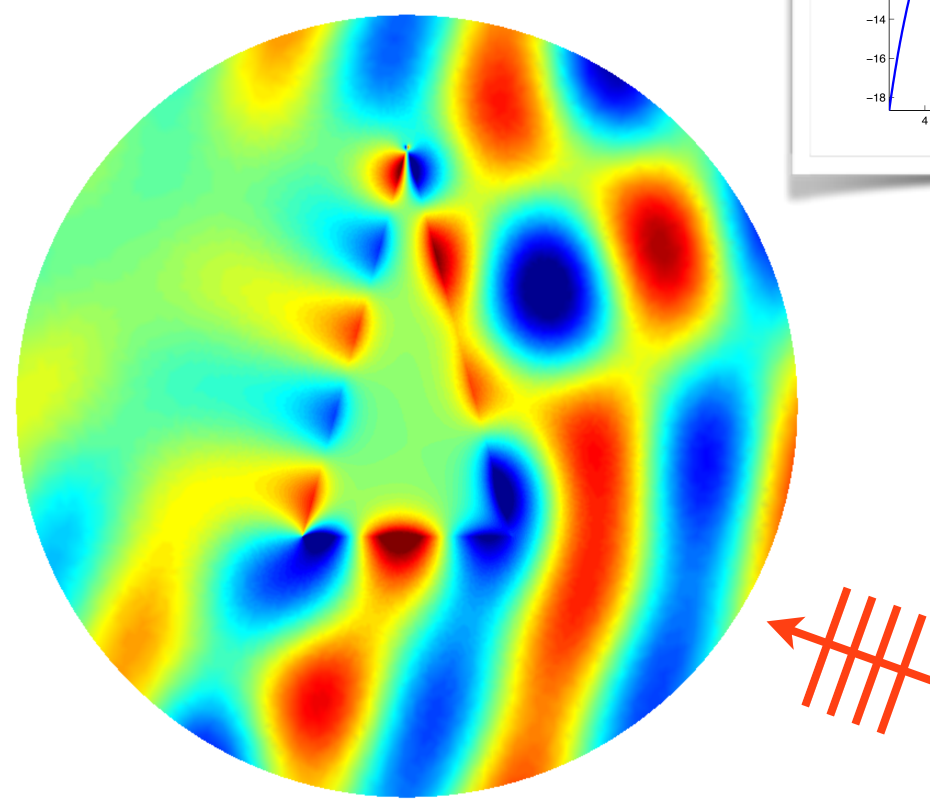

The solution is not stable ! Strong oscillations near the corners.
To understand the reasons of such instabilities and how to avoid them, we study a **limit problem by neglecting dissipation.**

Outline

- Introduction
- The limit problem
- Analysis at the corners
- Multiscale-FEM approach
- Extensions

The dissipationless Drude's model

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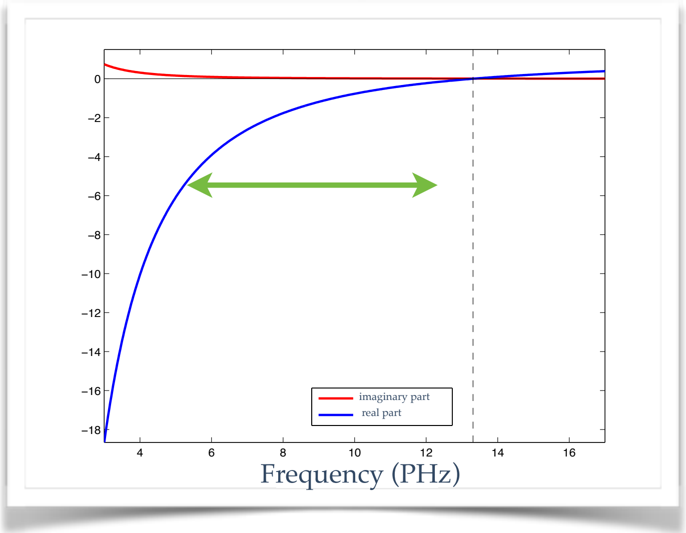

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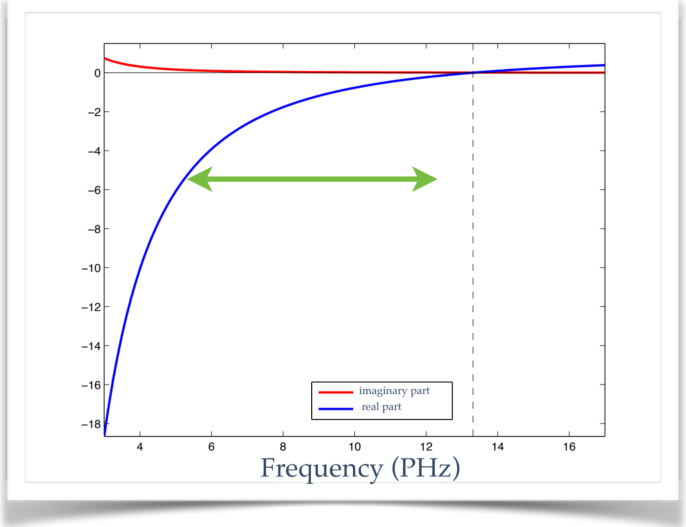

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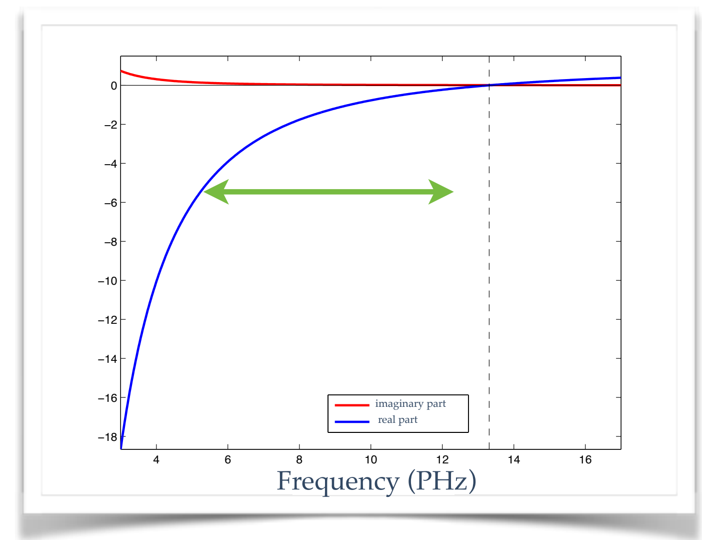

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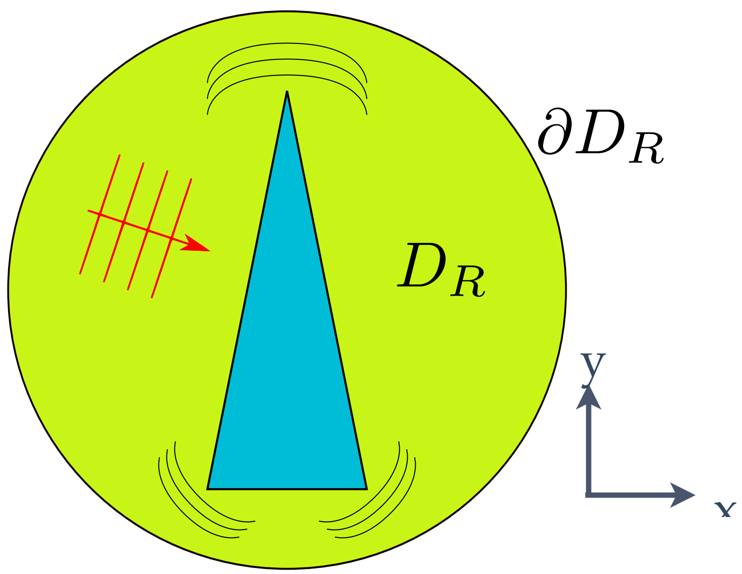

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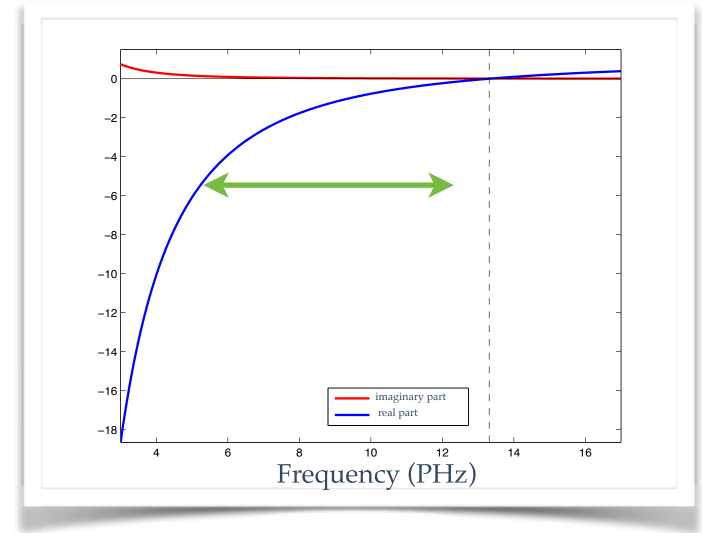

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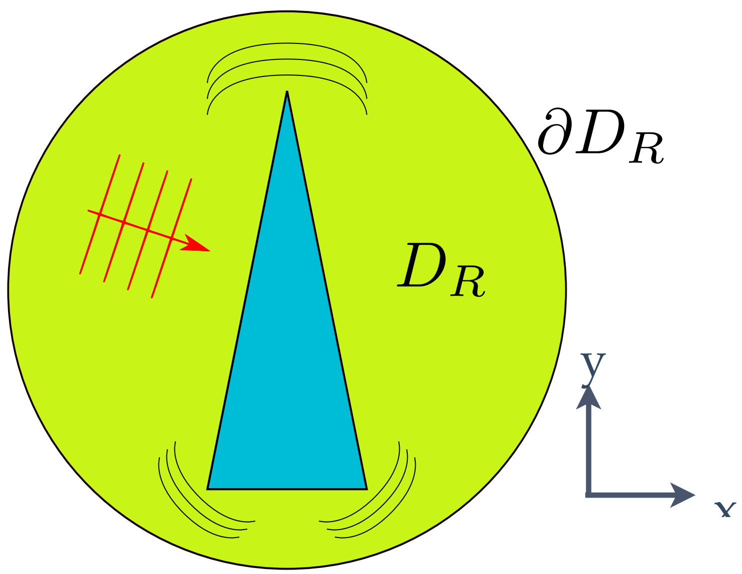

Mathematically this implies for our problem:
-difficulties to prove existence and uniqueness of the solution
-the corners of the inclusion may cause strong singular behavior
-standard approximation with Finite Elements Methods may fail

Well-posedness of the problem

Find $u := u^{\text{inc}} + u^{\text{sac}} \in H^1(D_R)$ such that: $\quad H^1(D_R) := \{u| \int_{D_R} |u|^2 + |\nabla u|^2 \, d\mathbf{x} < +\infty\}$

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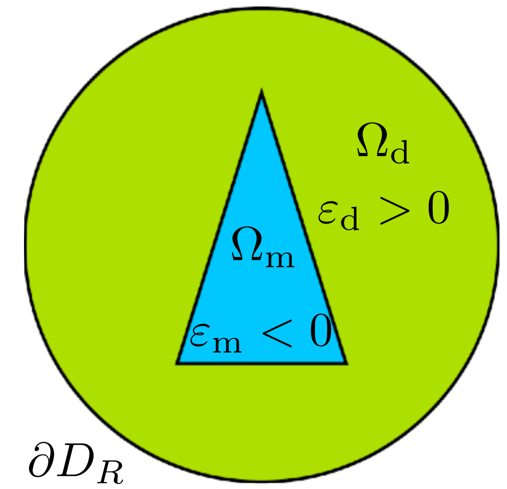

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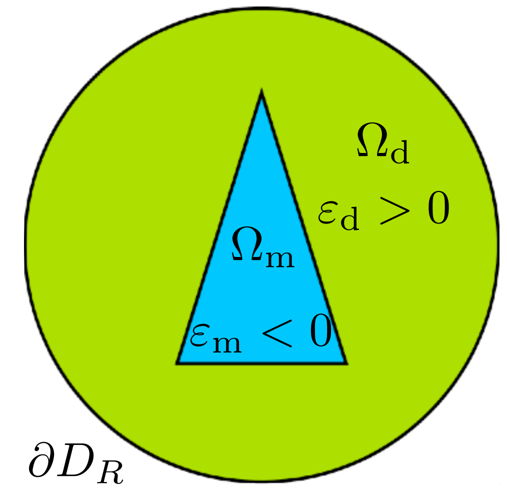

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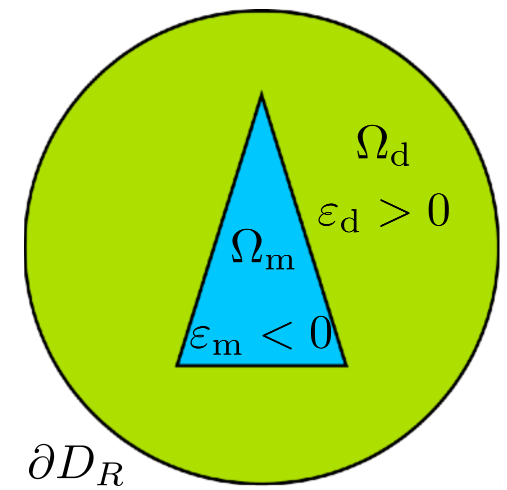

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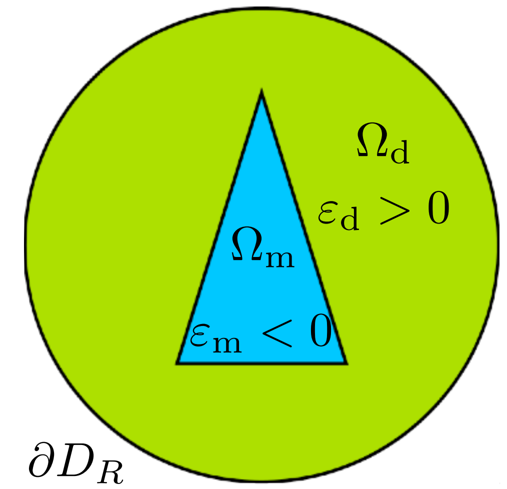

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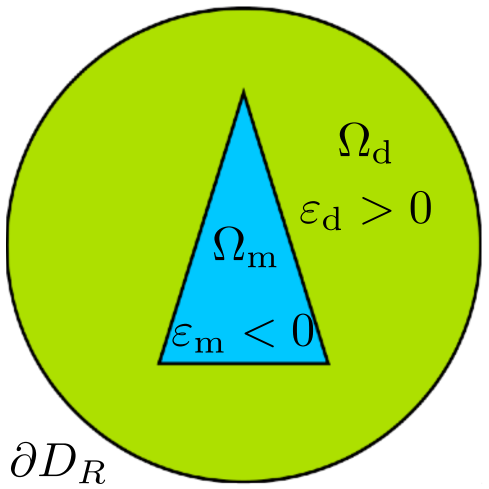
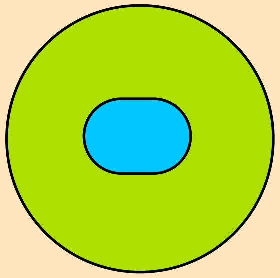


Thanks to the T-coercivity theory, one can prove well-posedness under some conditions on ε and the geometry.

Idea: build ad hoc isomorphisms to compensate the change of sign.

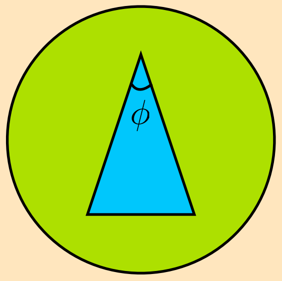
In our case: YES if and only if $\kappa_\varepsilon := \dfrac{\varepsilon_\text{m}}{\varepsilon_\text{d}} \notin I_c$ $\quad I_c$ is called critical interval.

If the interface is smooth:



$I_c = \{-1\}$

If the interface has corners:



$I_c = \left[\frac{\phi - 2\pi}{\phi}; \frac{\phi}{\phi - 2\pi}\right]$

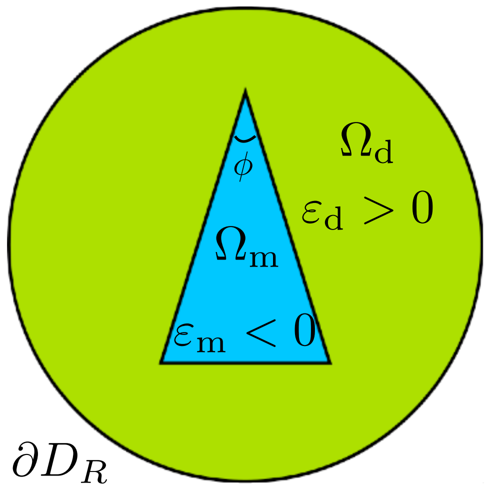
$\phi \to 0, \; I_c \to \mathbb{R}^-$

$\phi \to \pi, \; I_c \to \{-1\}$

Bonnet-Ben Dhia, Ciarlet, Zwölf (2010), Bonnet-Ben Dhia, Chesnel, Ciarlet (2012).

Critical interval and critical frequencies

$$I_c = \left[\frac{\phi - 2\pi}{\phi}; \frac{\phi}{\phi - 2\pi}\right]$$



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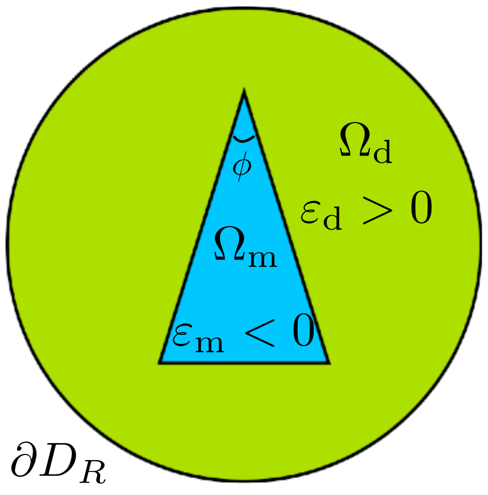

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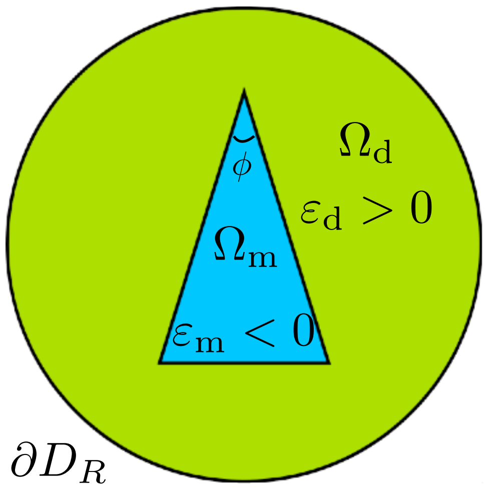

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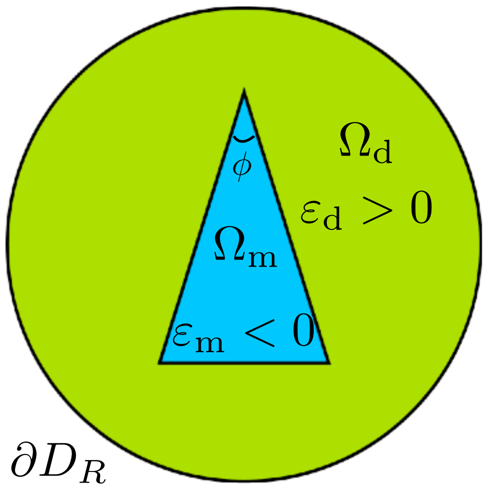

$$\kappa_\varepsilon = -1 \Longleftrightarrow \omega = \omega_{sp} := \frac{\omega_p}{\sqrt{1 + \varepsilon_\mathrm{d}}}$$ Surface plasmons frequency

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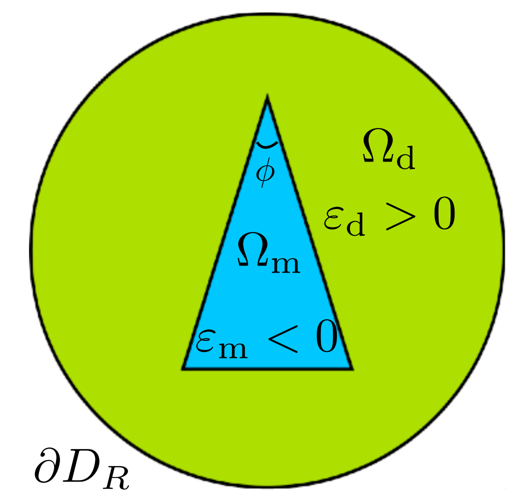

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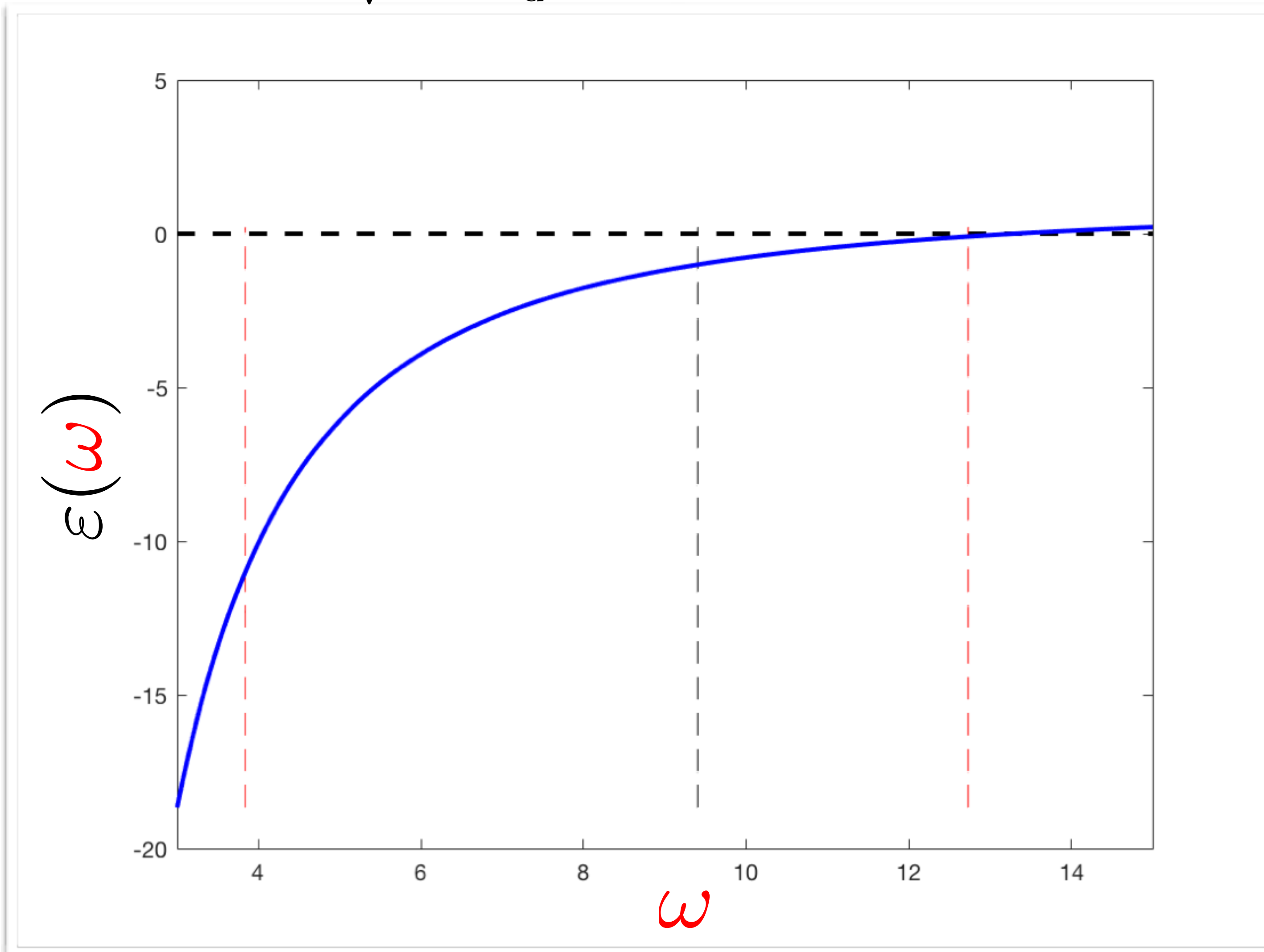

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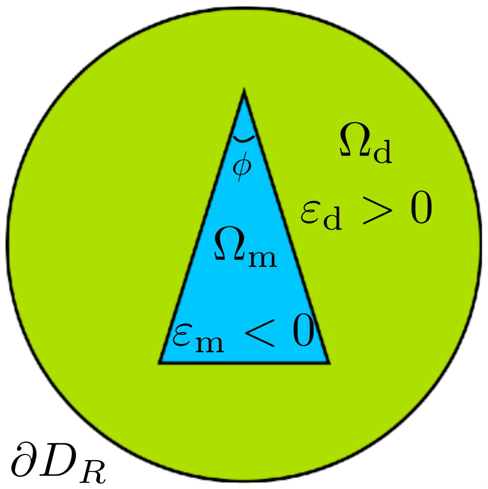

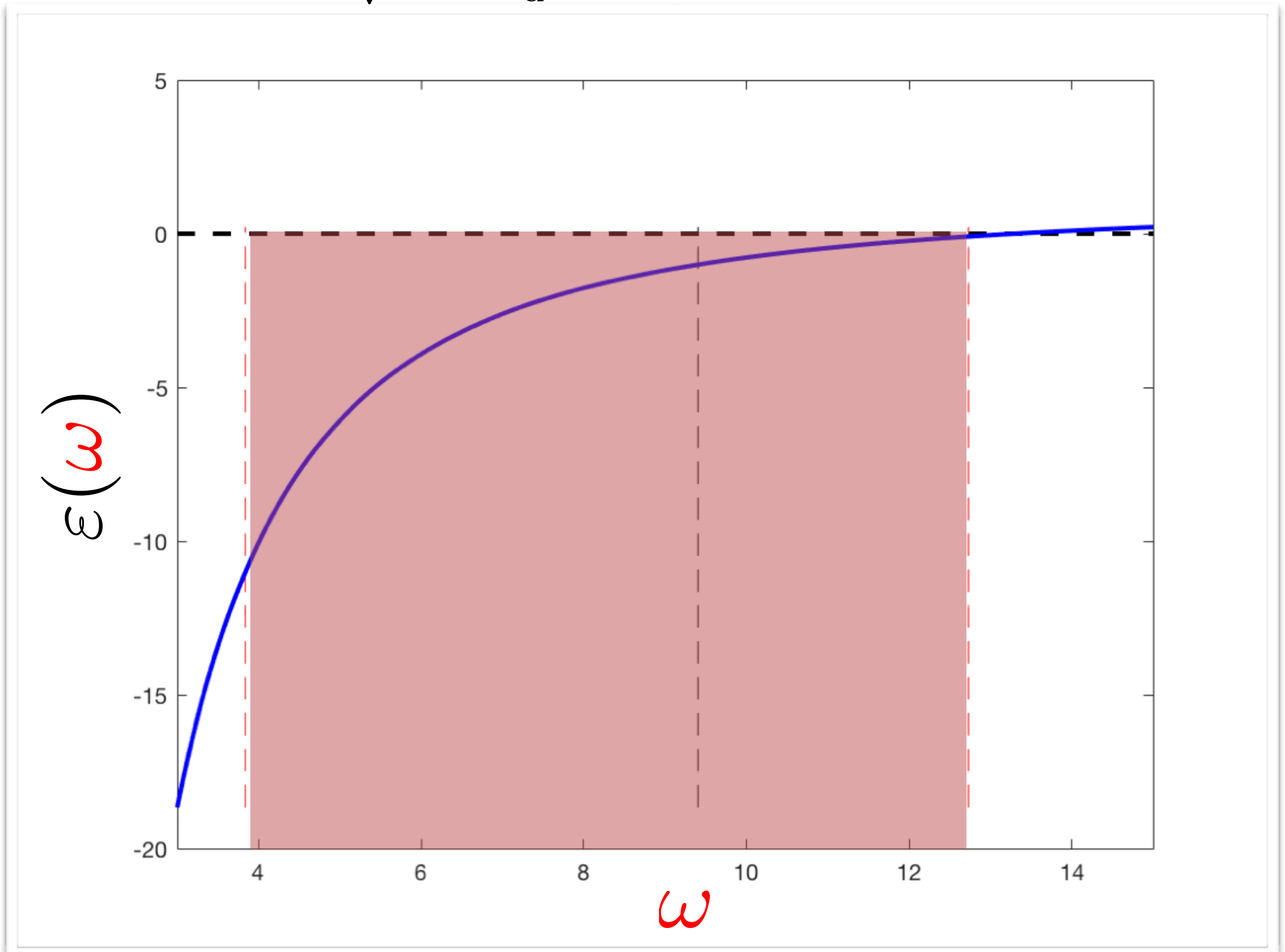

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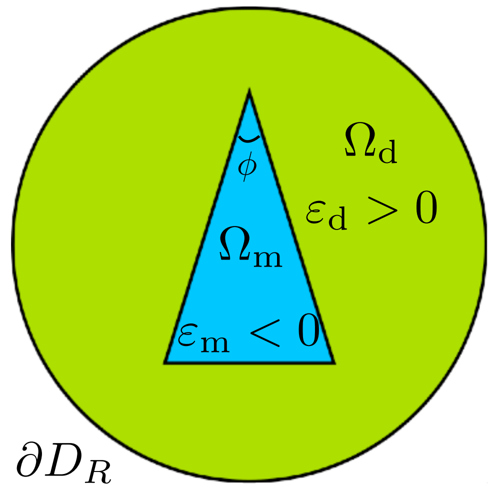

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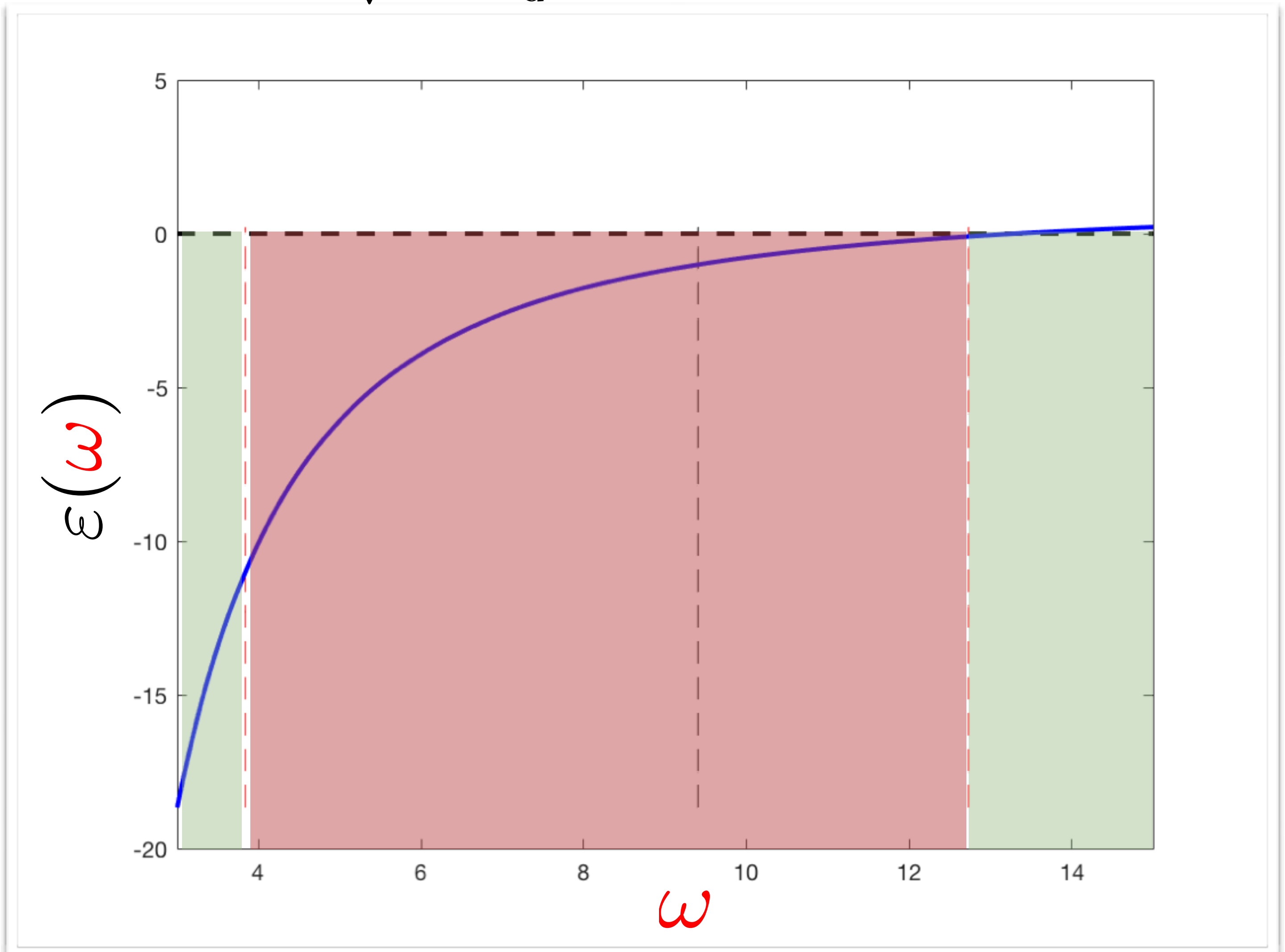
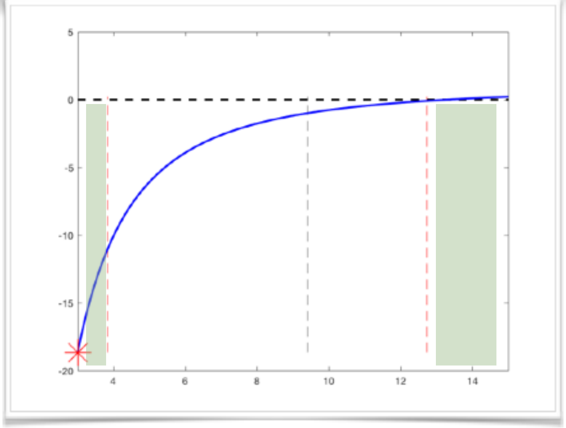


Two configurations (1)

Outside I_c (YES)

The scattering problem has a unique solution $u \in H^1(D_R)$

Finite Elements converge (under some condition on the mesh): design symmetric meshes near the interface to ensure optimal FE convergence



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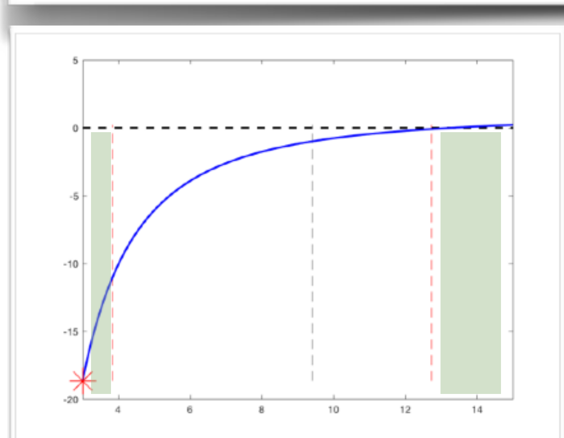

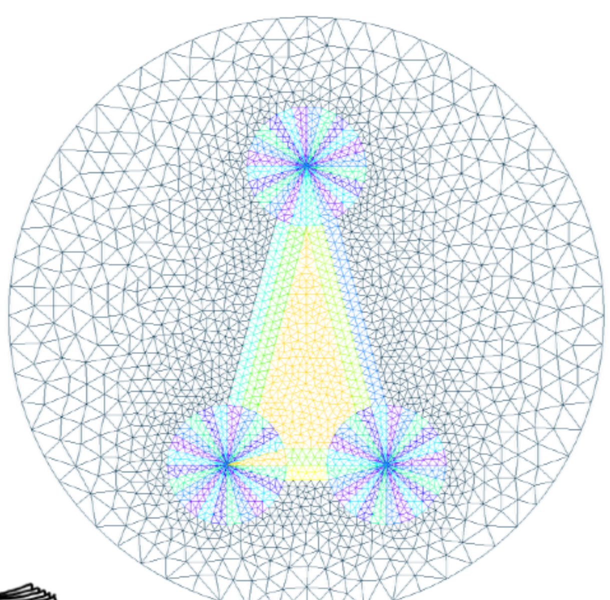

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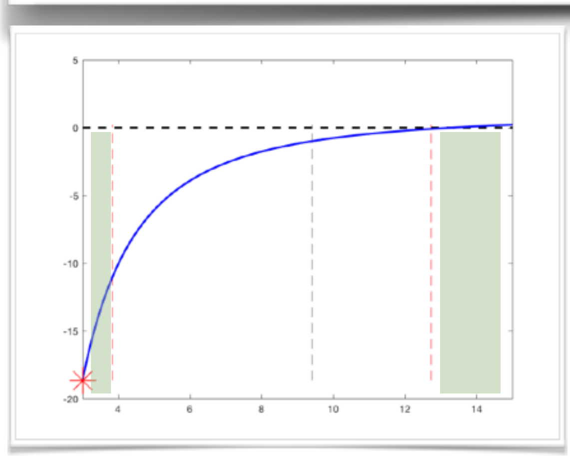
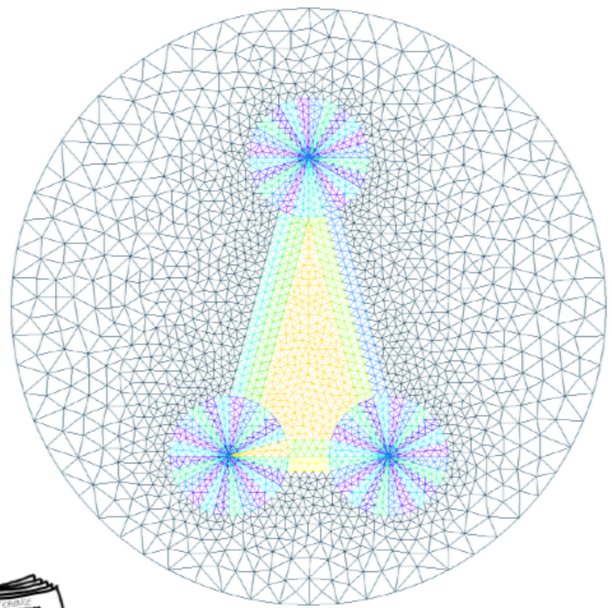


For silver: $\kappa_\varepsilon \in I_c \iff \omega \in [3.839 \text{ PHz}; 12.733 \text{ PHz}]$.

Results for $\omega = 3.7$ PHz



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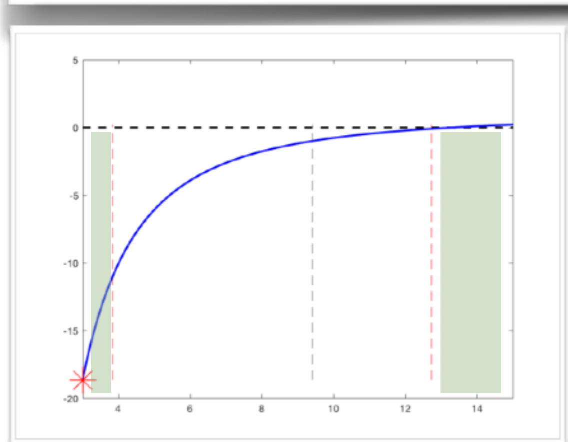

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Standard Meshes

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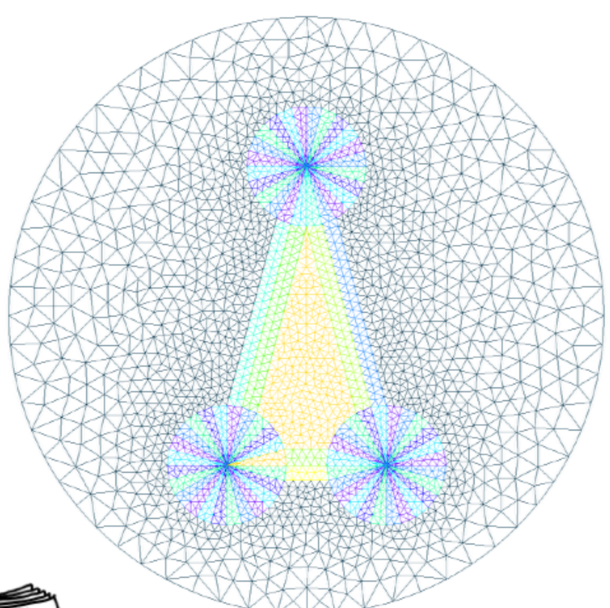

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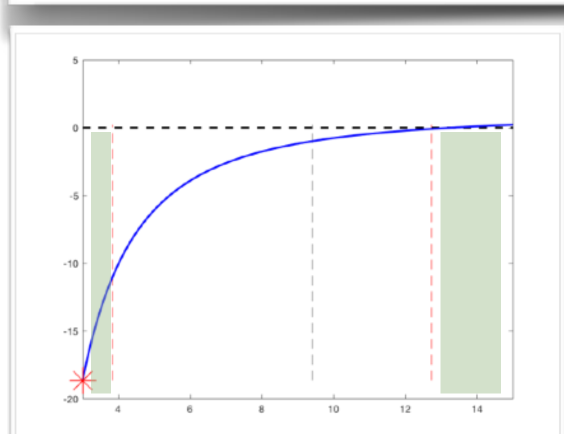

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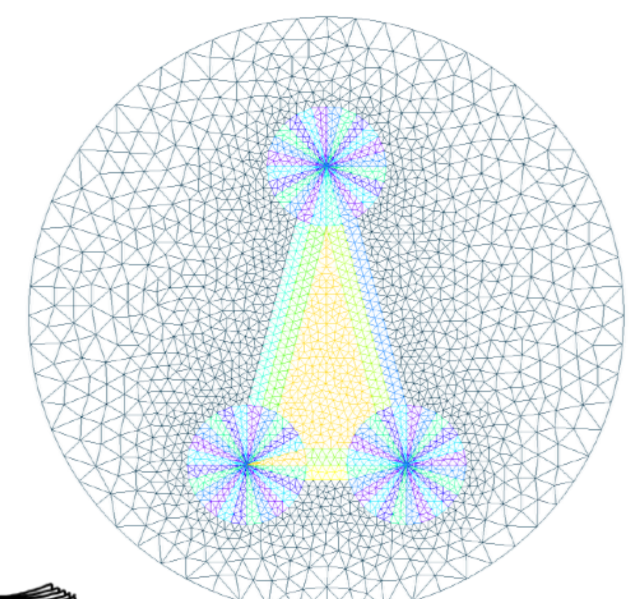

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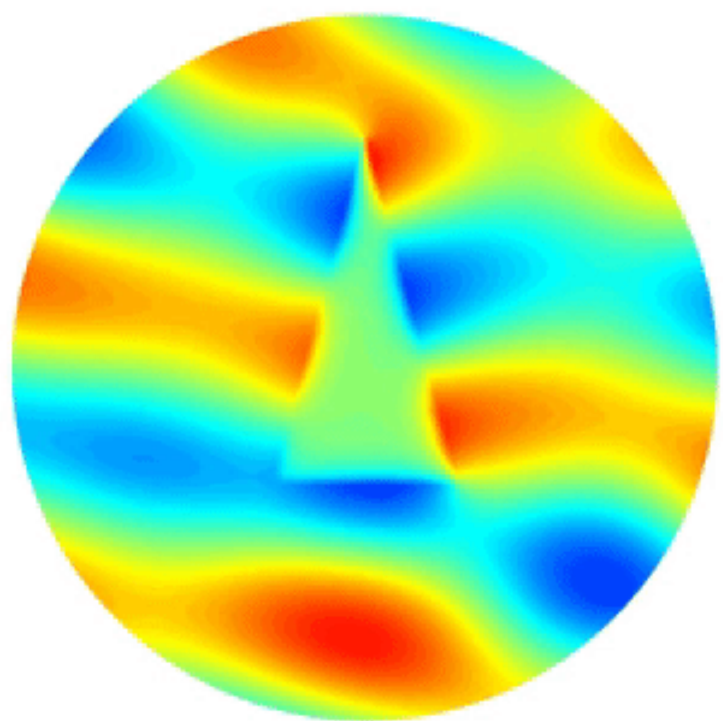

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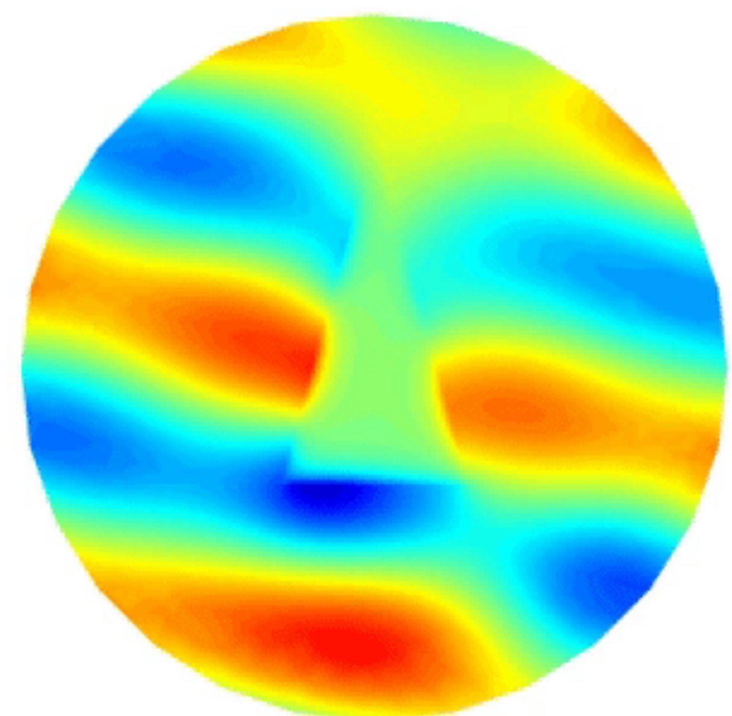

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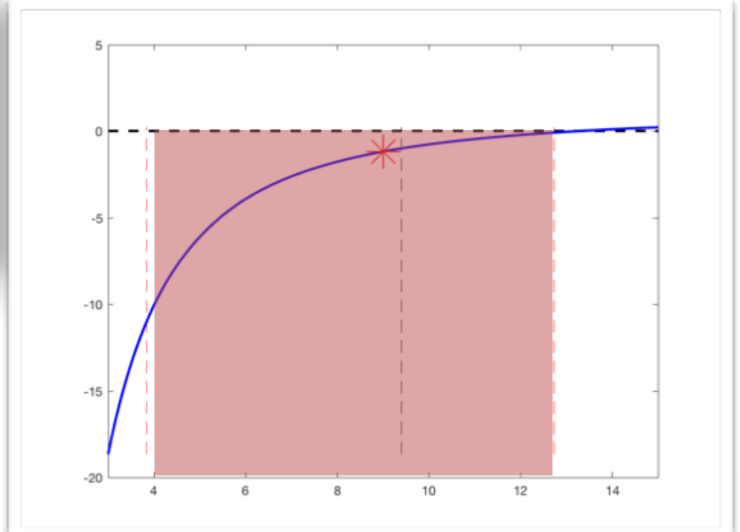
Inside I_c (NO)	The scattering problem is ill-posed in $H^1(D_R)$ No FEM convergence



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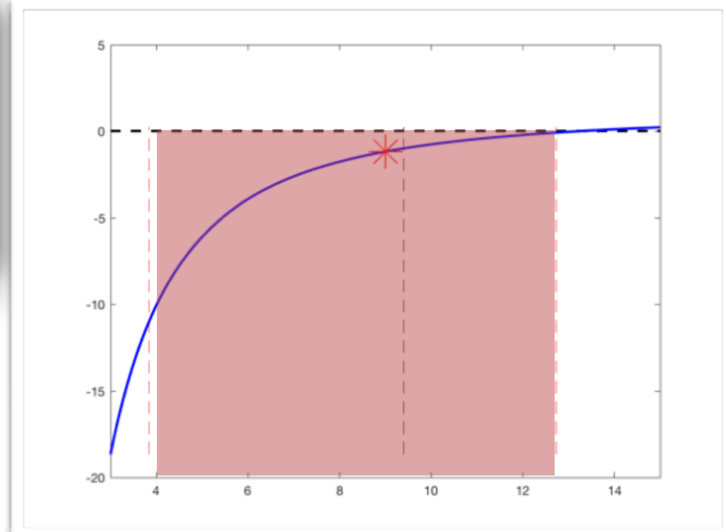

Numerical results for triangular silver inclusion in vacuum for $\kappa_\varepsilon \in I_c$

$$\kappa_\varepsilon \in I_c \iff \omega \in [3.839 \text{ PHz}; 12.733 \text{ PHz}].$$

Results for $\omega = 9$ PHz.

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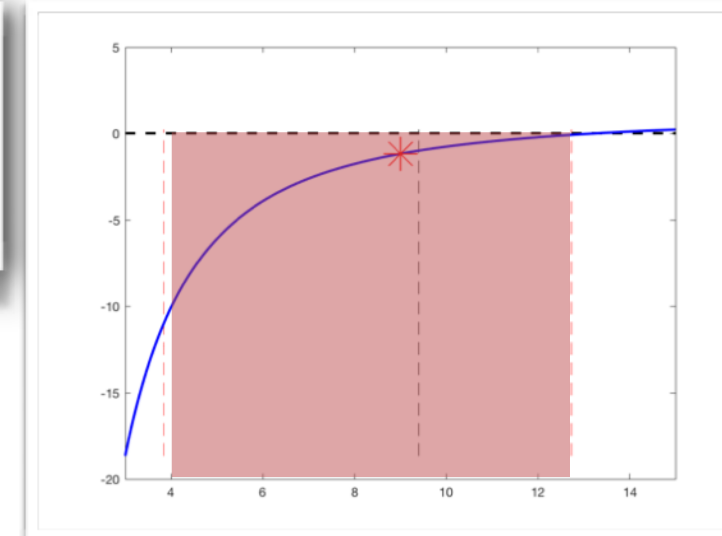

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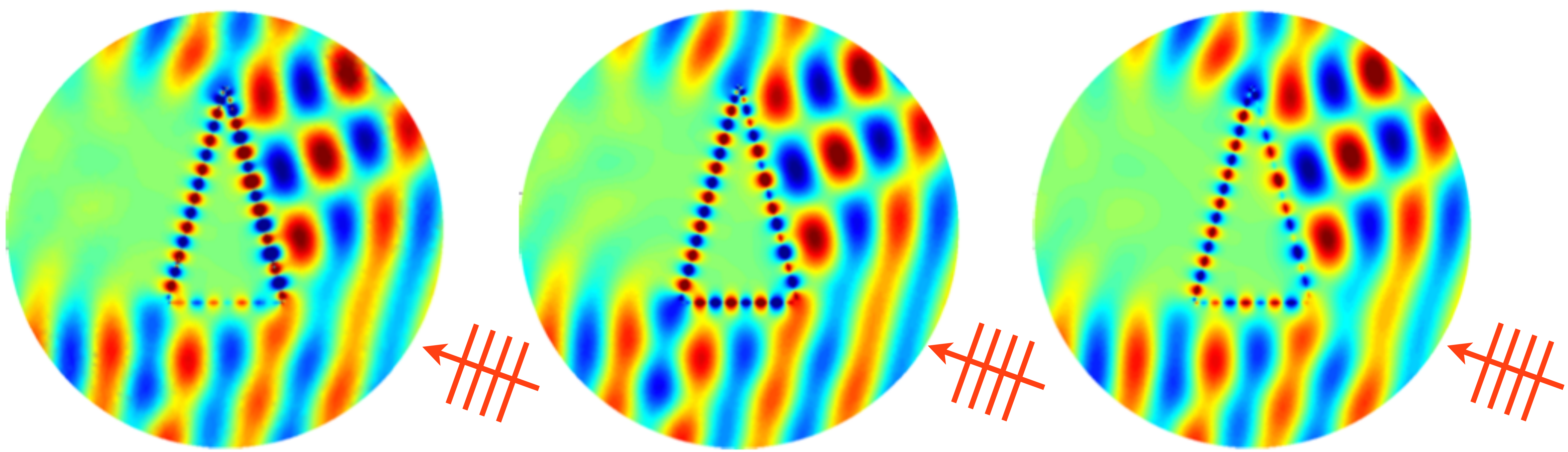

coarse mesh intermediate mesh refined mesh

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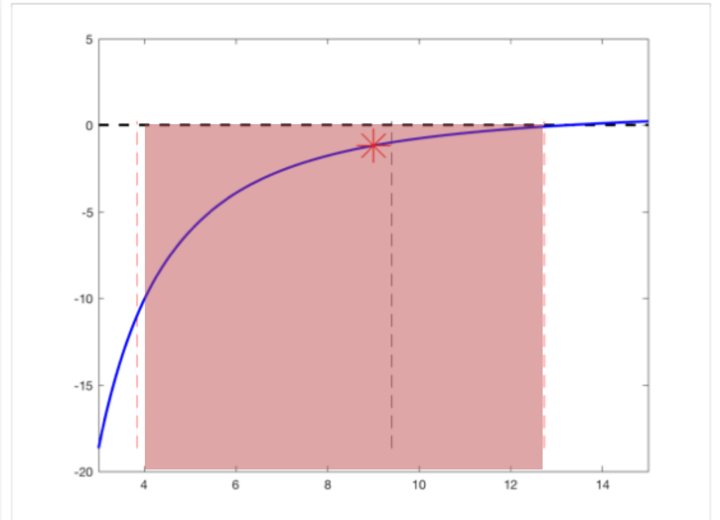

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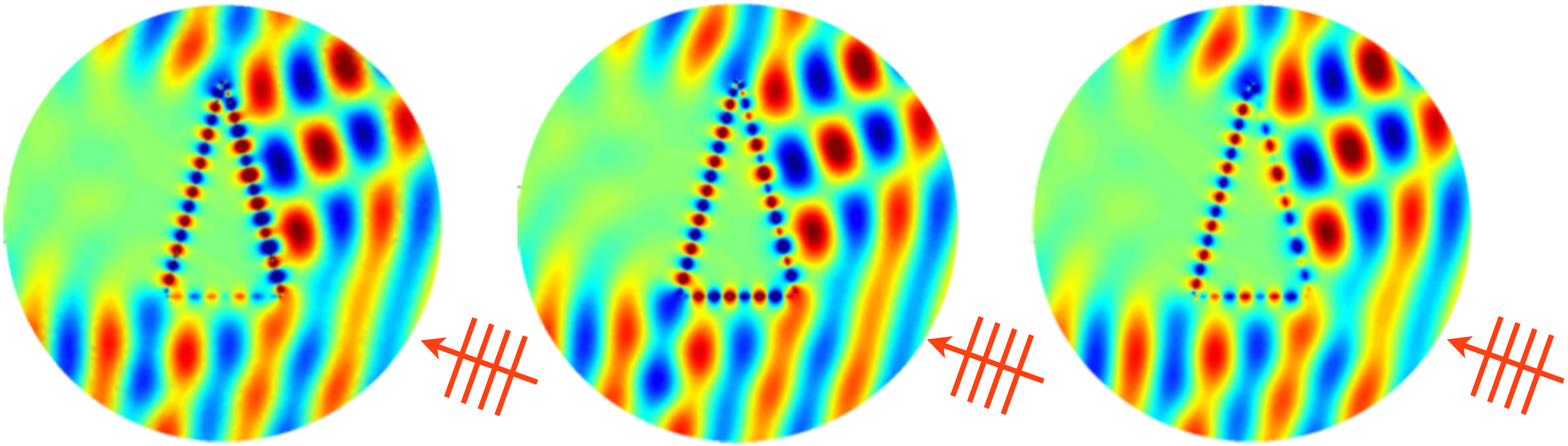


coarse mesh intermediate mesh refined mesh

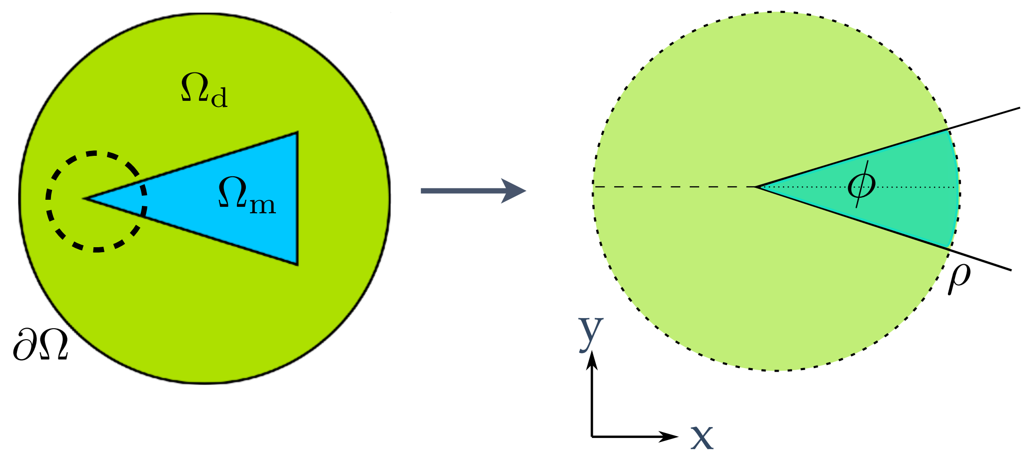
Singular behavior to near the corners to understand

Outline

- Introduction
- The limit problem
- Analysis at the corners
- Multiscale-FEM approach
- Extensions

Analysis and scaling at the corners

For simplicity, we consider only one corner.



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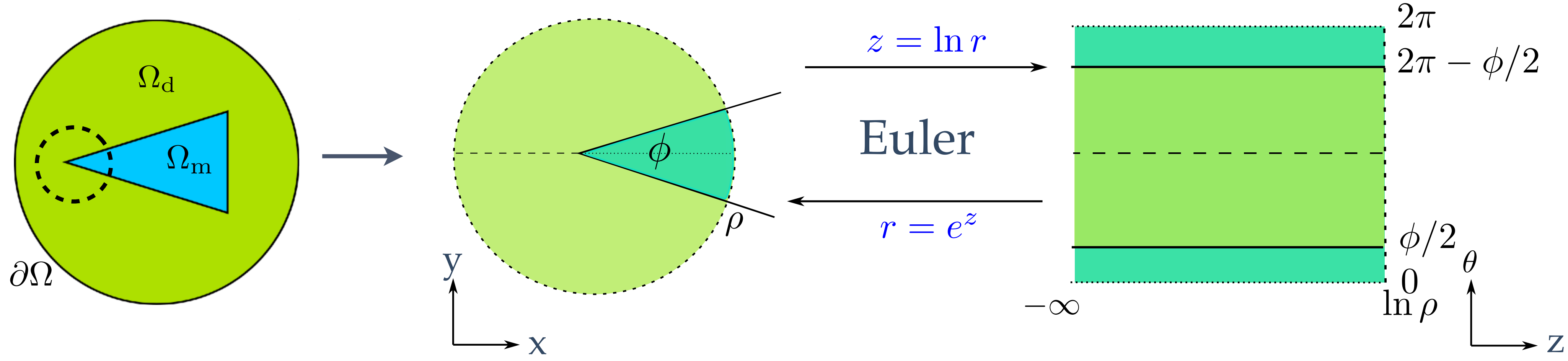

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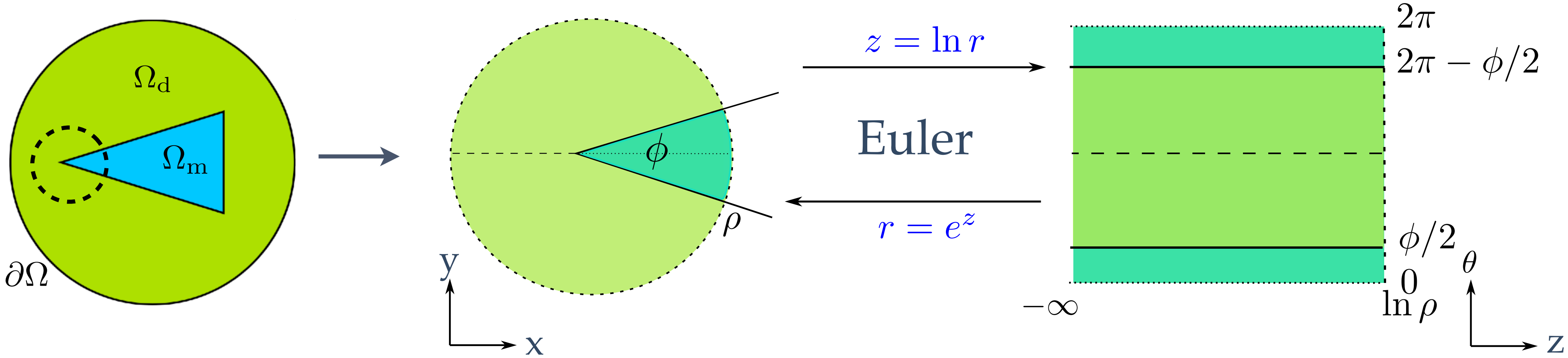

Limit behaviour at the corner

Behaviour at infinity in the strip

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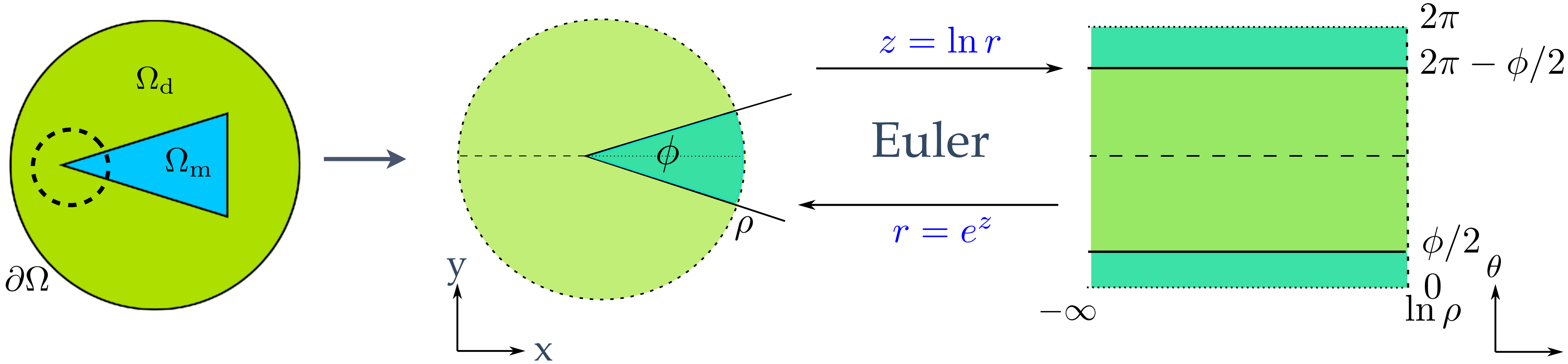

Limit behaviour at the corner

$$-\varepsilon^{-1} r\partial_r(r\partial_r u) - \partial_\theta\left(\varepsilon^{-1}\partial_\theta u\right) + \omega^2 \mu r^2 u = 0$$

Behaviour at infinity in the strip

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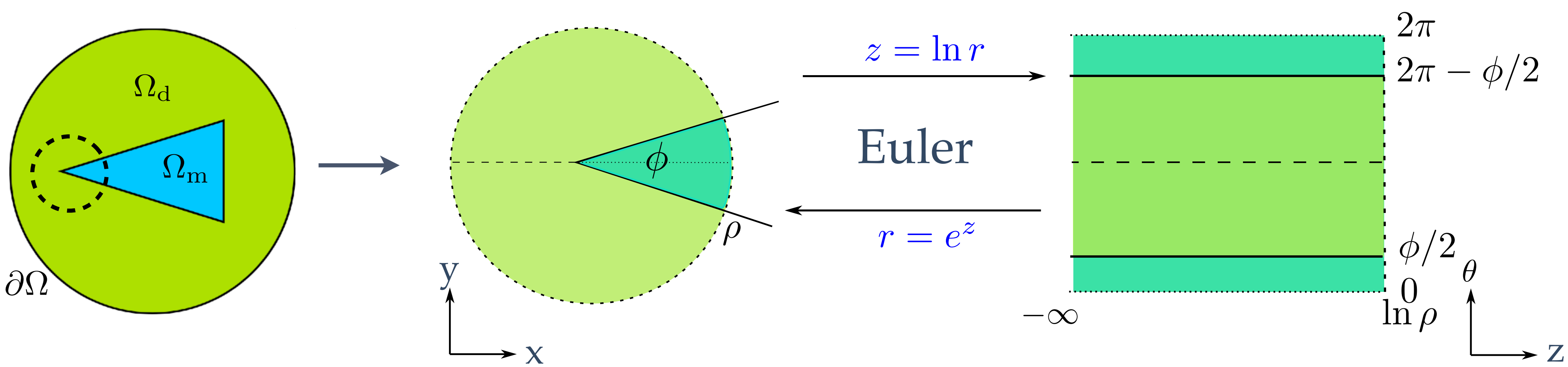

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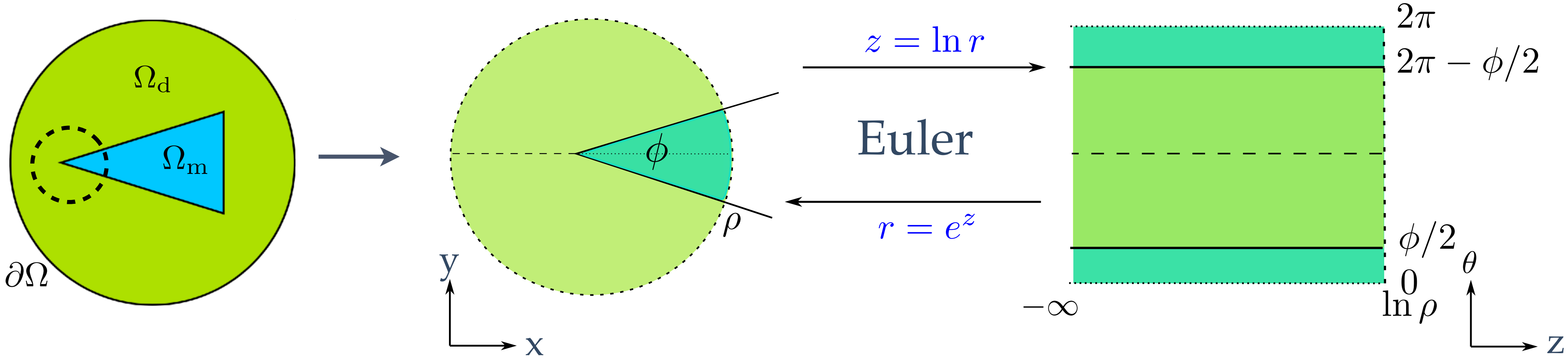

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λ are called singular exponents.

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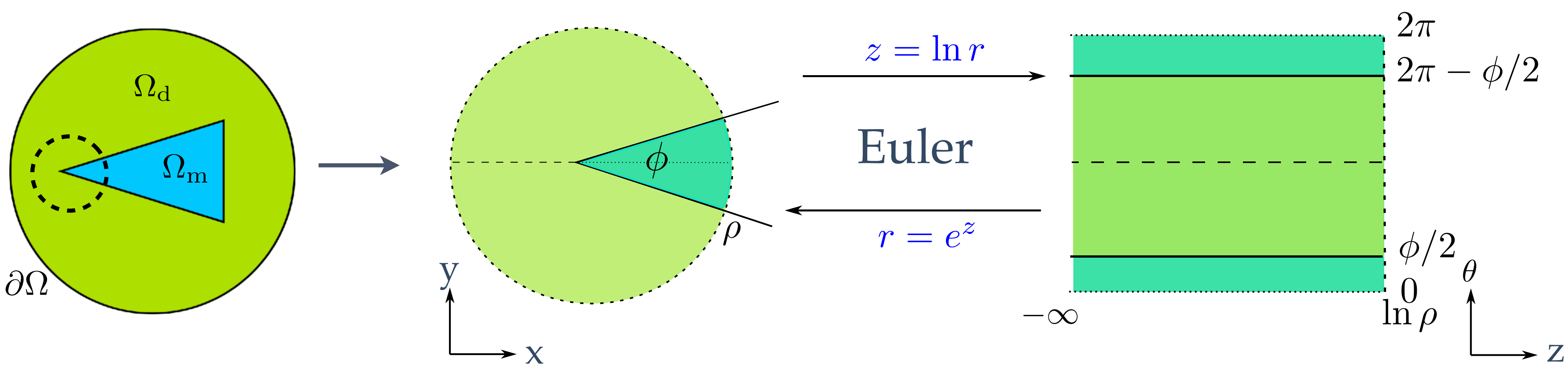

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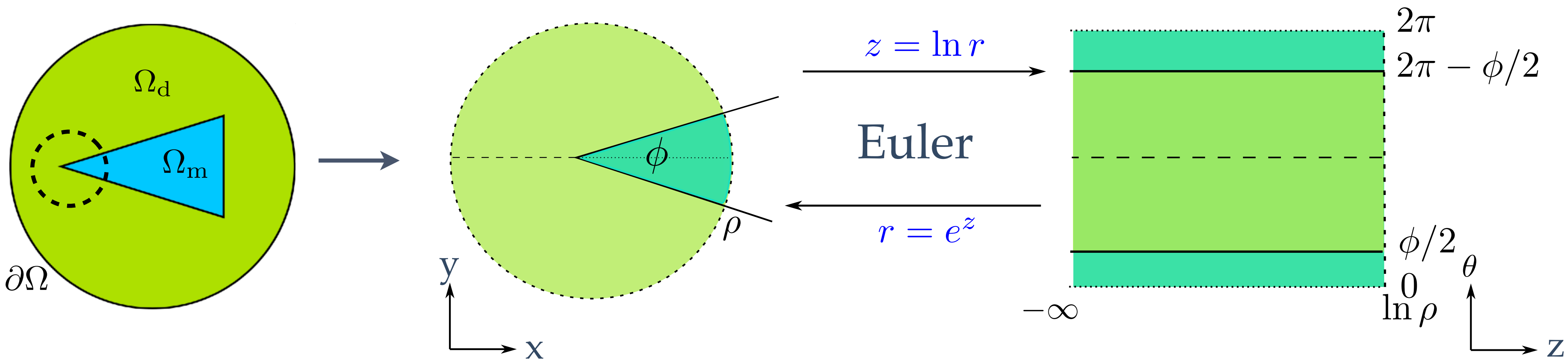

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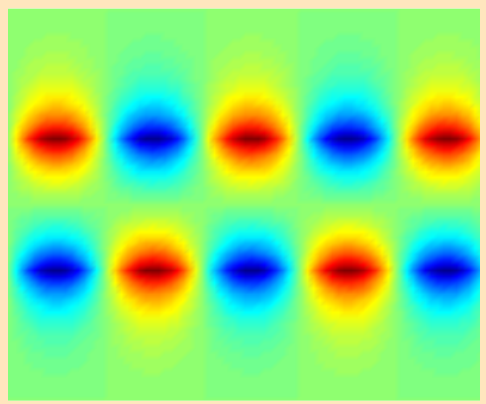
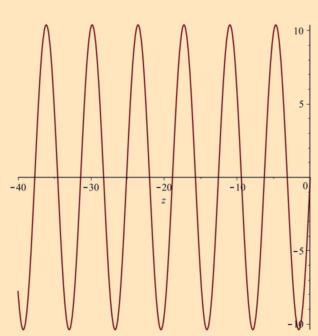
$\kappa_\varepsilon \in I_c$ appearance of a propagative mode

$$s(z,\theta) = e^{i\eta z}\phi(\theta) \notin H^1$$





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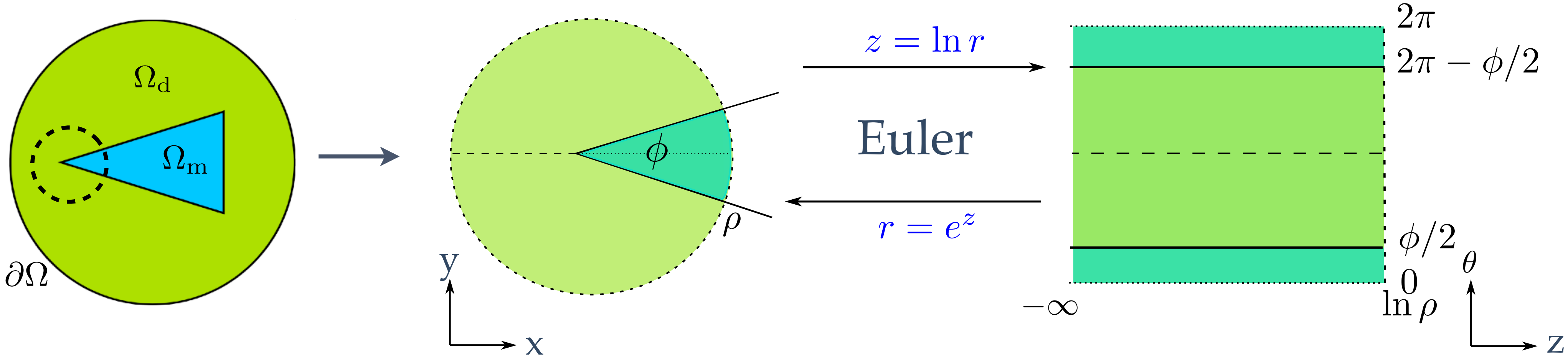

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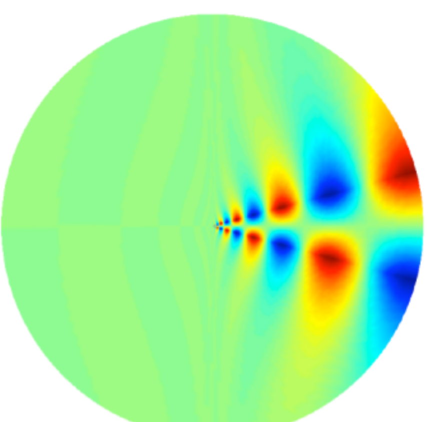
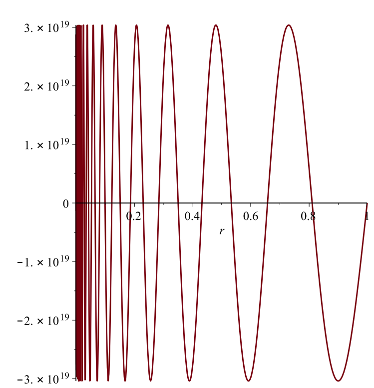
Appearance of an oscillating hypersingularity $s(r,\theta) = e^{i\eta \ln r}\phi(\theta) \notin H^1$





Black-hole wave.

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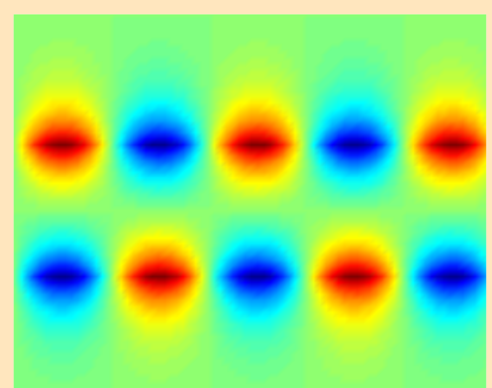
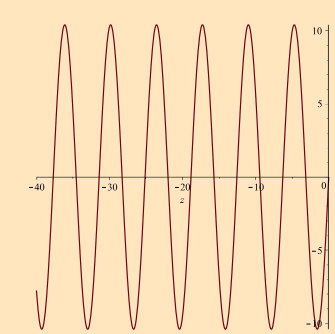
$\boxed{\kappa_\varepsilon \in I_c}$ appearance of a propagative mode $s(z,\theta) = e^{i\eta z}\phi(\theta) \notin H^1$





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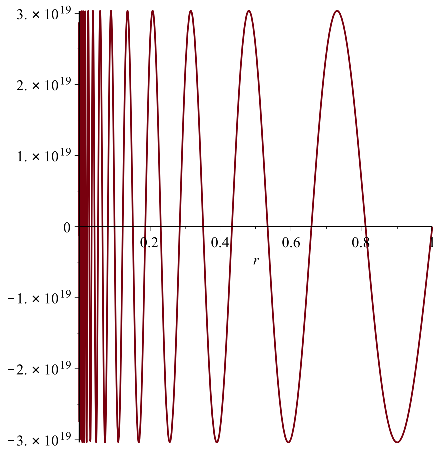

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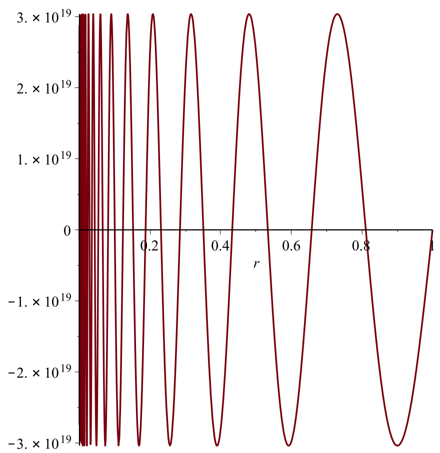

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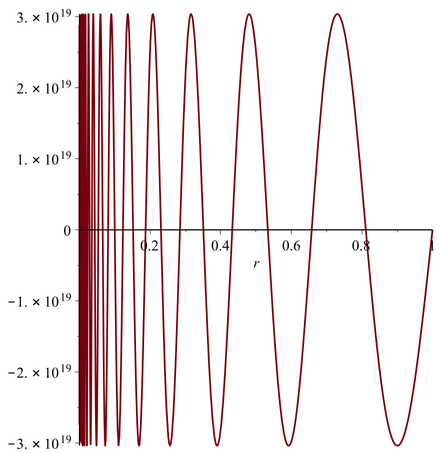

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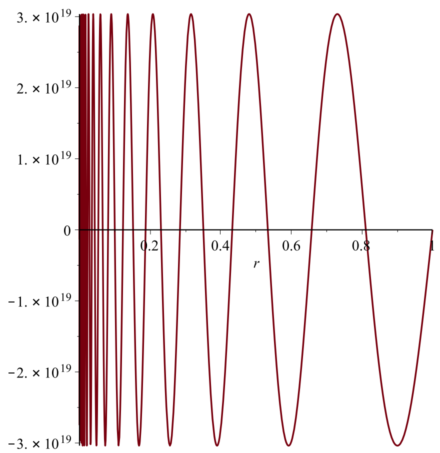

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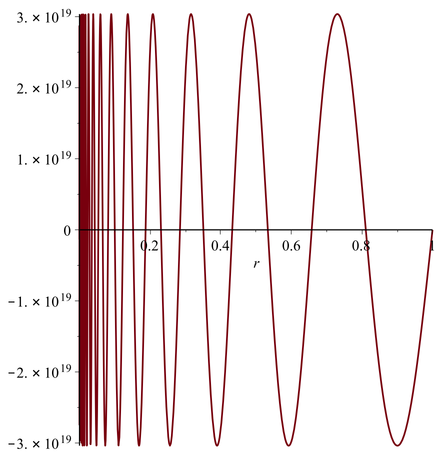

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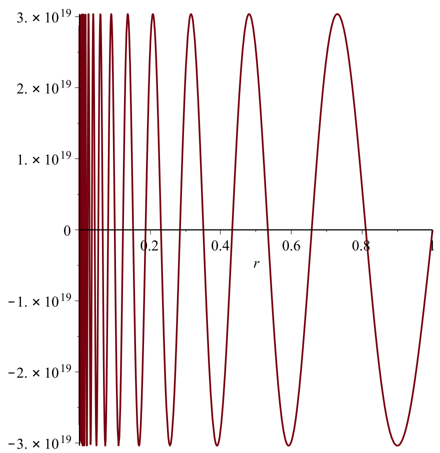

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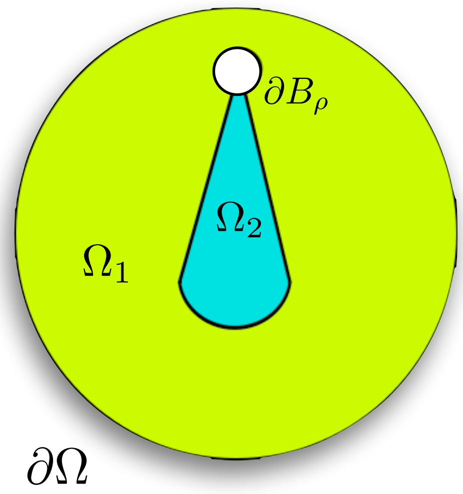

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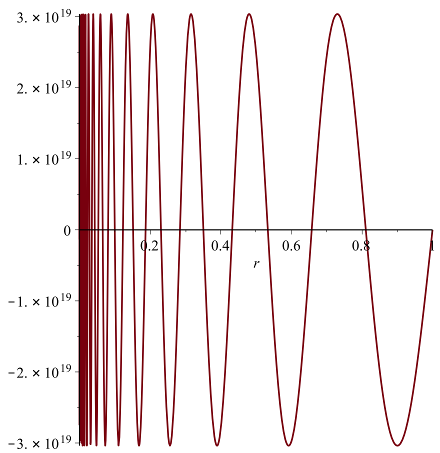

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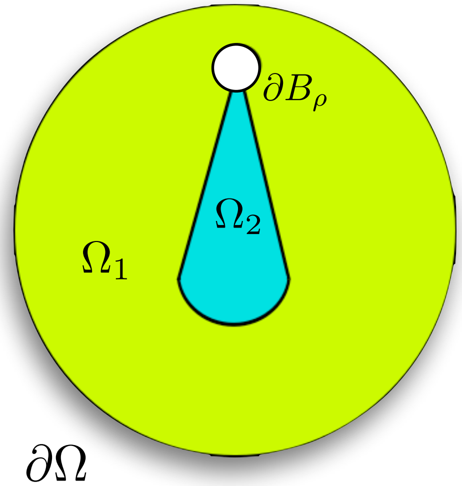

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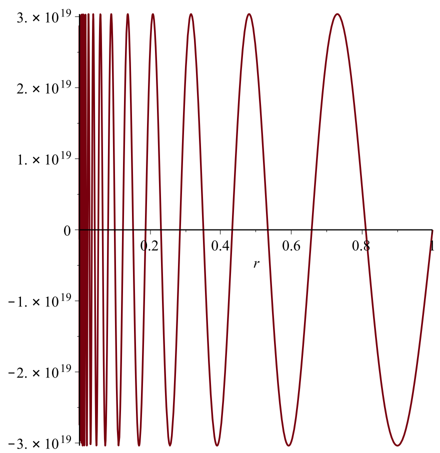

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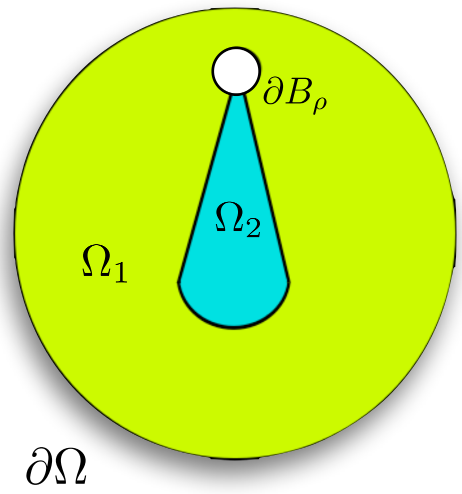

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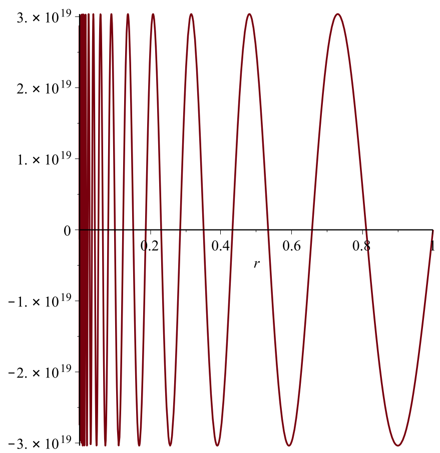

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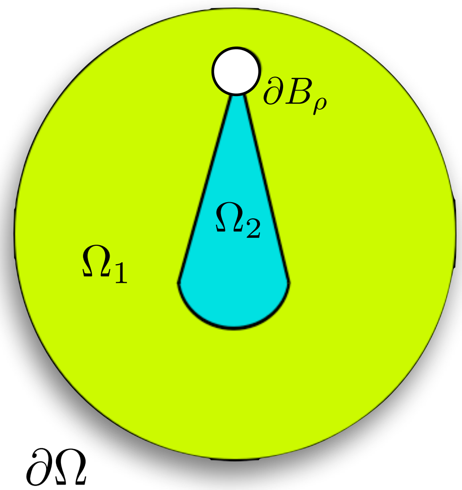

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How to proceed numerically to select the good singularity ?

Outline

- Introduction
- The limit problem
- Analysis at the corners
- Multiscale-FEM approach
- Extensions

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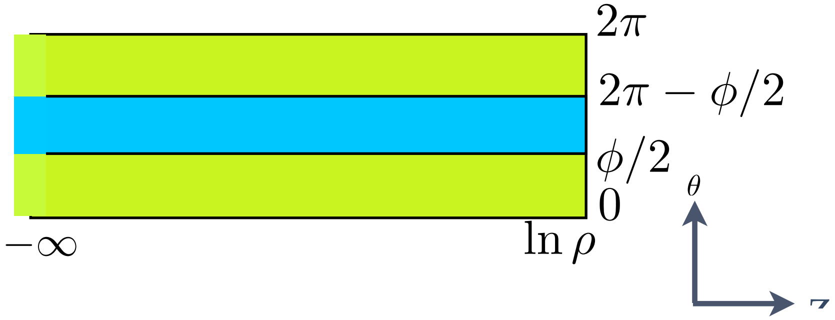

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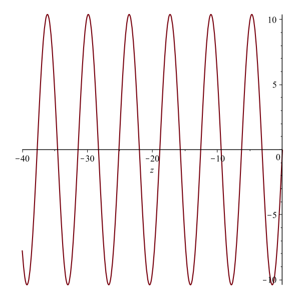

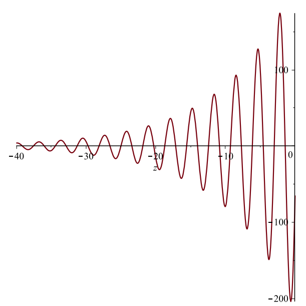

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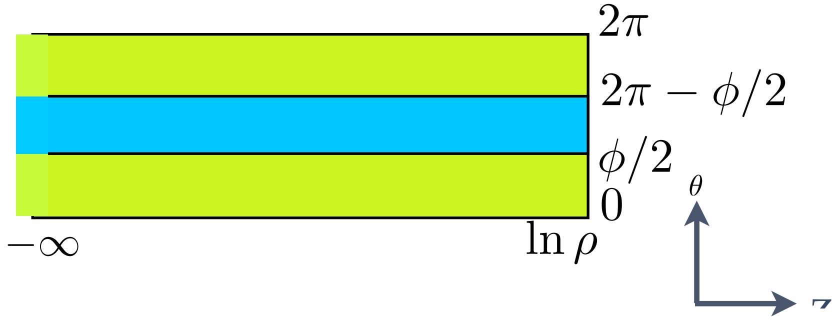

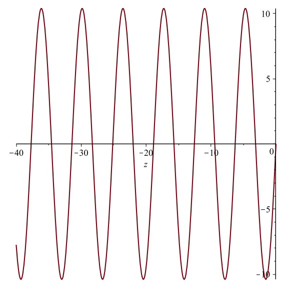

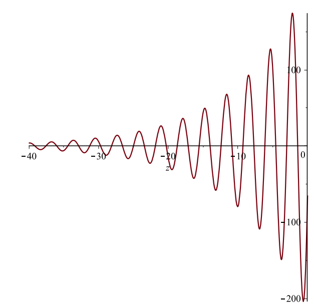

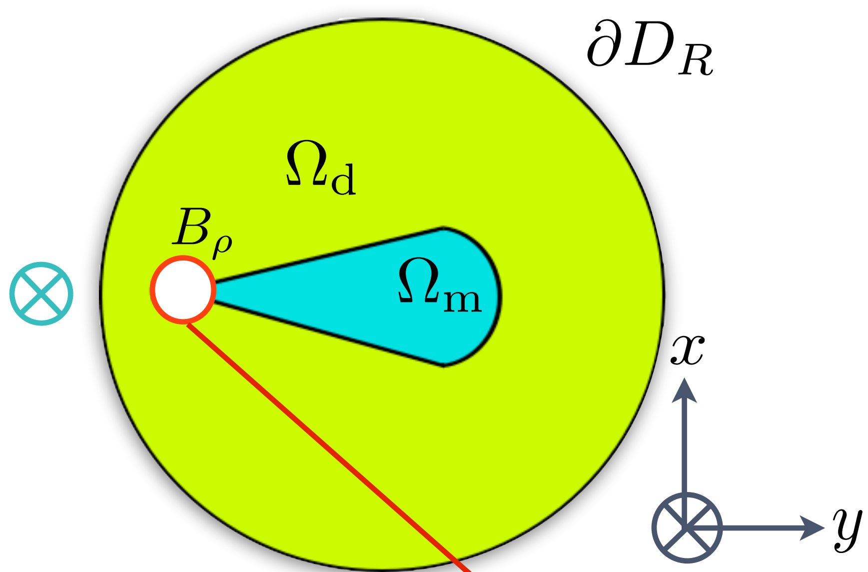

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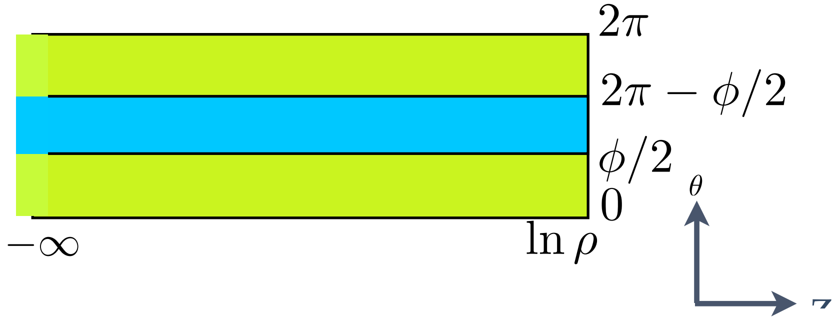

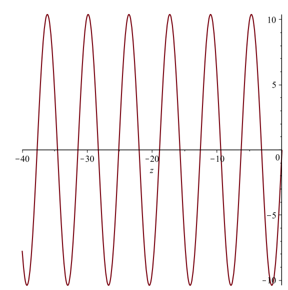

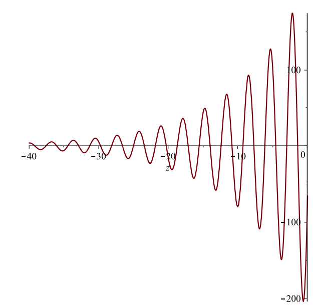

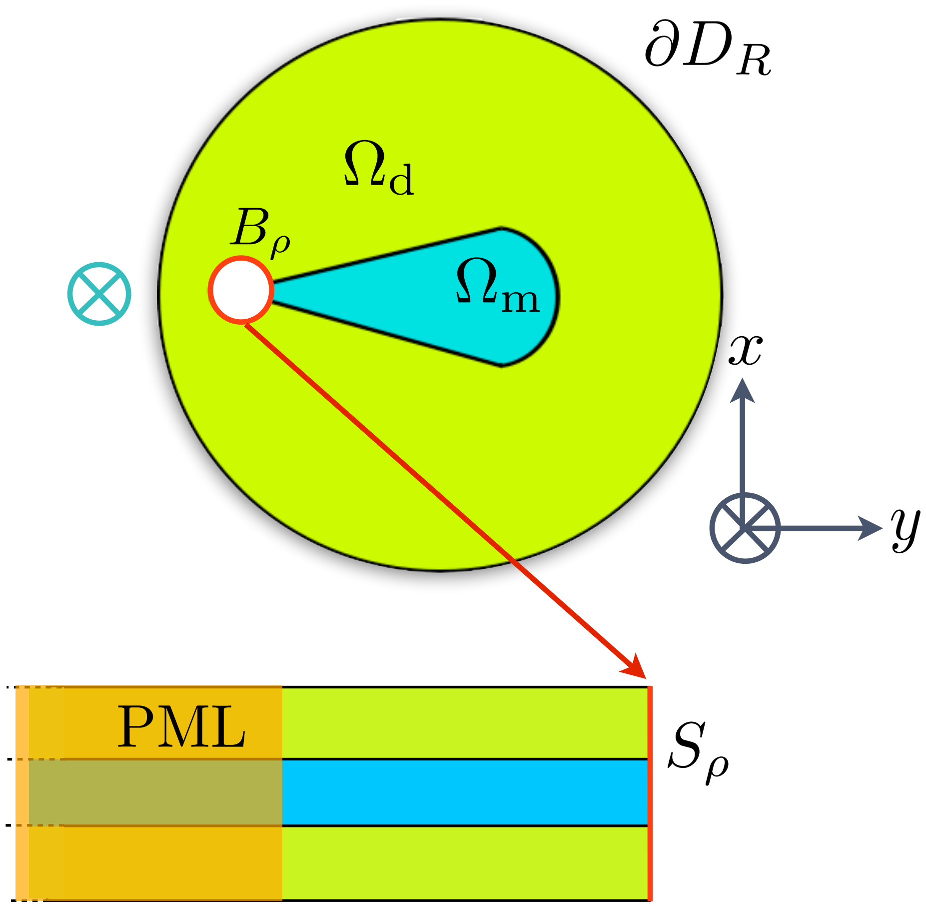

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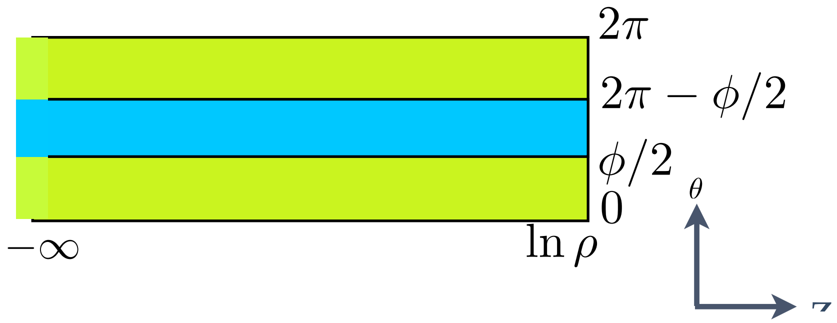

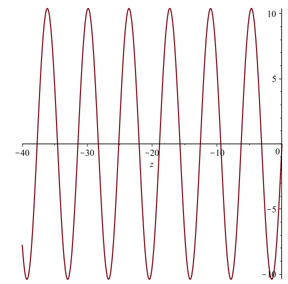

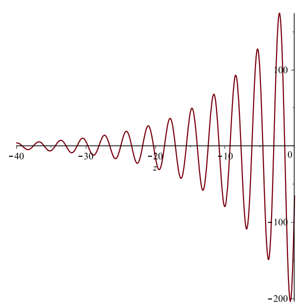

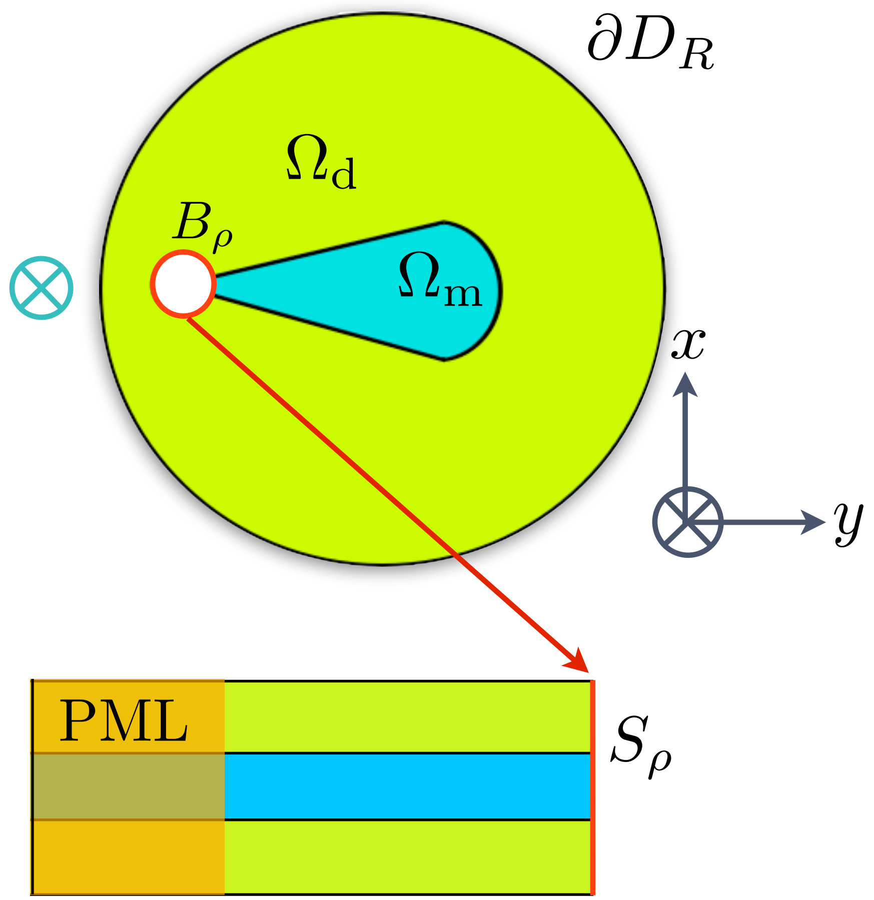

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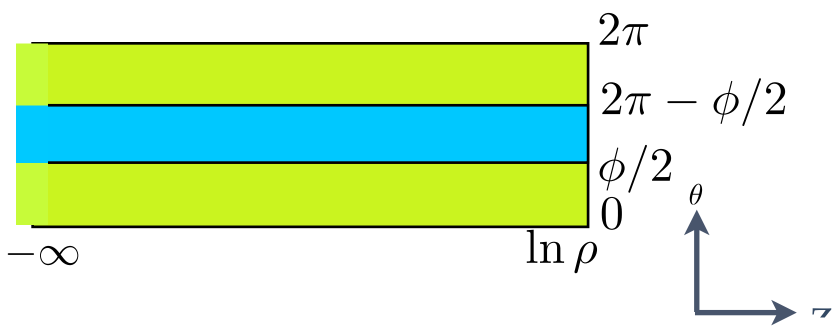

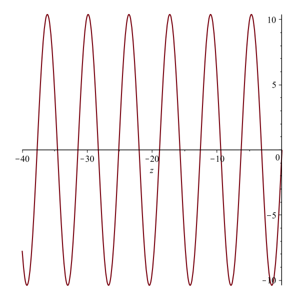

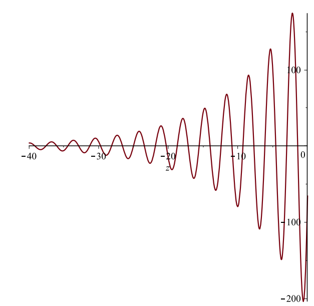

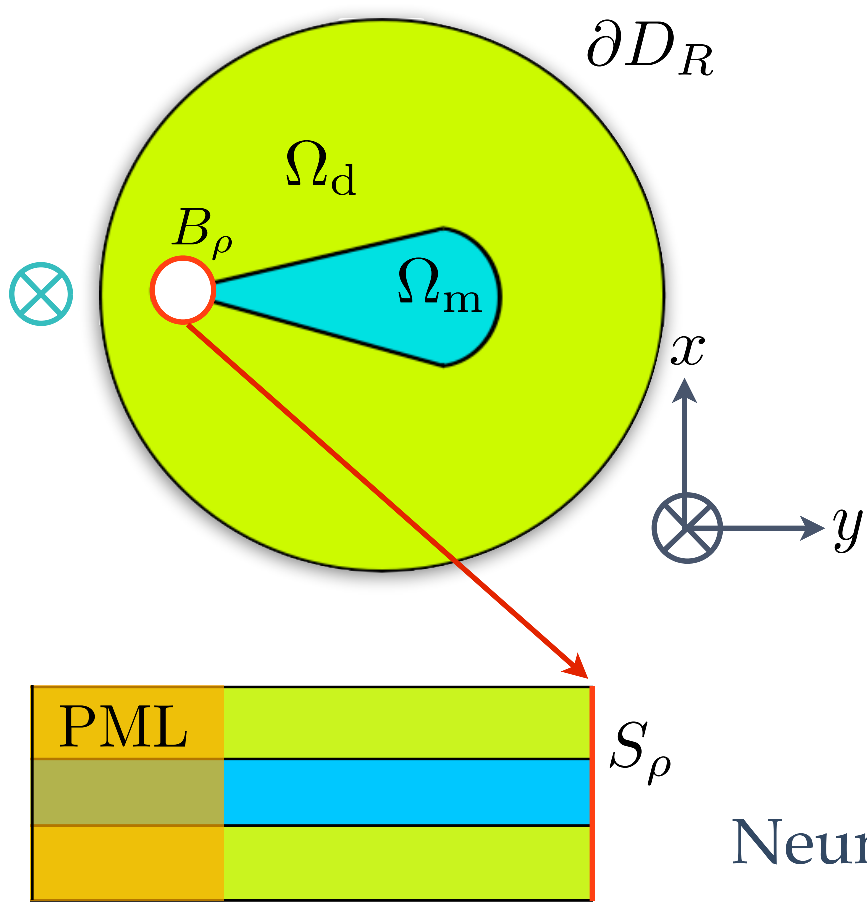

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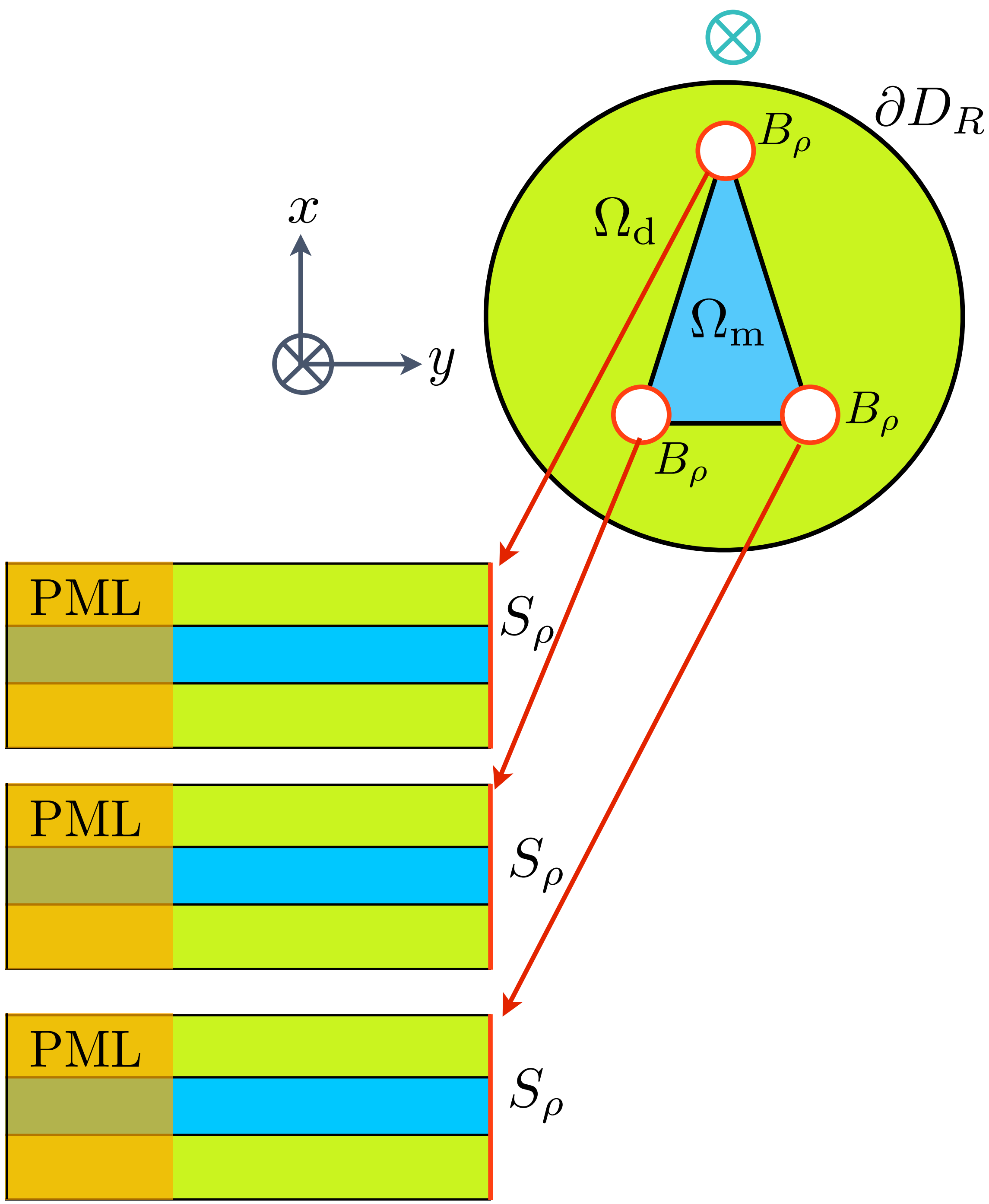
Neumann condition due to the constant mode

With several corners



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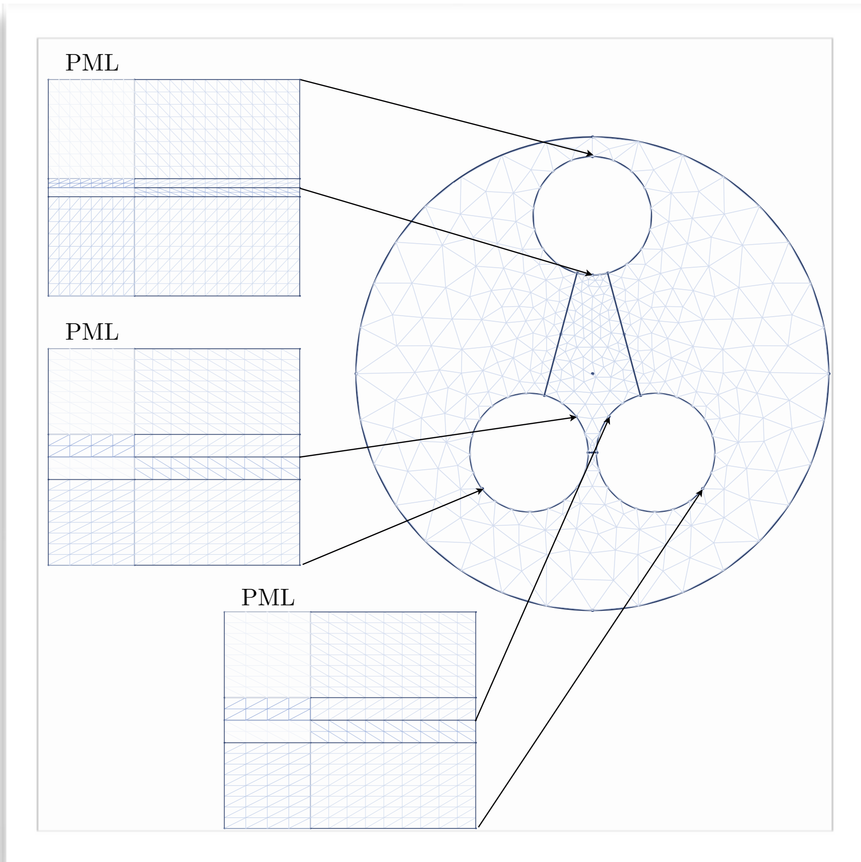

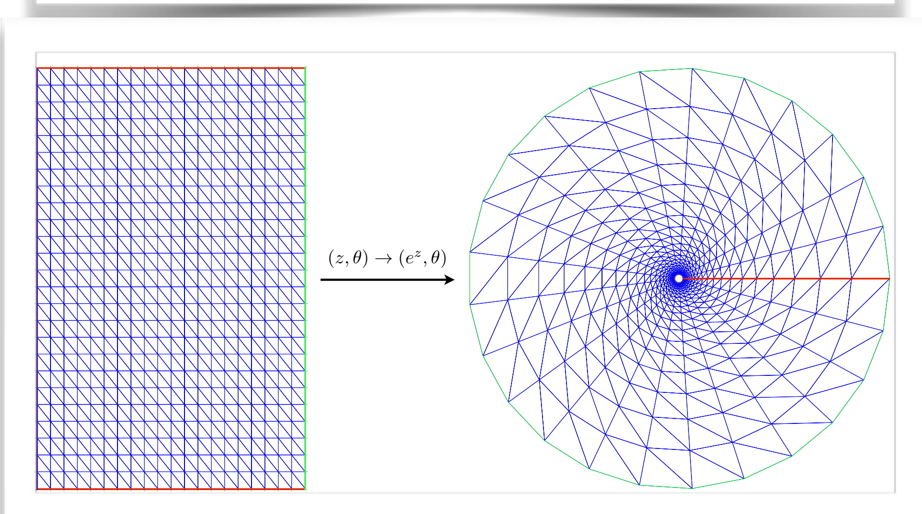

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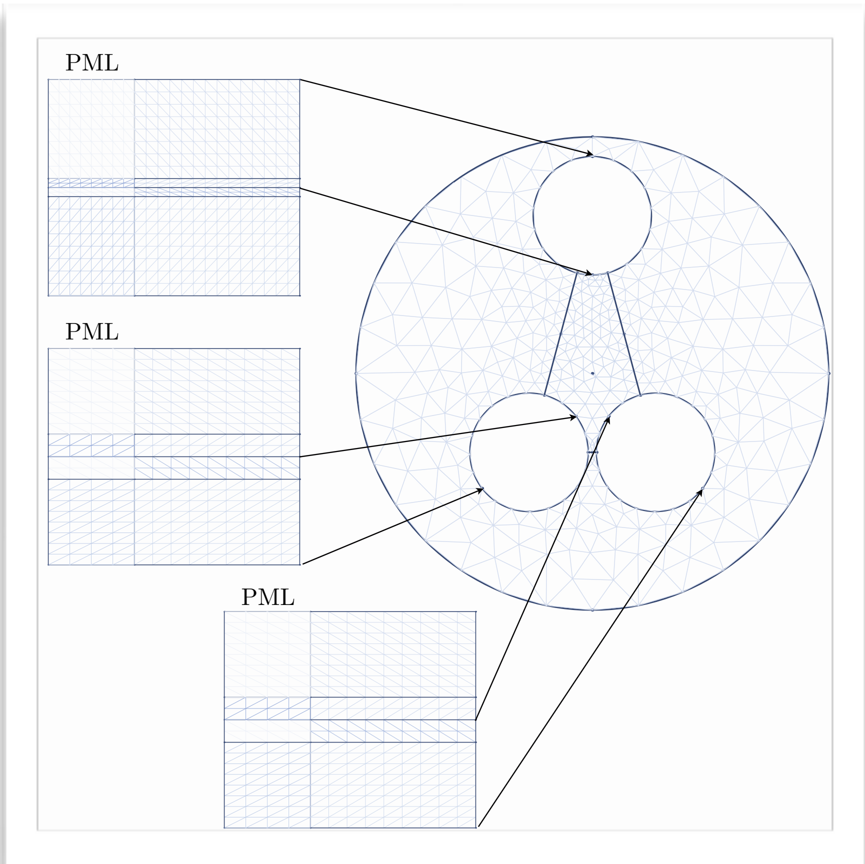

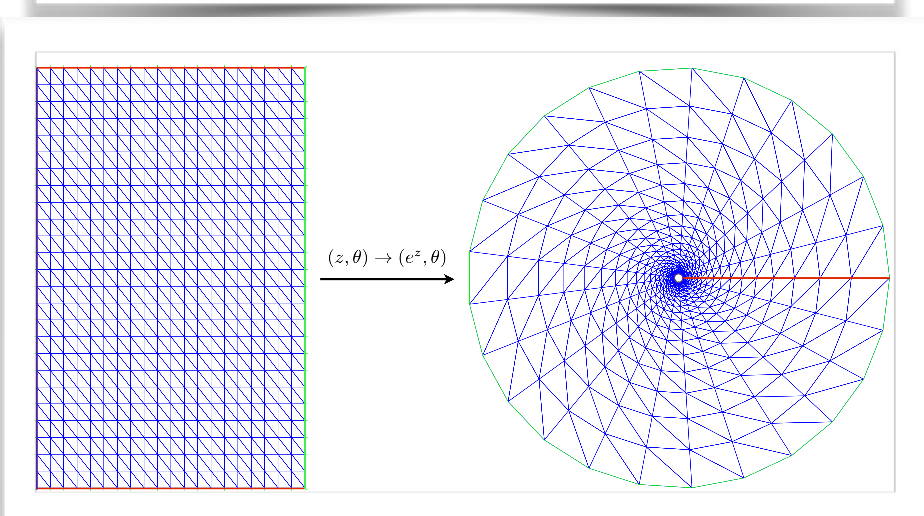

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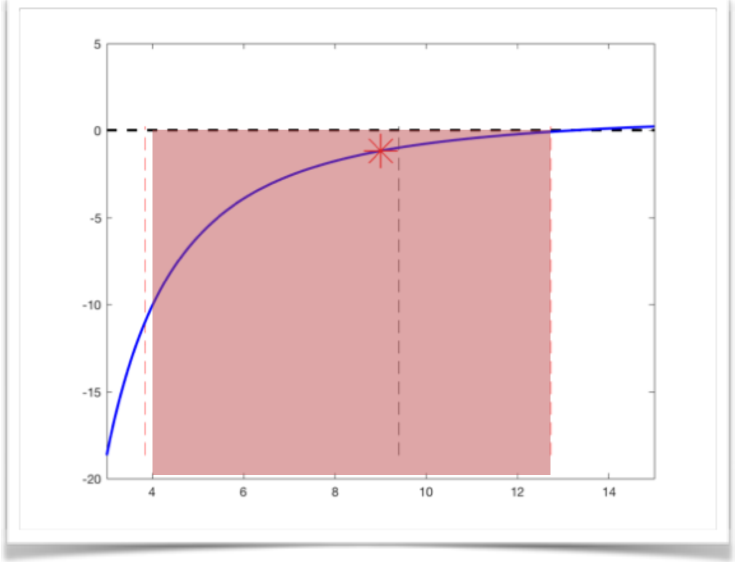
Computation with Lagrange FE of order 2 with a Matlab code

Numerical results with the multiscale-FEM

Numerical illustrations for triangular silver inclusion in vacuum:

$\kappa_\varepsilon \in I_c \quad \Longleftrightarrow \quad \omega \in [3.839 \text{ PHz}; 12.733 \text{ PHz}].$

Results for $\omega = 9$ PHz.



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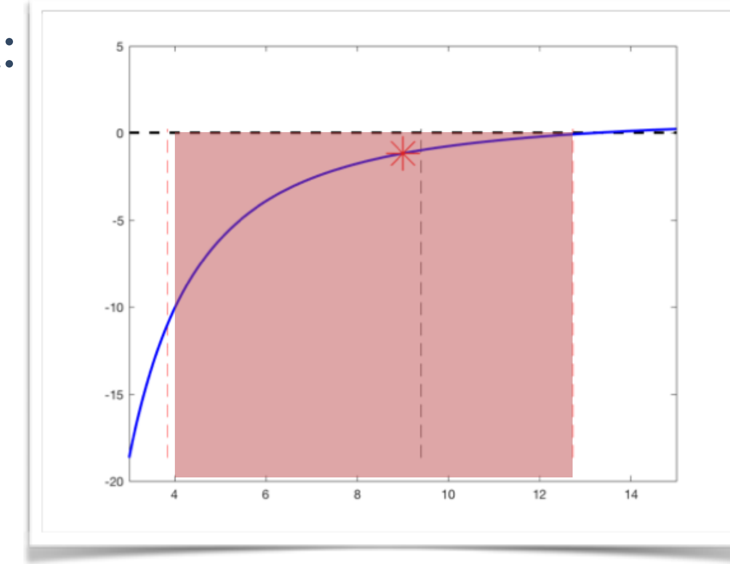
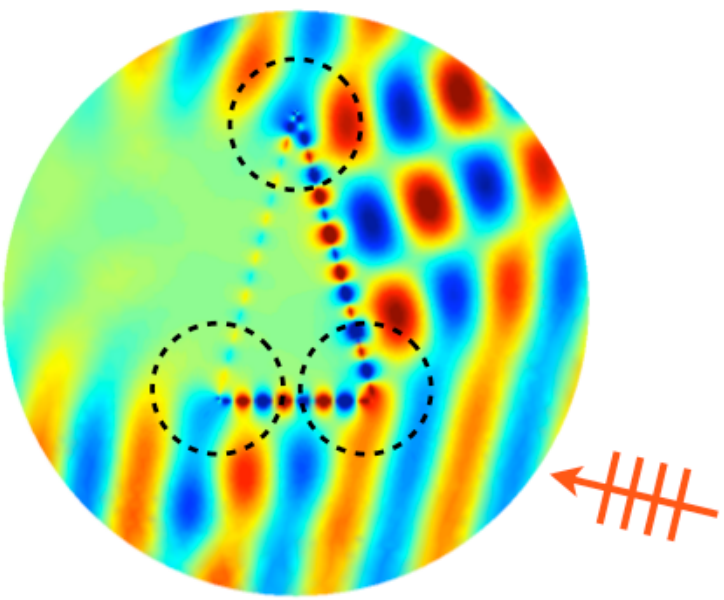
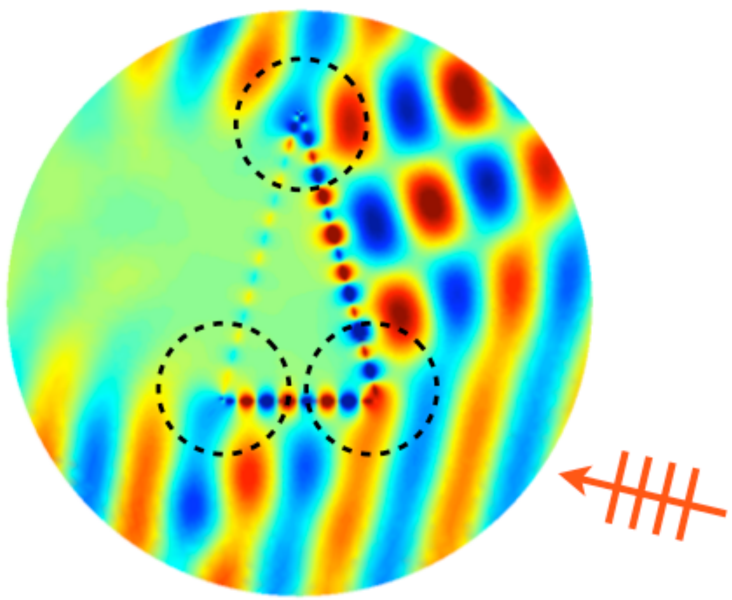
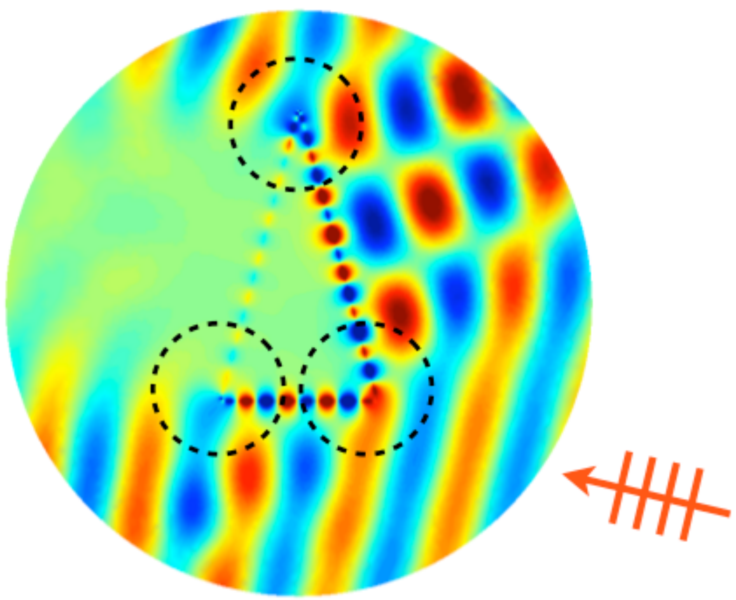




coarse mesh



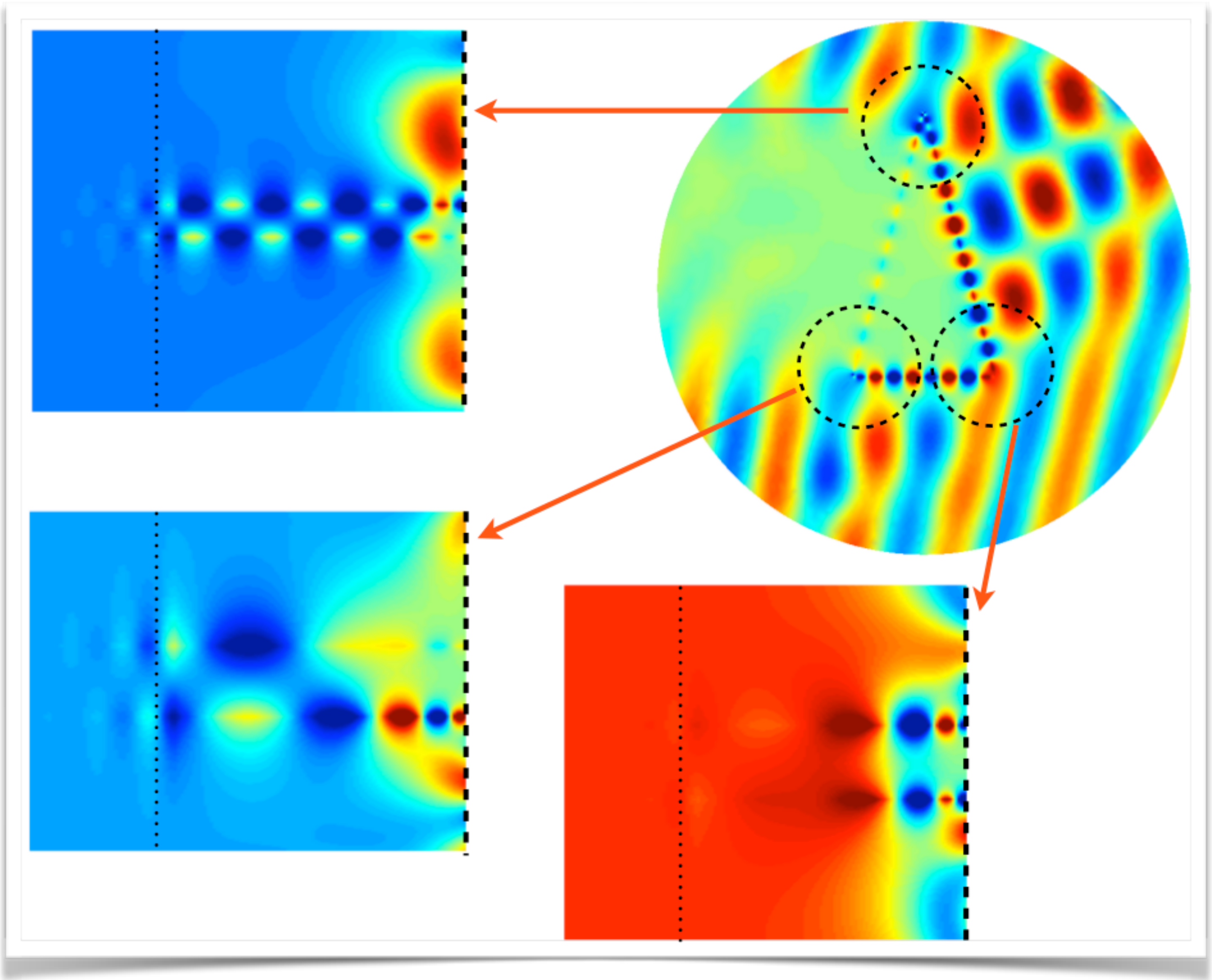
intermediate mesh



refined mesh

Numerical results with the multiscale-FEM

Numerical illustrations for triangular silver inclusion in vacuum: $\kappa_\varepsilon \in I_c$



Back to dissipative medium

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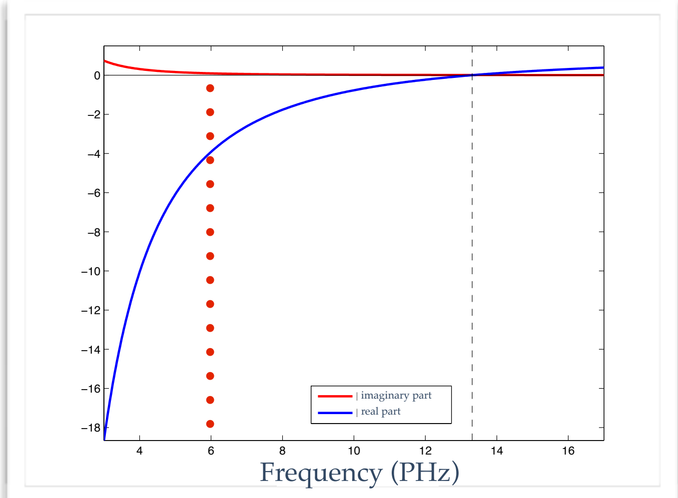

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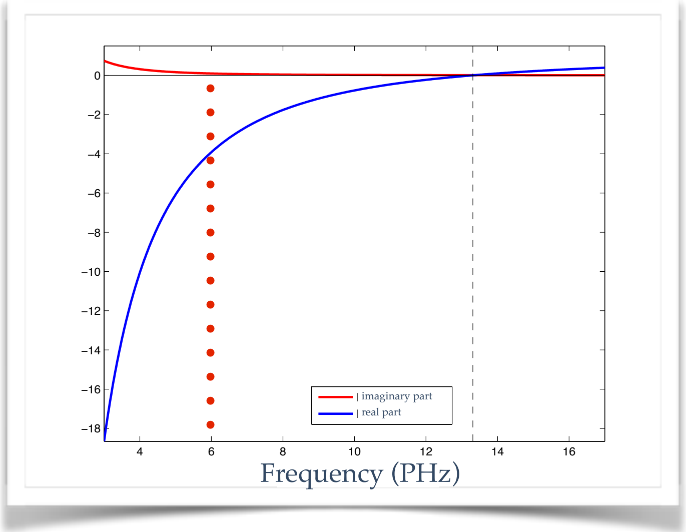

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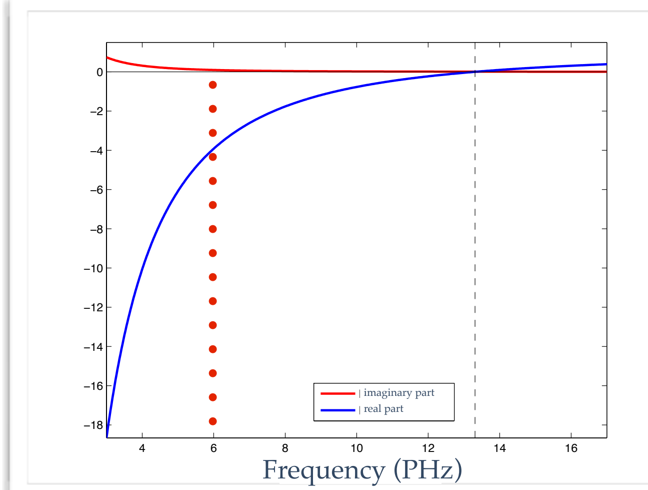

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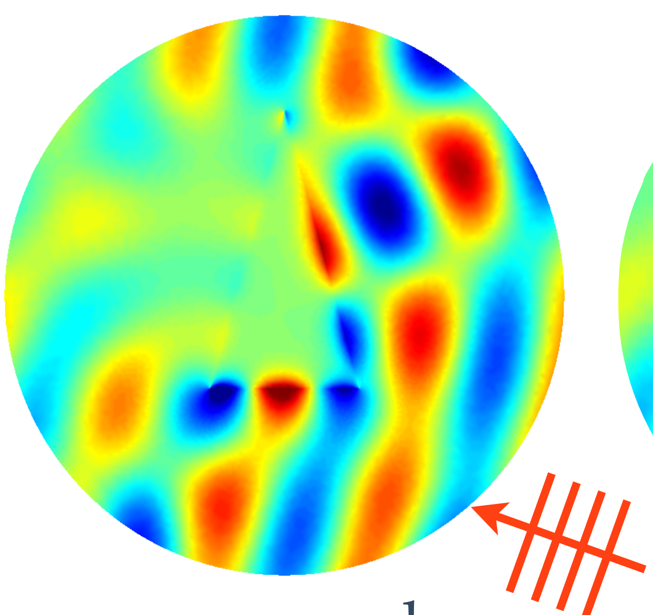
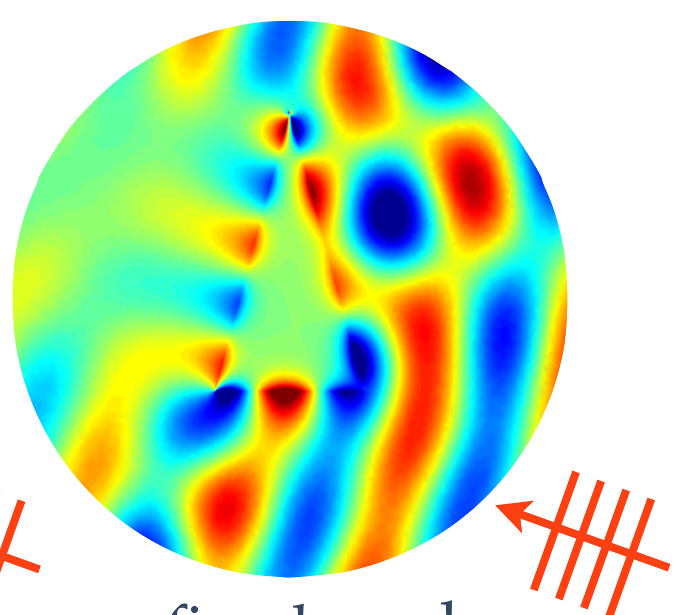


coarse mesh



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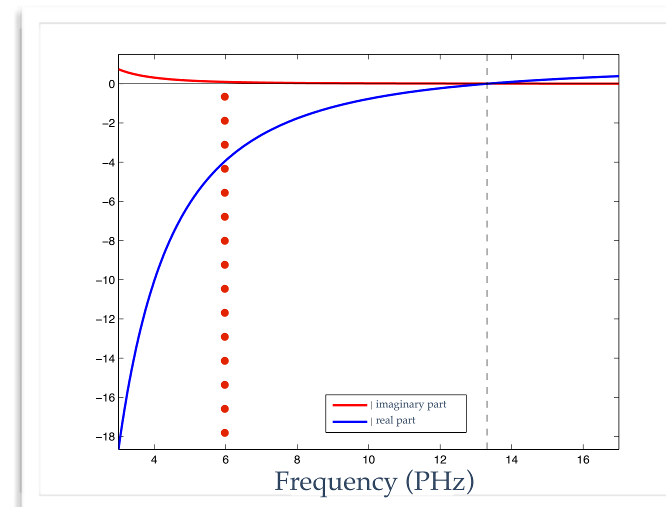

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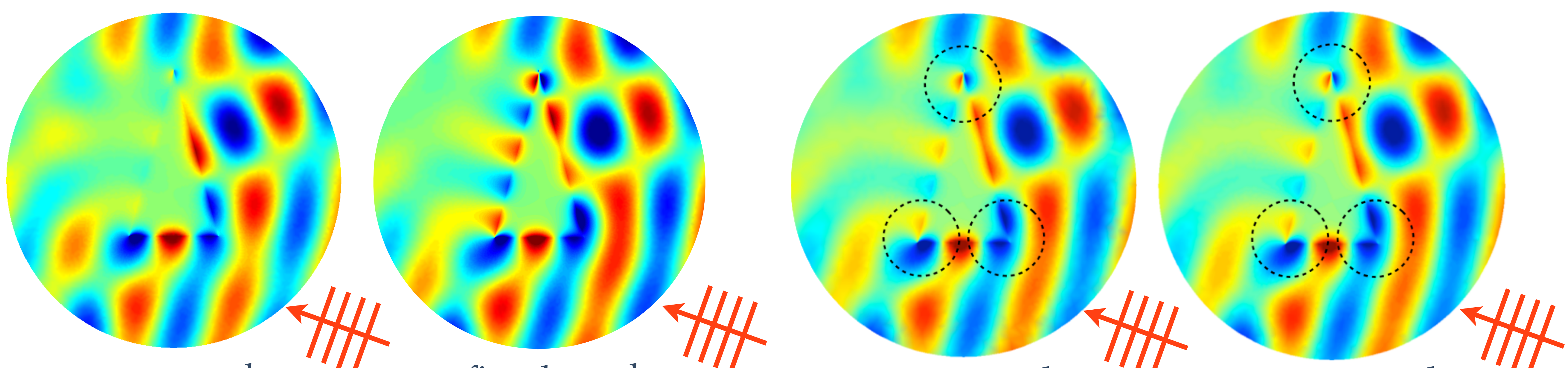
Without PMLs | With PMLs



coarse mesh | refined mesh | coarse mesh | refined mesh

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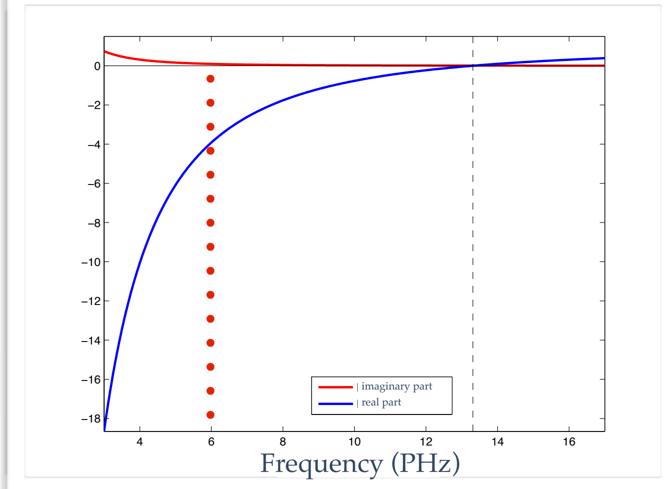

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Animation in time $\Re e(u\, e^{-i\omega t})$

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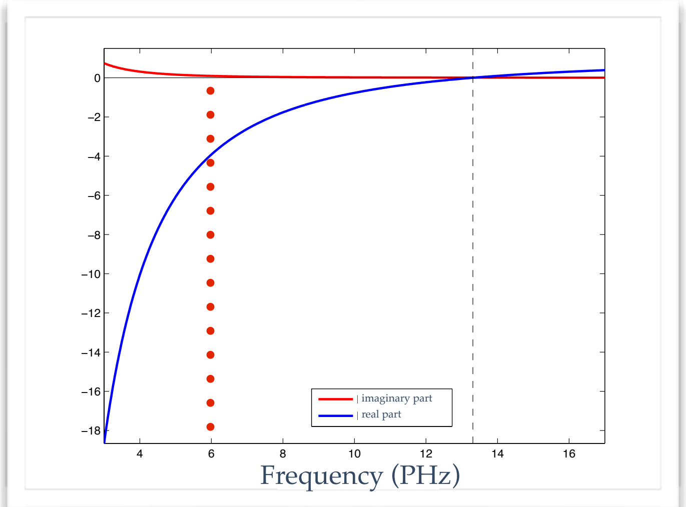

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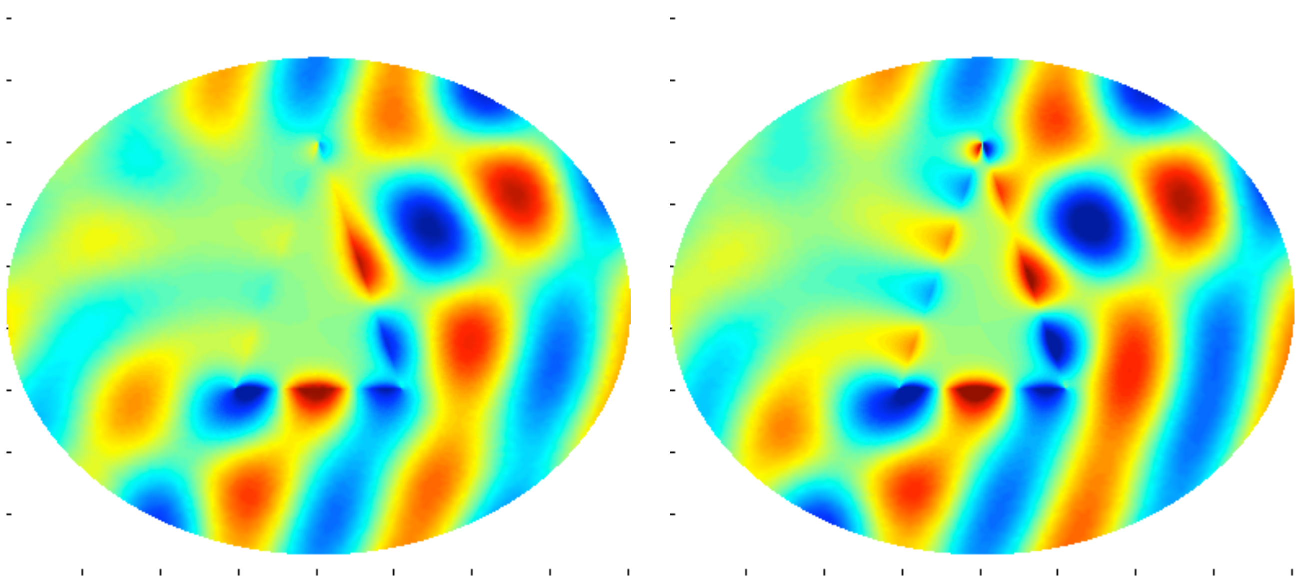

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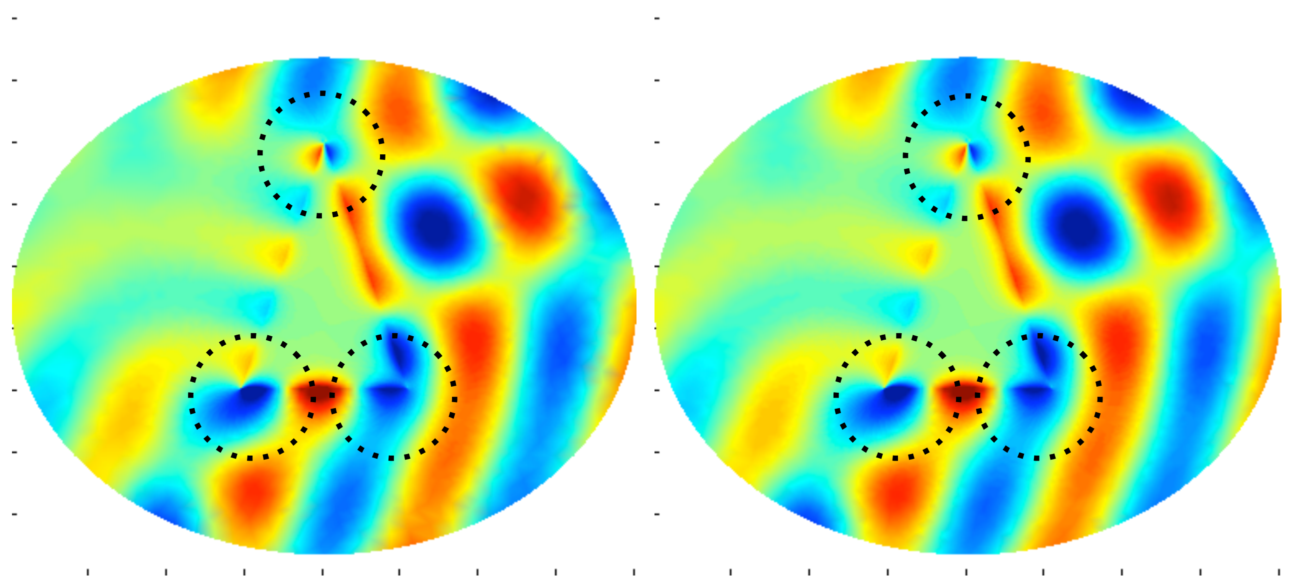

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Outline

- Introduction
- The limit problem
- Analysis at the corners
- Multiscale-FEM approach
- Extensions

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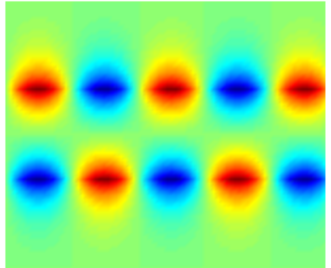

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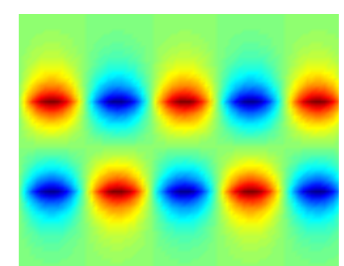

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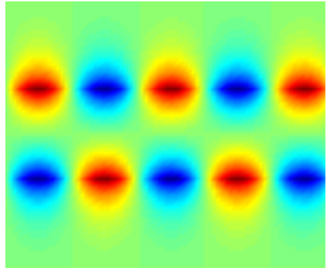

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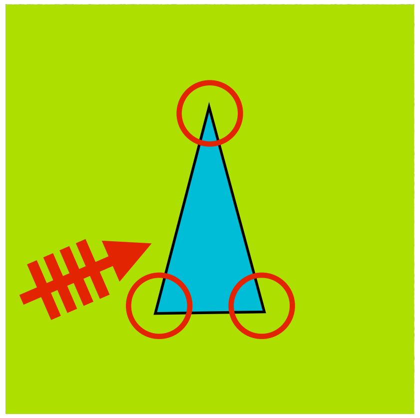

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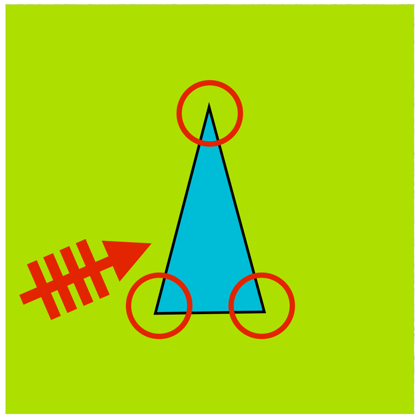

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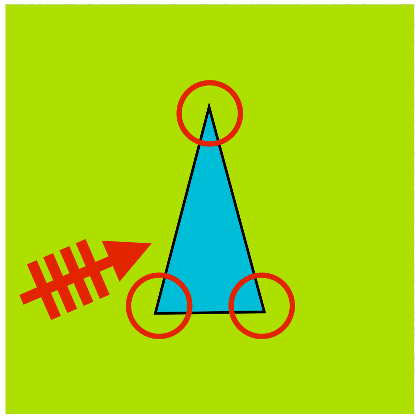

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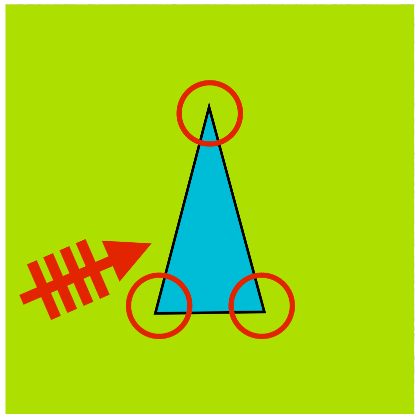

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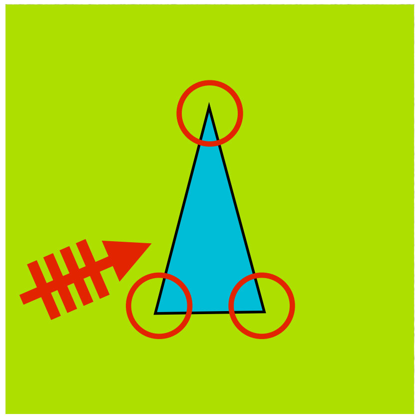

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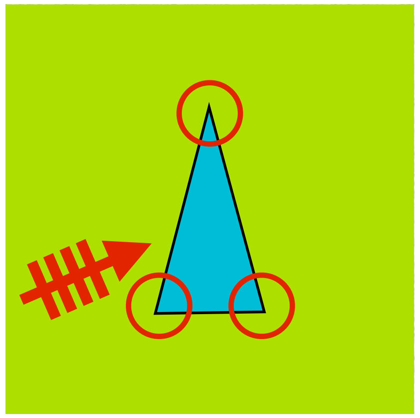

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Introduce one extra problem to solve (technical) but it has to be solved only once !

Carvalho, Ciarlet (in preparation).

Future work

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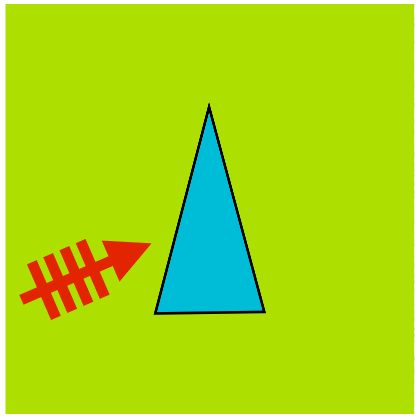
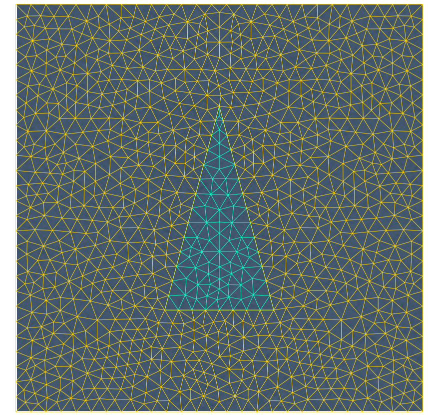


Variational-based approach

(multiscale- FEM)



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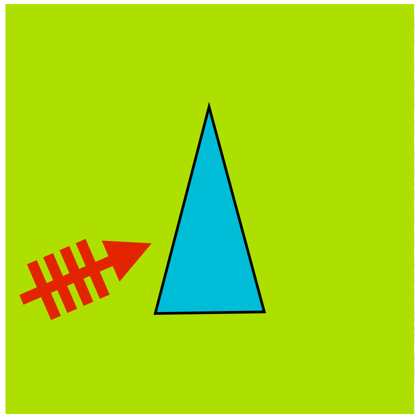

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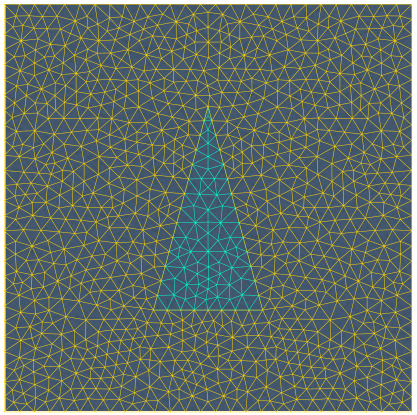

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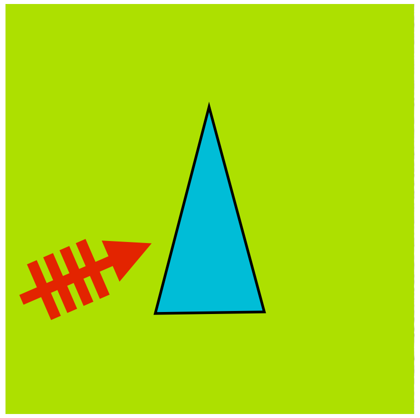

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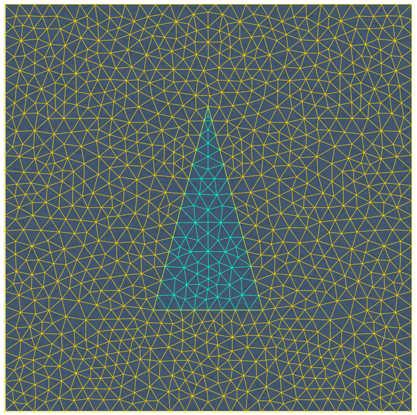

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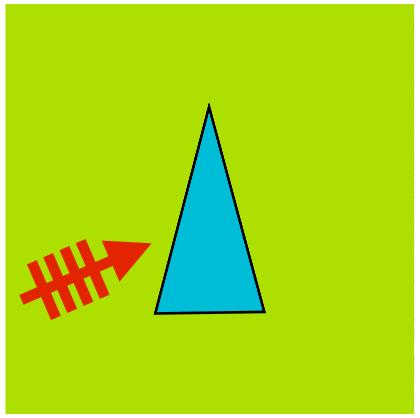

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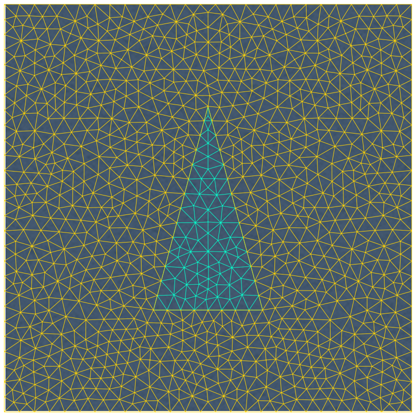

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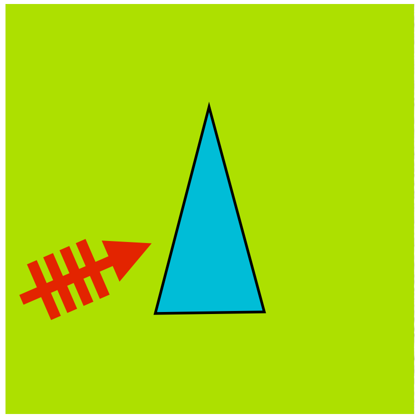

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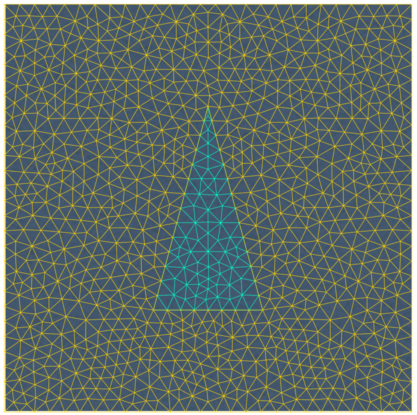

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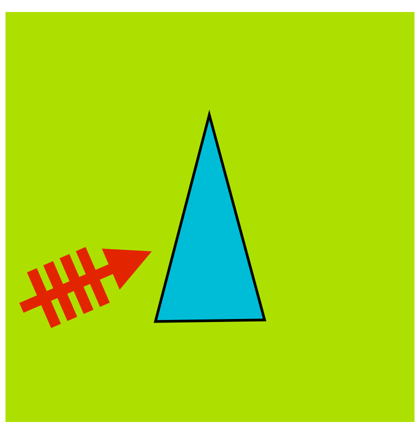
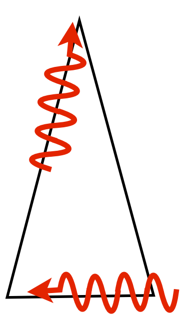


Multiscale asymptotic boundary integral approach



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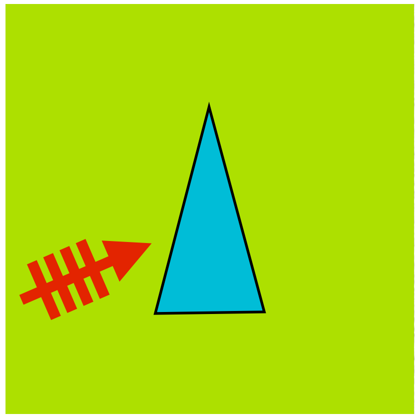

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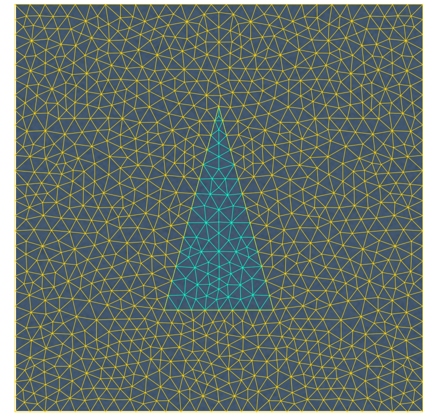

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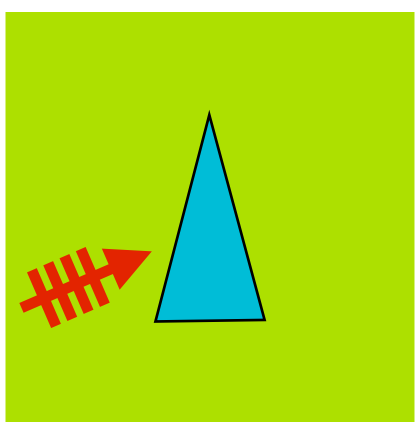

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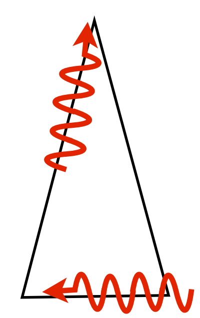

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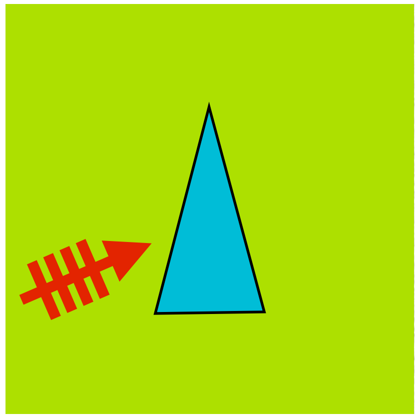

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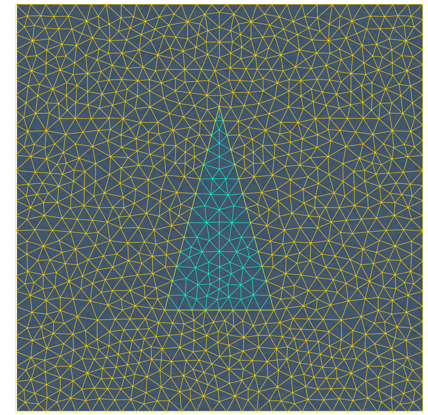

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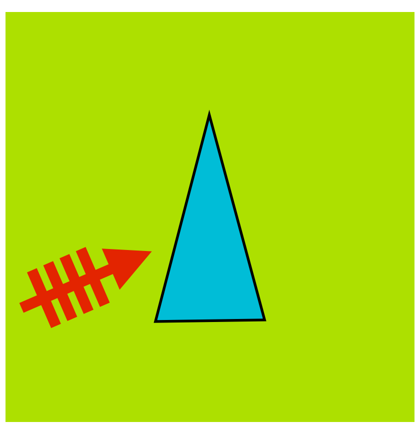

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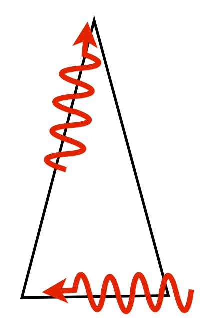

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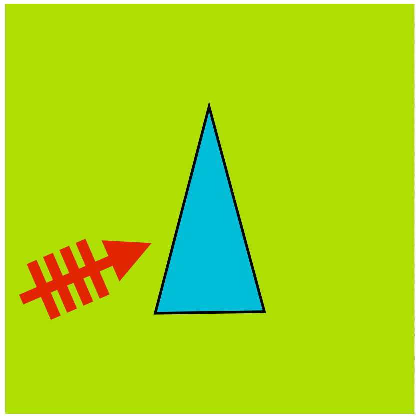

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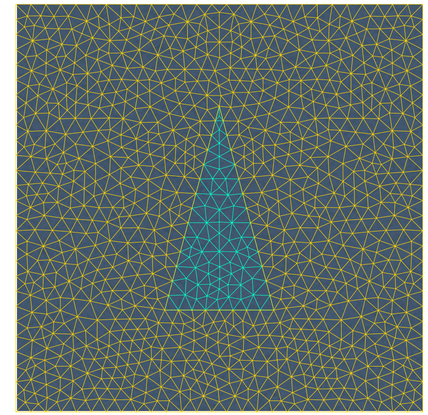

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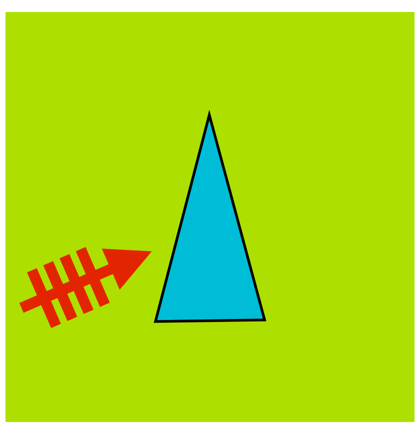

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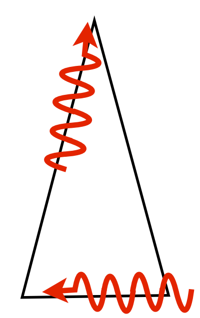

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The black-hole is of “infinite" energy. What does it mean in the time domain ?

Thank you for your attention.