Mathematical and numerical study of plasmonic structures with corners

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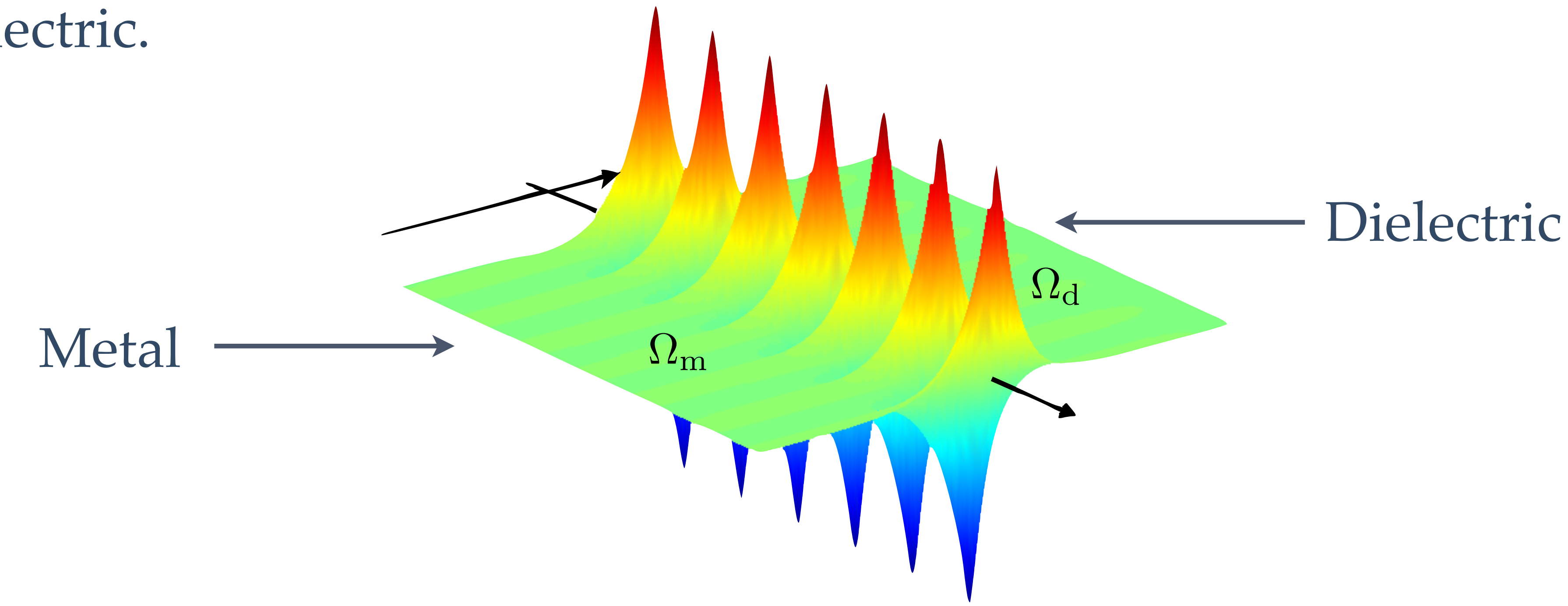

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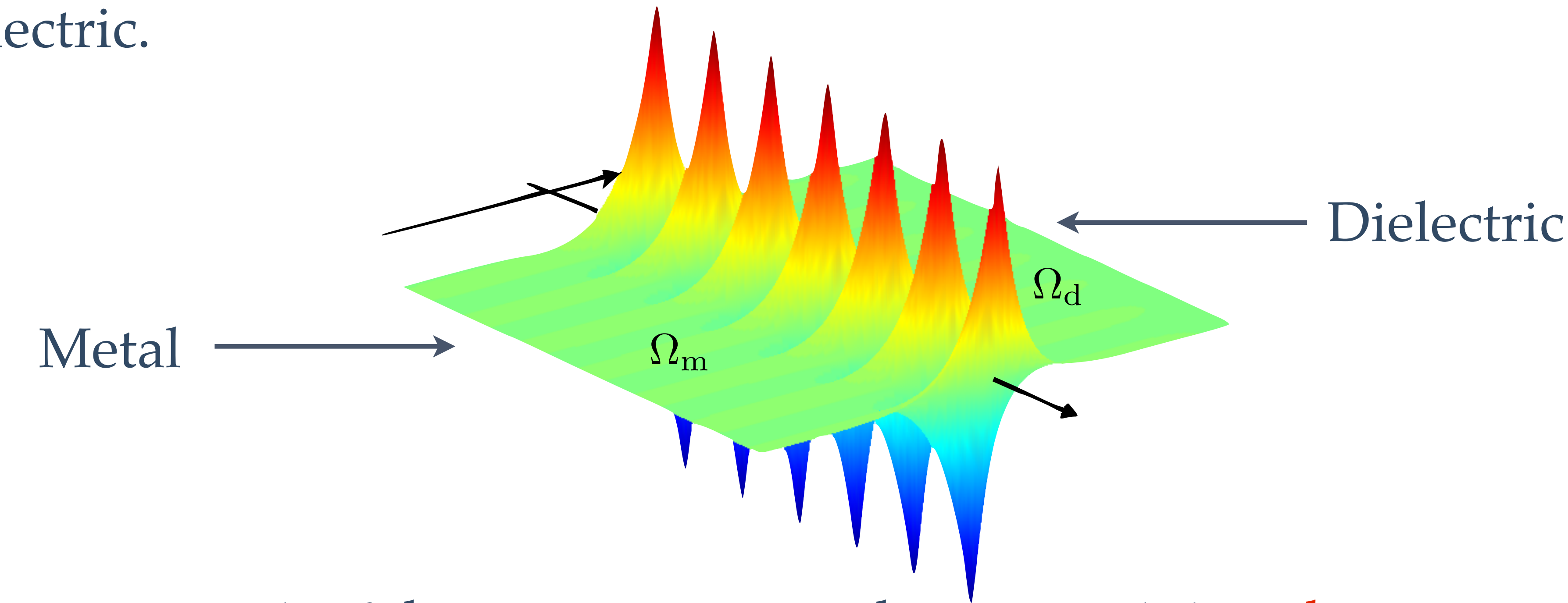

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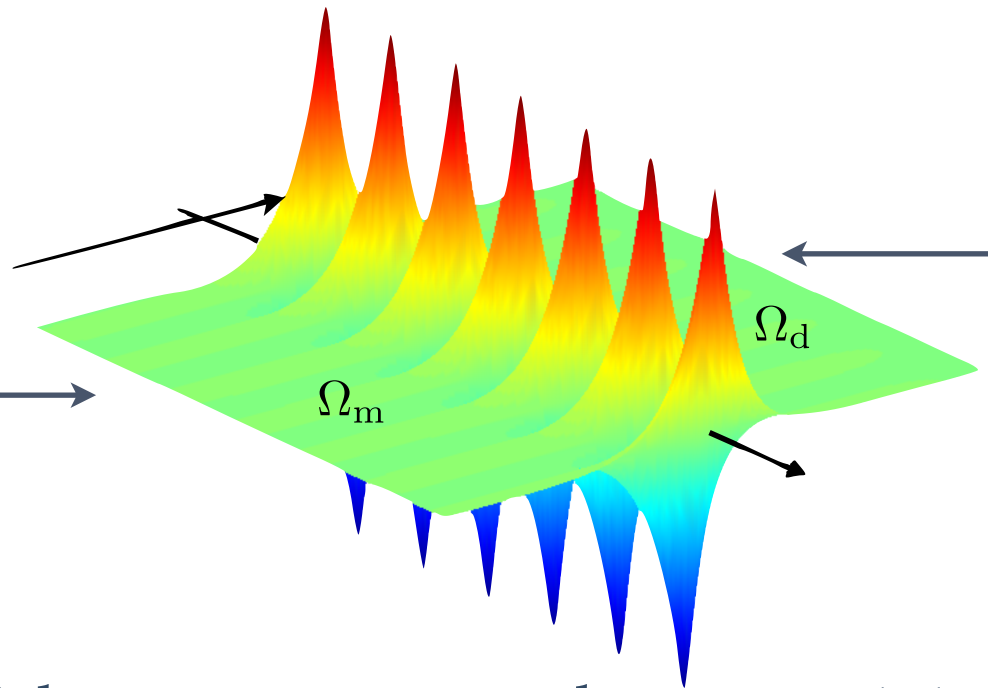

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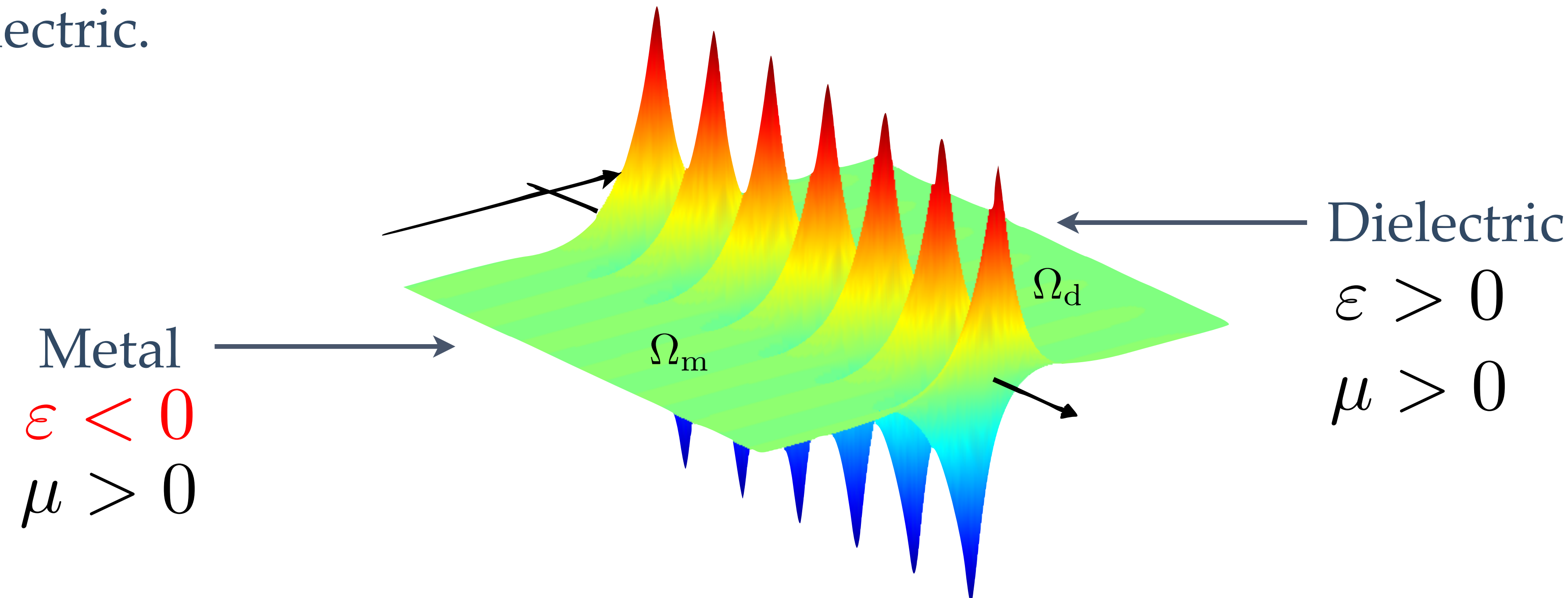

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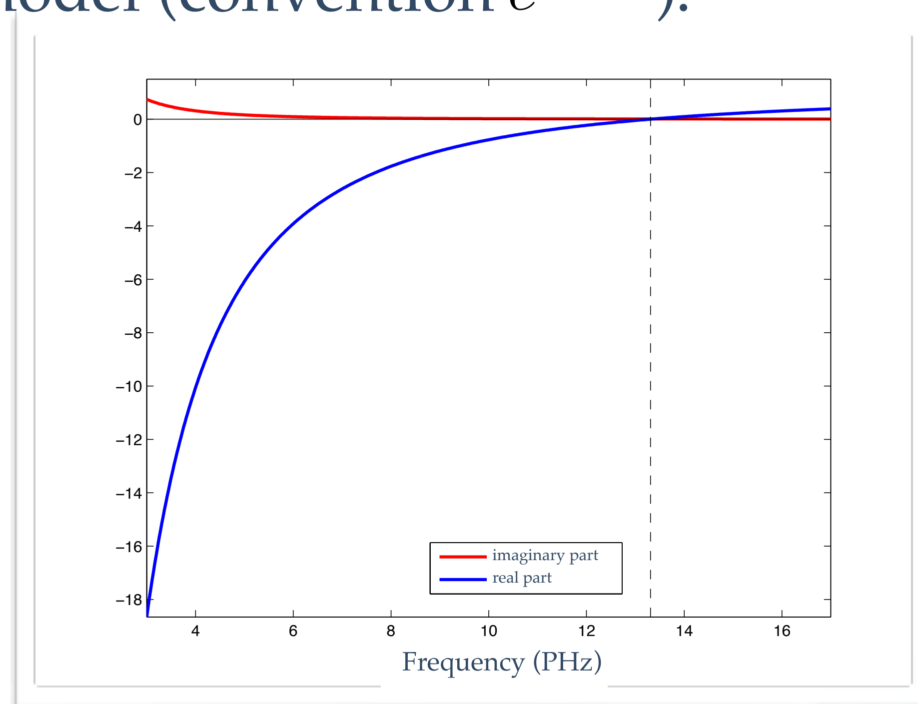
One simple model of permittivity: Drude's model (convention $e^{-i\omega t}$).

$$\boxed{\varepsilon = \varepsilon^{\gamma}(\omega) := 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}}$$



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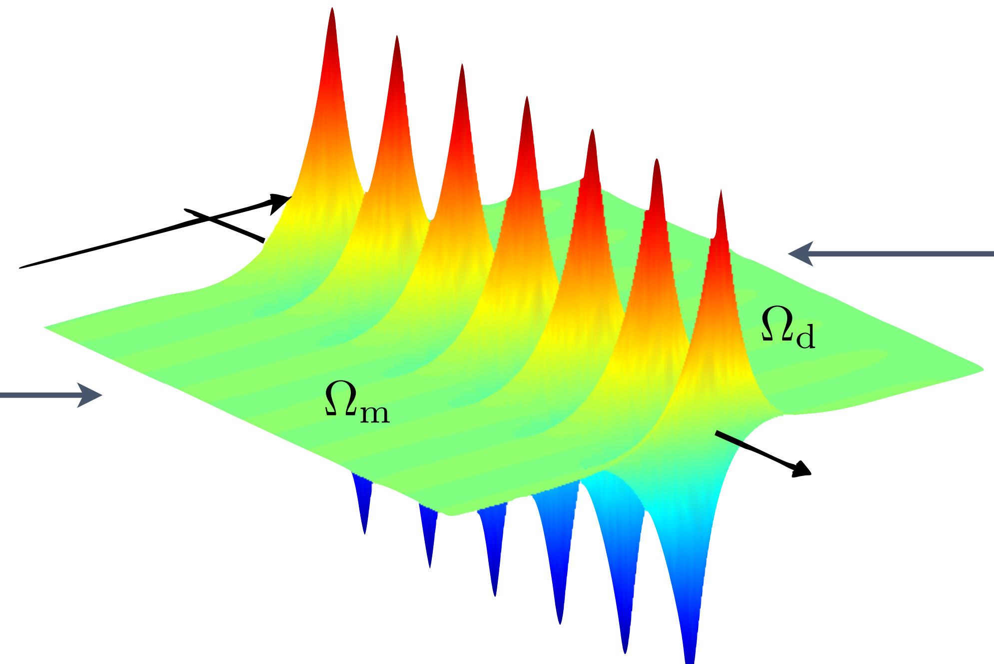

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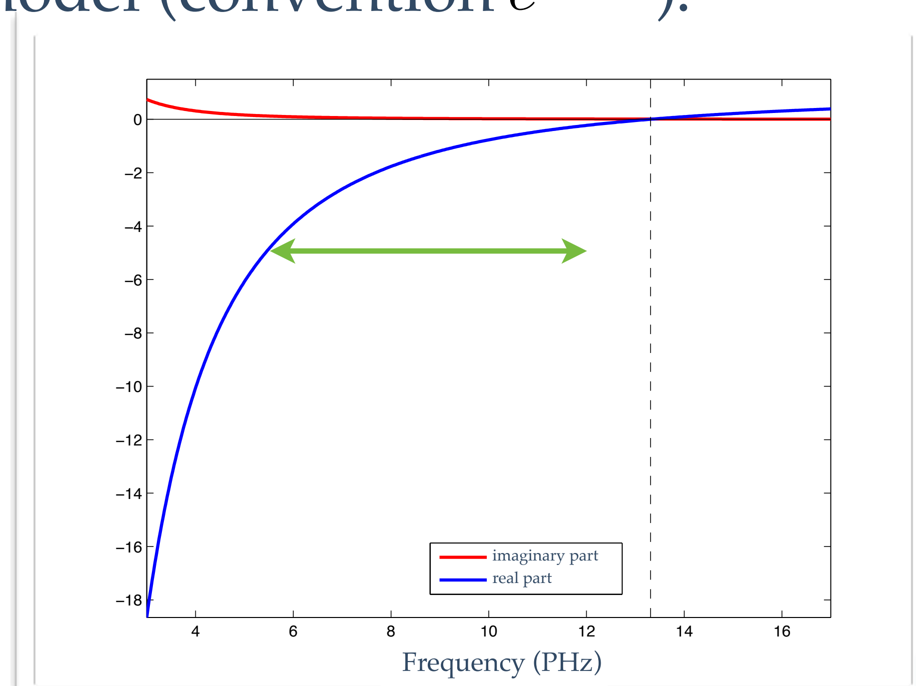
At optical frequencies ($\gamma \ll \omega < \omega_p$), ε has a negative real part and a neglectable imaginary part.



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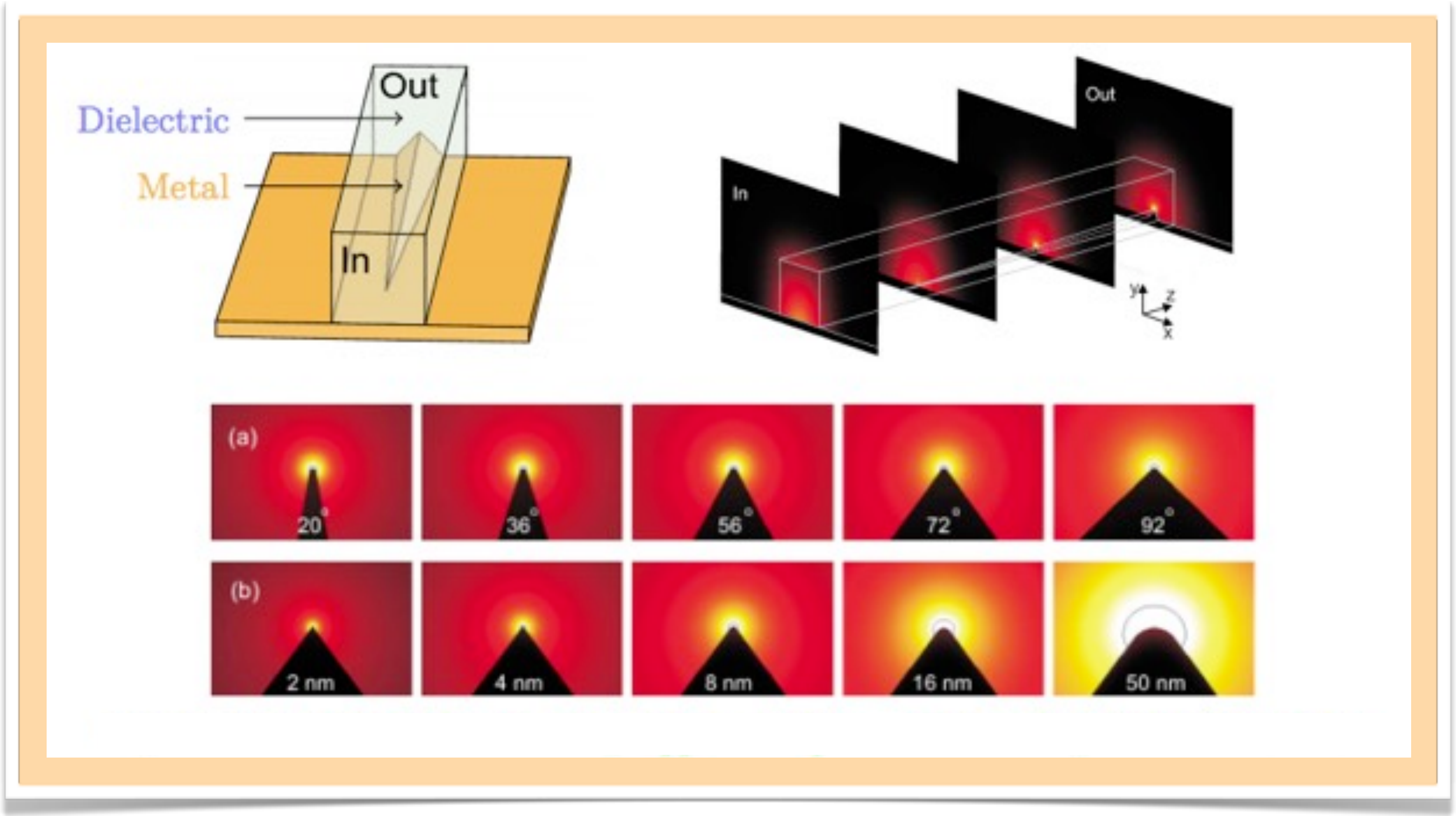

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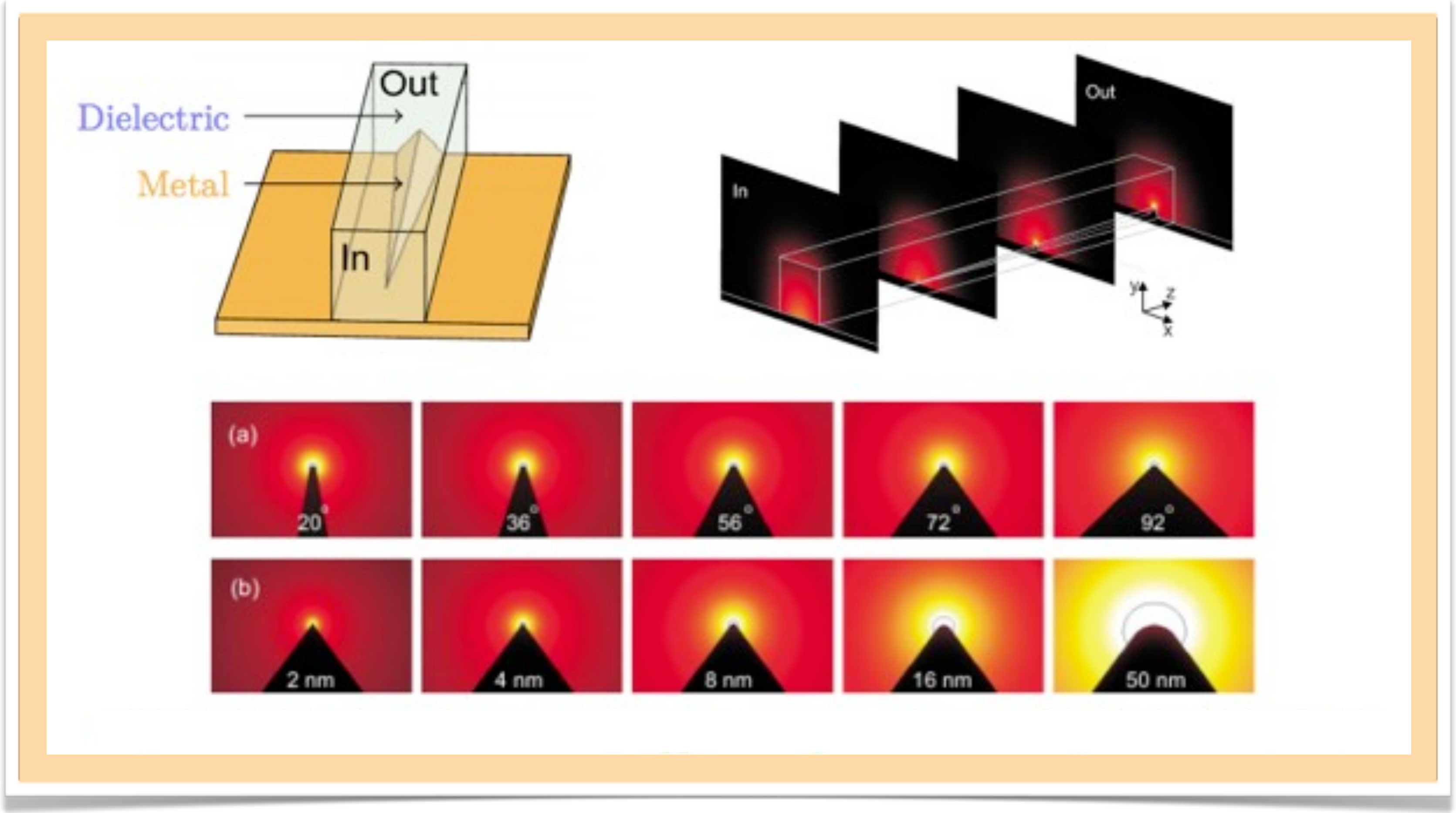

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However these waves are very sensitive to the geometry of the interface between the two media.

Explicit computations of surface plasmons

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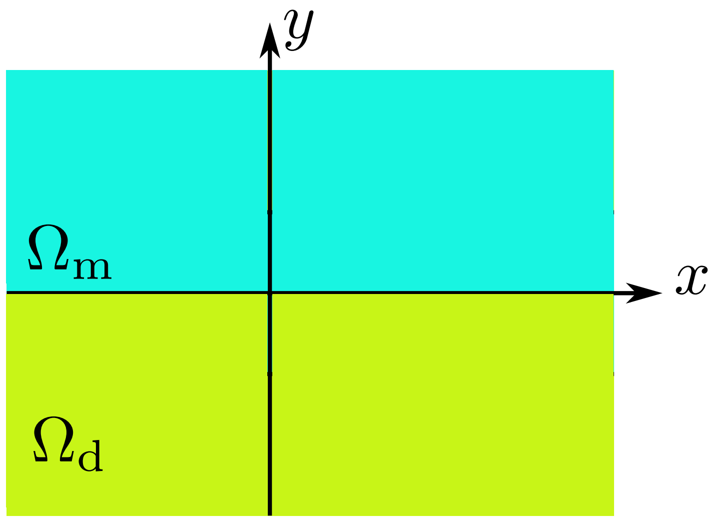

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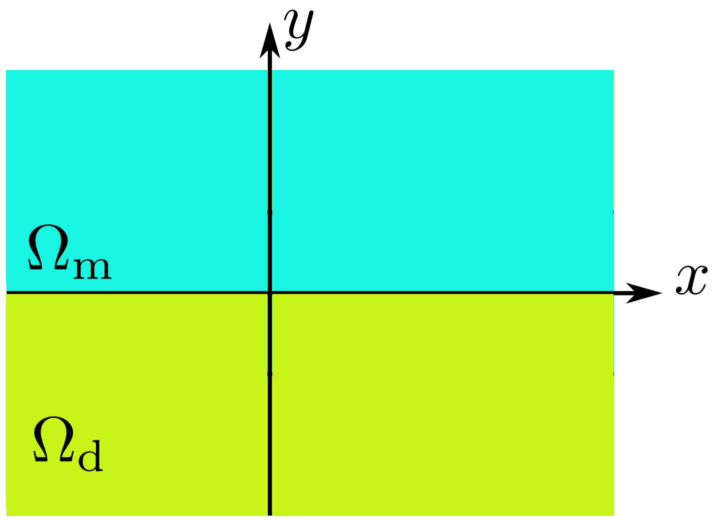

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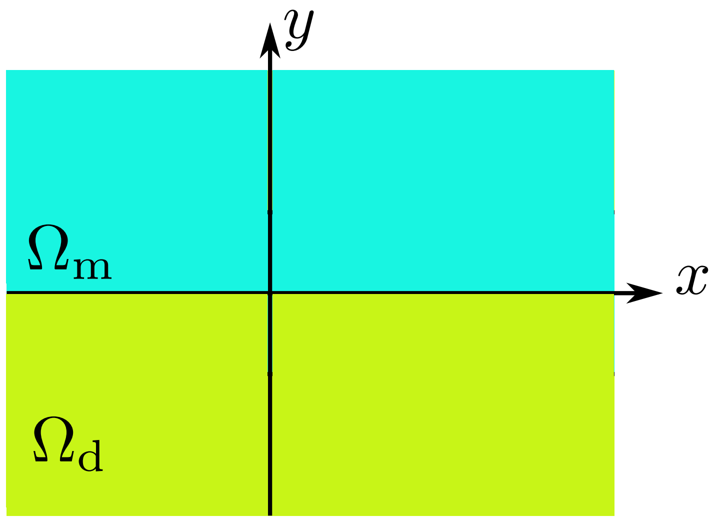

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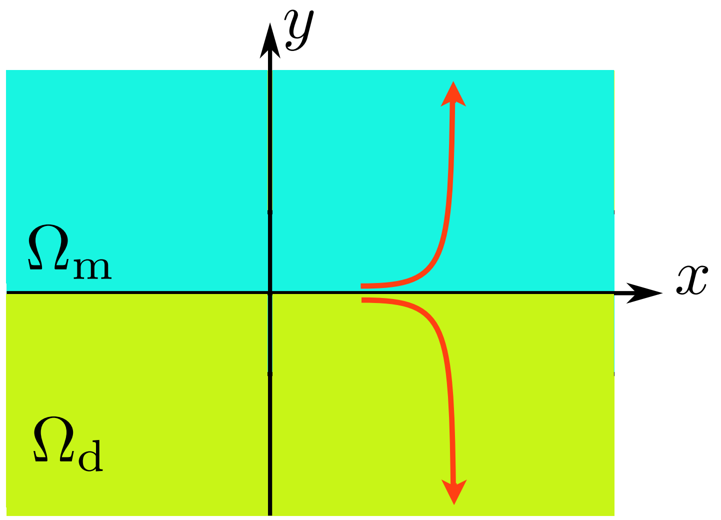

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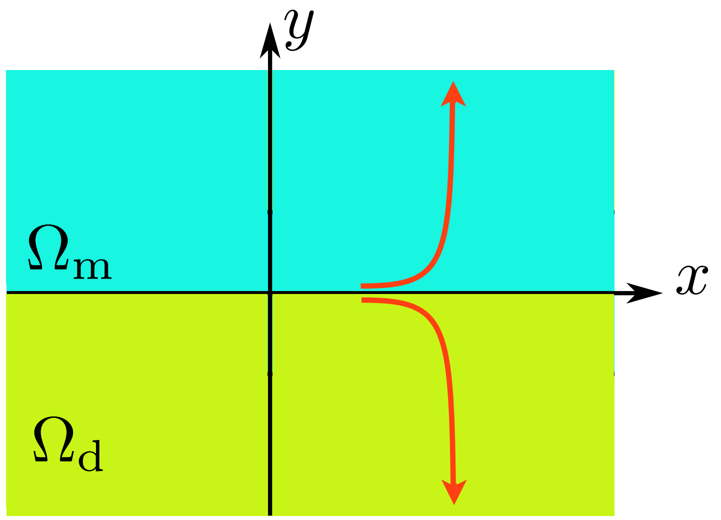

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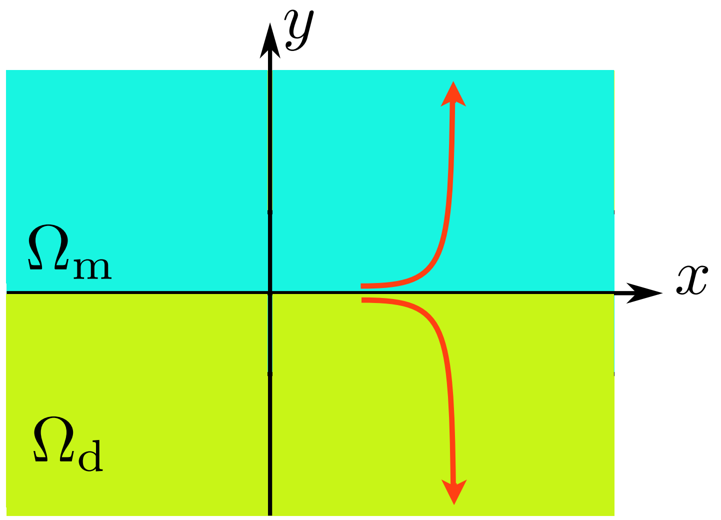

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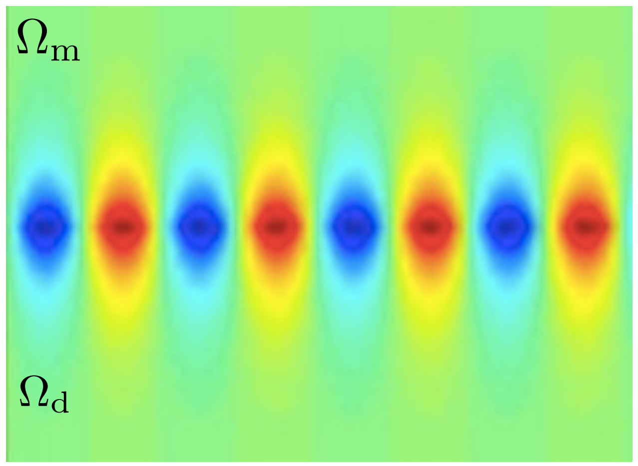

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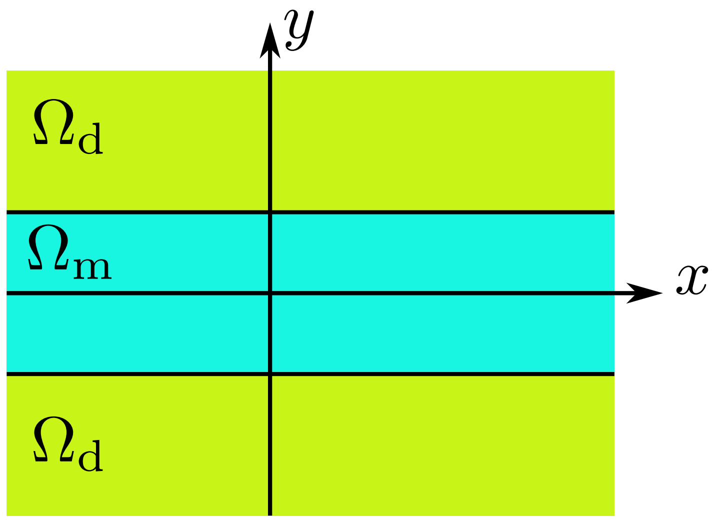

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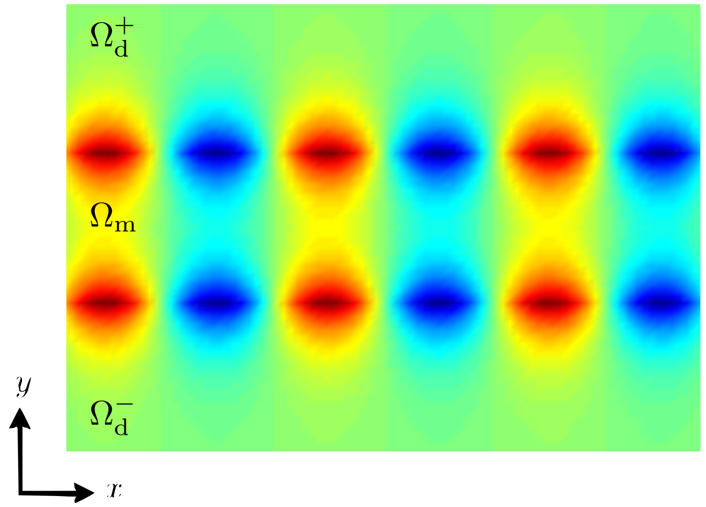

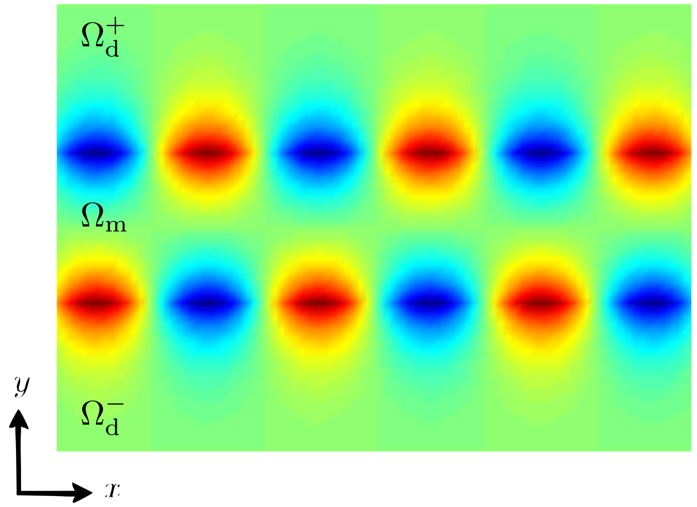

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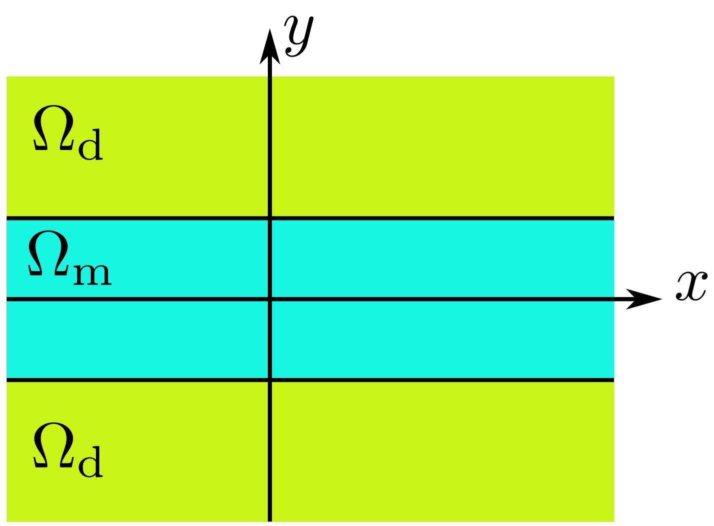

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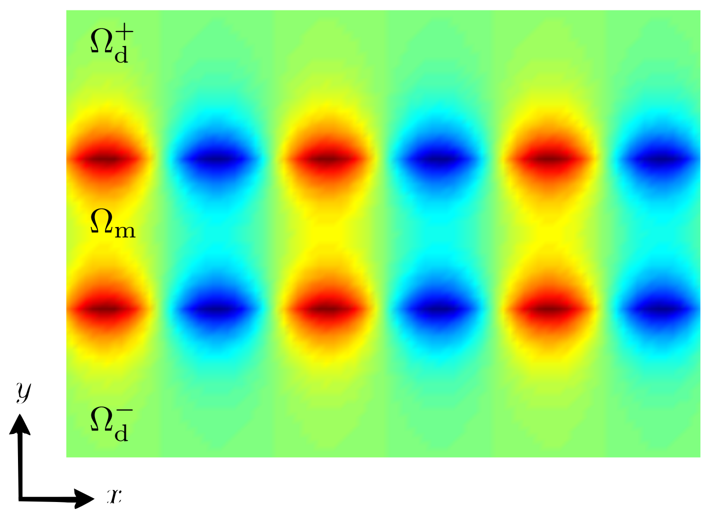

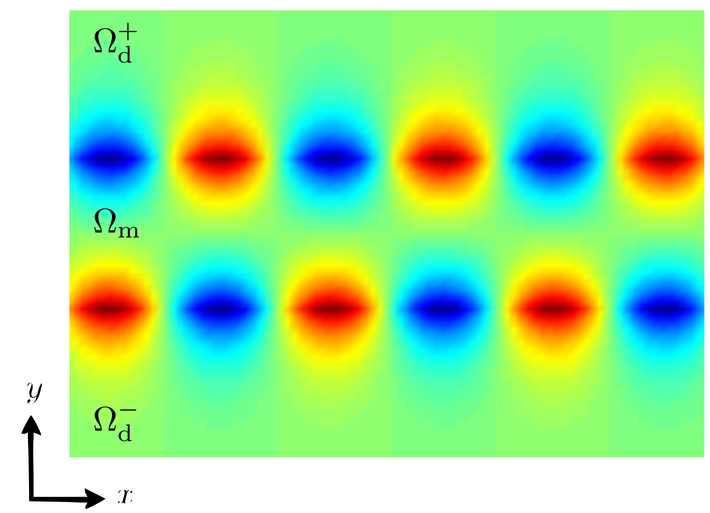

How to compute surface plasmons in more complex geometries ?

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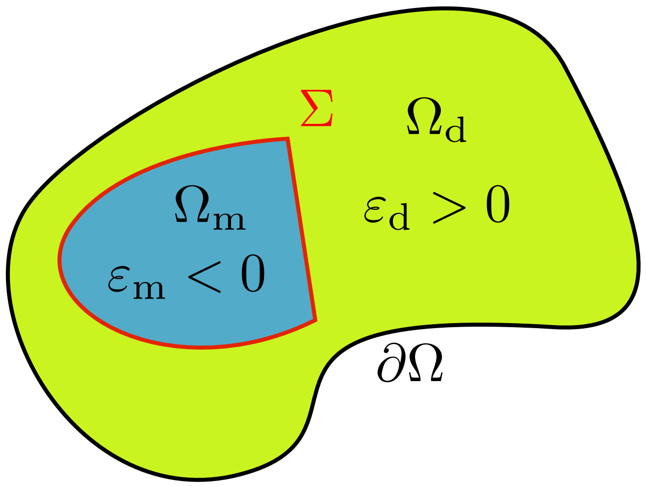
Example: a 2D transmission problem in a bounded domain.

$$\left|\begin{array}{l}\text{Find } u \in H_0^1(\Omega) \text{ such that:}\\ \operatorname{div}(\varepsilon^{-1}\nabla u) + \omega^2 \mu u = -f \quad \text{in } \Omega\end{array}\right.$$



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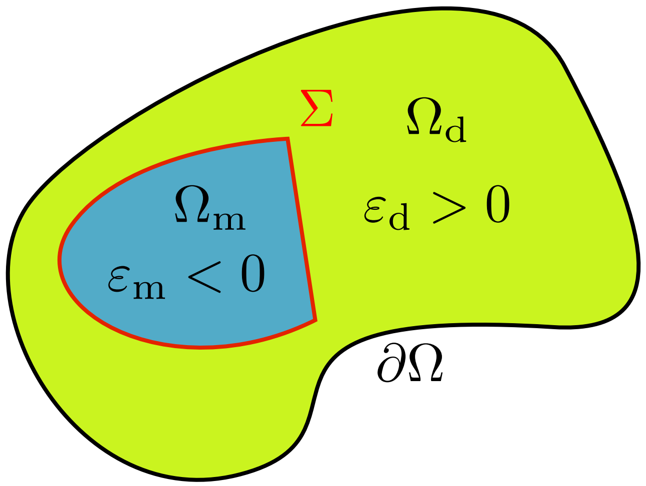

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The variational formulation writes:

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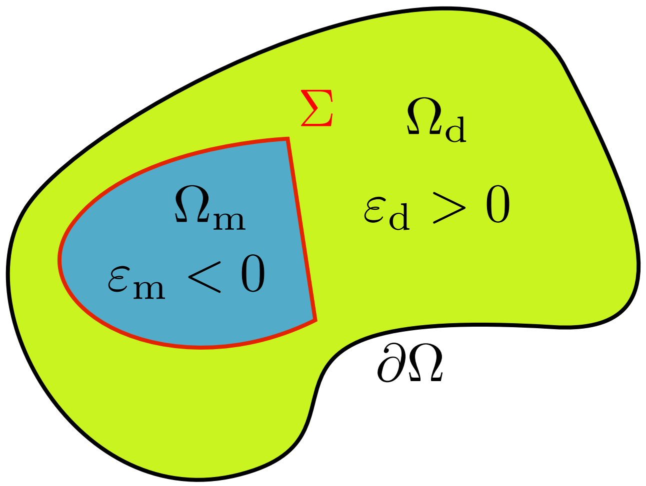

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$$a(u,u) \geq C\|u\|^2_{H_0^1(\Omega)} \quad \forall u \in H_0^1(\Omega)$$

Classically, for $\varepsilon > 0$:

$a(\cdot,\cdot)$ is coercive and $c(\cdot,\cdot)$ is a compact perturbation: problem of Fredholm type.

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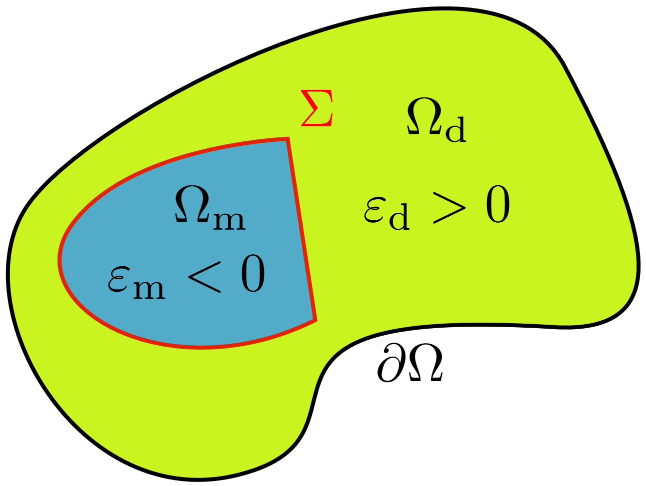

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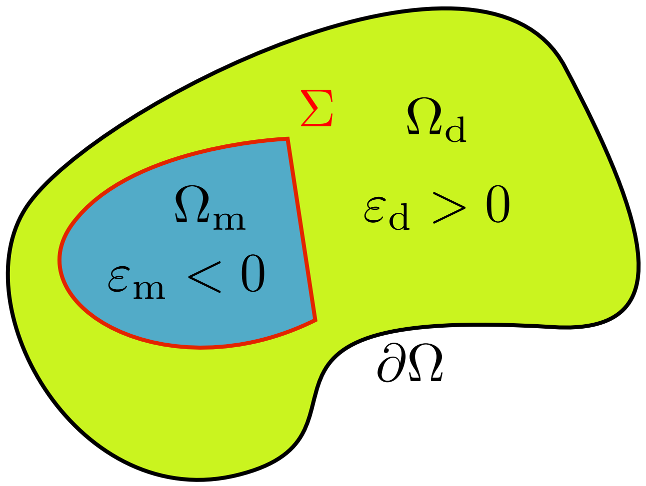

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The problem may be ill-posed for certain values of the contrast $\kappa_\varepsilon := \dfrac{\varepsilon_\mathrm{m}}{\varepsilon_\mathrm{d}} < 0$.

The T-coercivity approach

Find $u \in H_0^1(\Omega)$ such that:

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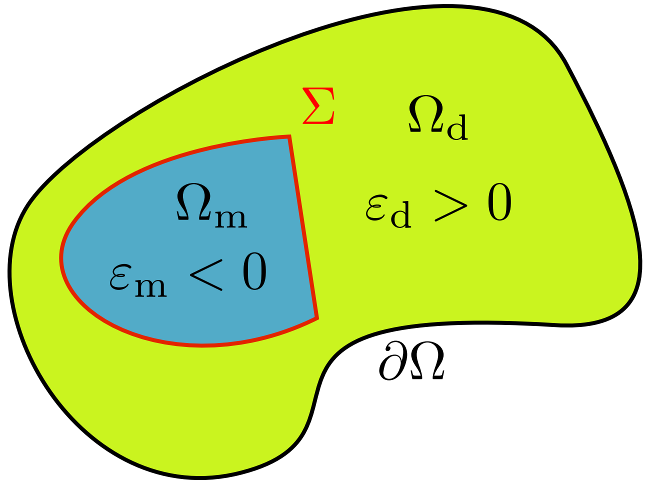

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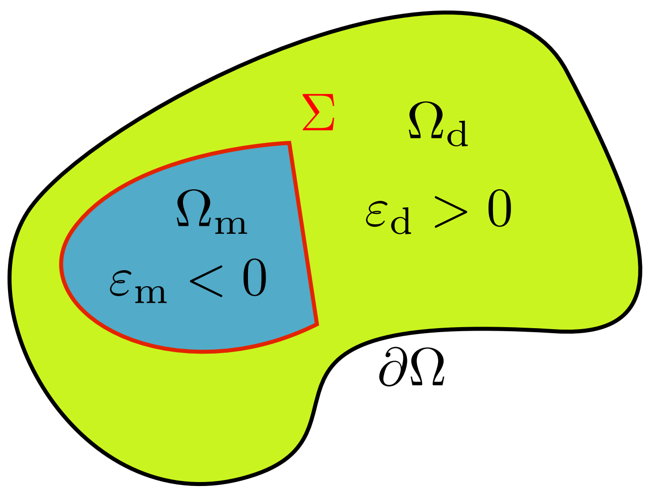

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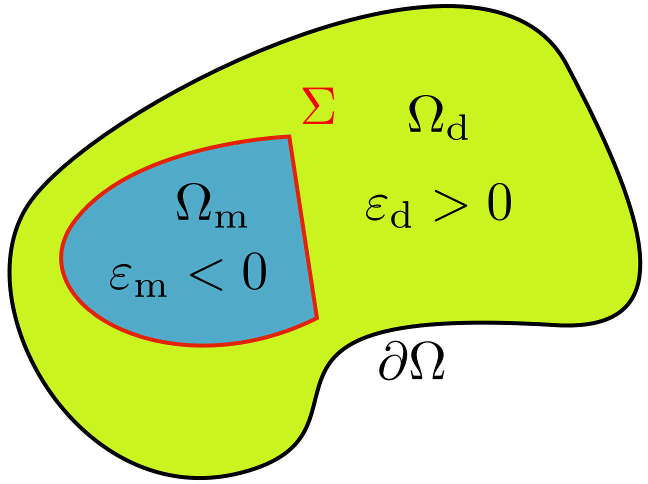

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Idea: build an isomorphism $\mathtt{T}$ of $H_0^1(\Omega)$ such that the following problem is coercive+compact

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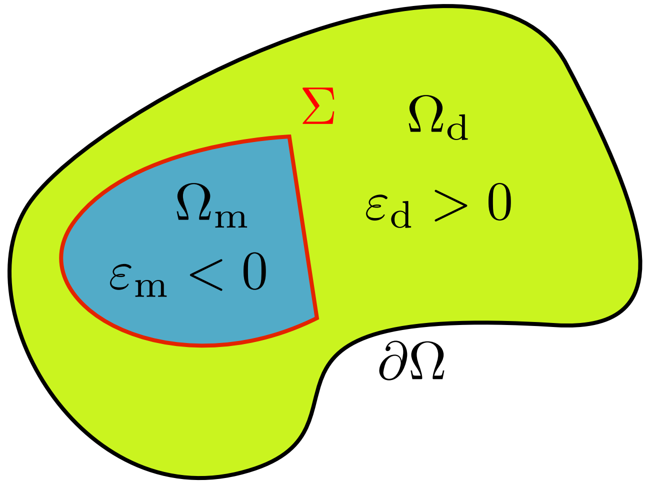

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The problem is of Fredholm type if and only if $\kappa_\varepsilon \notin I_c$, I_c is called critical interval.

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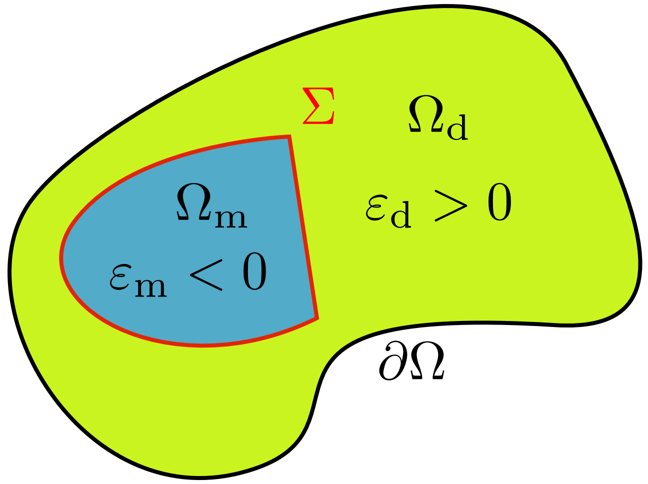

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$$\left| \begin{array}{l} \text{Find } u \in H_0^1(\Omega) \text{ such that:} \\ a(u,\mathtt{T}v) + c(u,\mathtt{T}v) = \langle f, \mathtt{T}v \rangle \quad \forall v \in H_0^1(\Omega) \end{array} \right.$$

Introduced in Zwölf (2008).

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I_c always contain $\{-1\}$.

The T-coercivity approach

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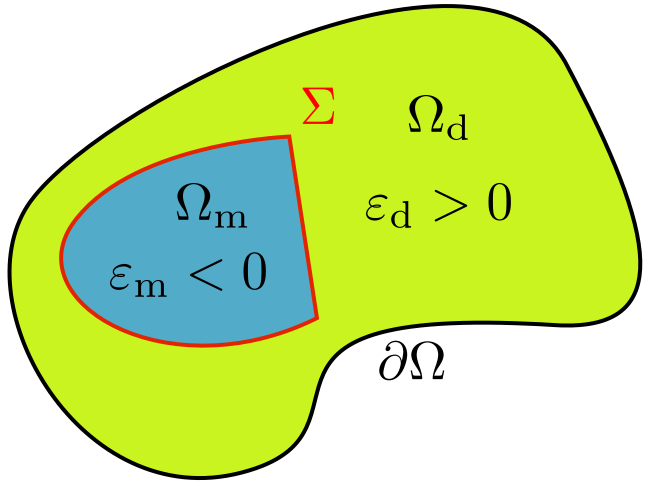
$$\kappa_\varepsilon := \frac{\varepsilon_\mathrm{m}}{\varepsilon_\mathrm{d}} < 0$$



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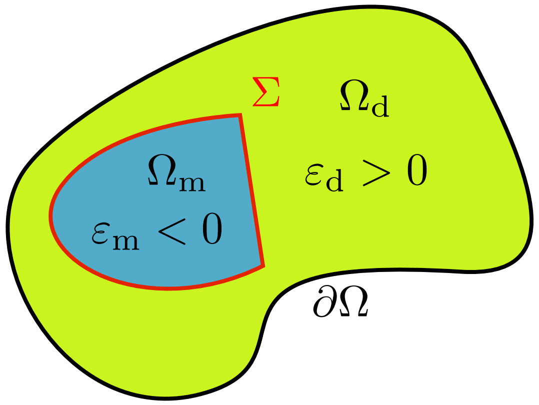
The case $\kappa_\varepsilon = -1$ is particularly problematic, we will not talk about it.

Ola (1995), Nguyen (2015).

Results

$$\left|\begin{array}{l}\text{Find } u \in H_0^1(\Omega) \text{ such that:} \\ \operatorname{div}(\varepsilon^{-1}\nabla u) + \omega^2 \mu u = -f \quad \text{in } \Omega\end{array}\right.$$



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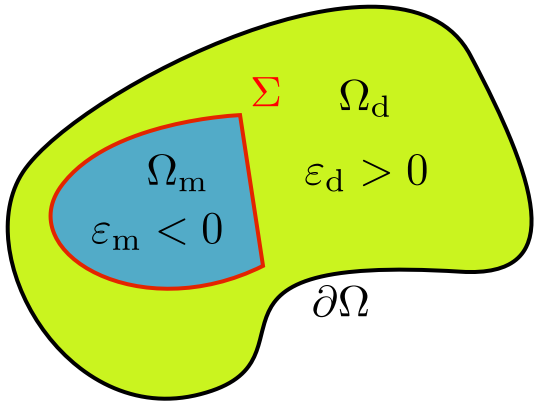

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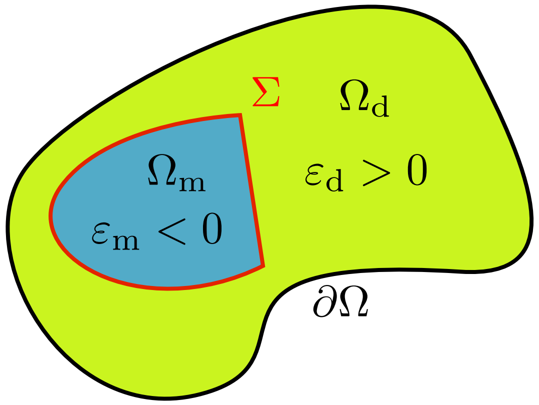

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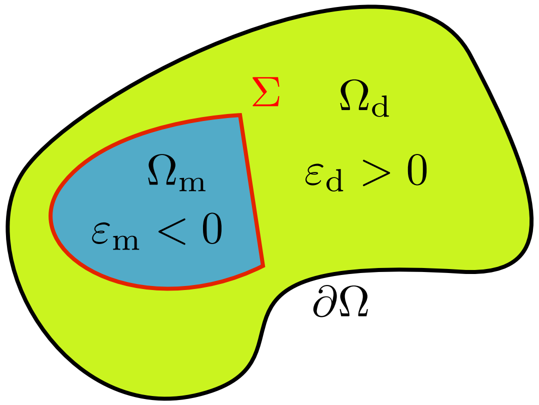

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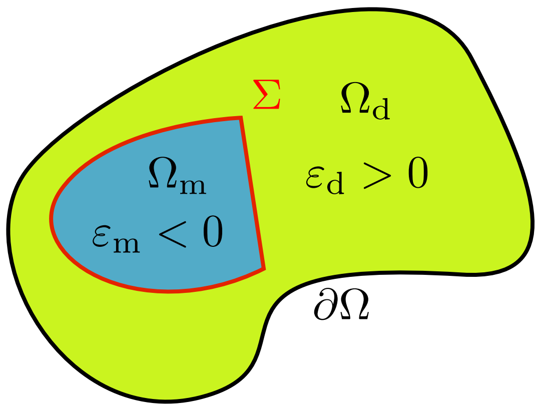

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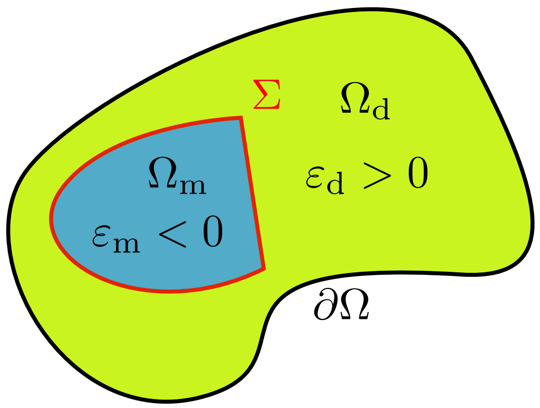

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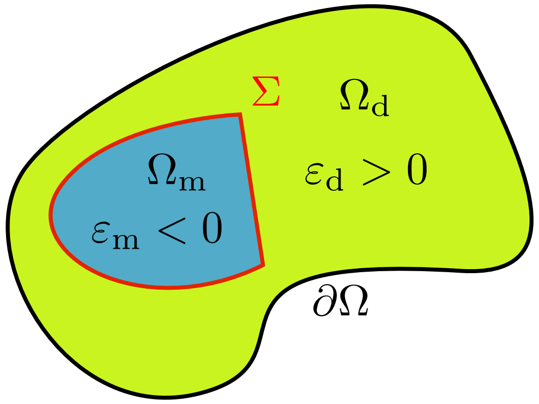

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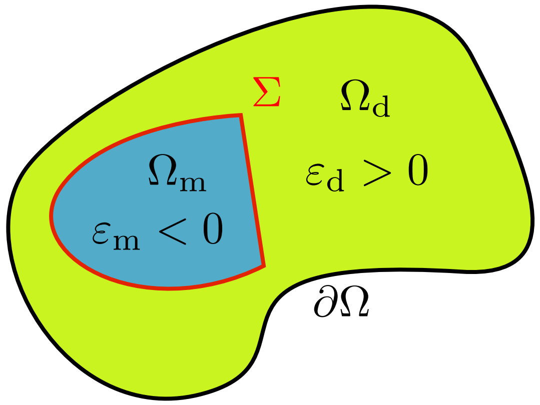

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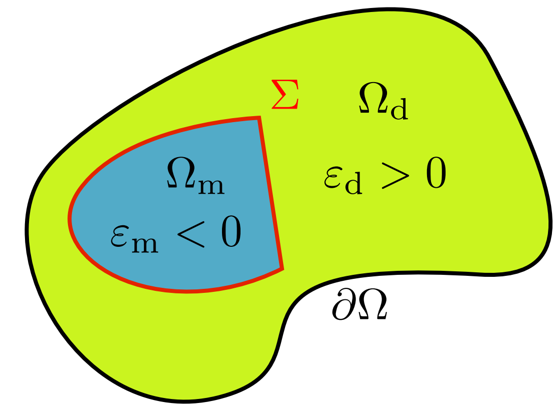

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Outline

- Part I: meshing rules for the corners case for $\kappa_\varepsilon \notin I_c$
- Part II: scattering problem with sign-changing coefficients
- Perspectives

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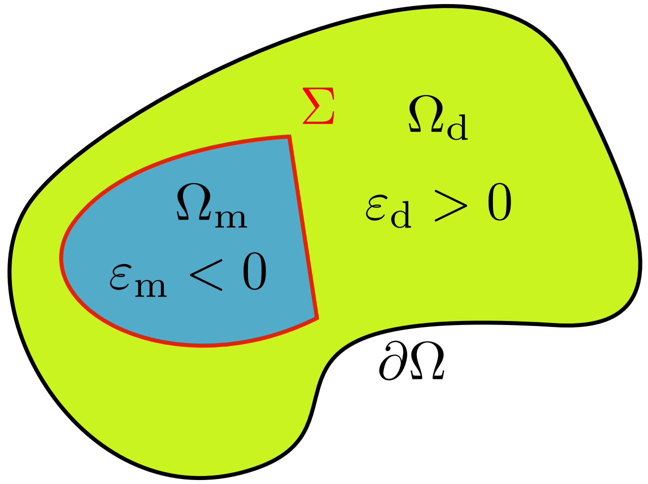
- Part I: meshing rules for the corners case for $\kappa_\varepsilon \notin I_c$

Transmission problem and T-coercivity

Goal: build an isomorphism $\mathtt{T}$ of $H^1_0(\Omega)$ such that the form a is $\mathtt{T}$-coercive: $\forall u \in H^1_0(\Omega)$

$$\boxed{a(u, \mathtt{T}u) \geq C\|u\|^2_{H^1_0(\Omega)} \quad \text{with} \quad a(u,v) = \int_\Omega \varepsilon^{-1}\nabla u \cdot \overline{\nabla v}}$$



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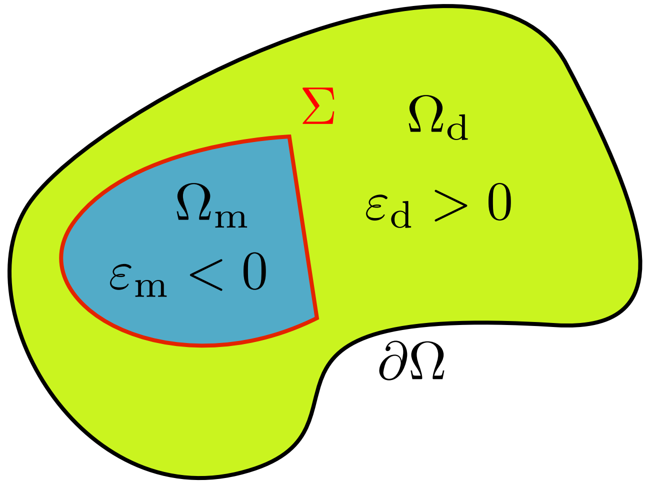

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1) compensate the change of sign of ε

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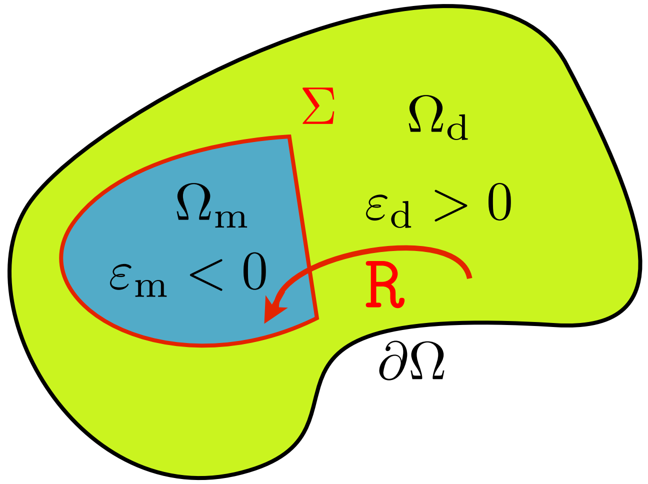

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$$\mathtt{T}u = \begin{cases} u_\mathrm{d} & \text{in } \Omega_\mathrm{d} \\ -u_\mathrm{m} + 2\mathtt{R}u_\mathrm{d} & \text{in } \Omega_\mathrm{m} \end{cases}$$

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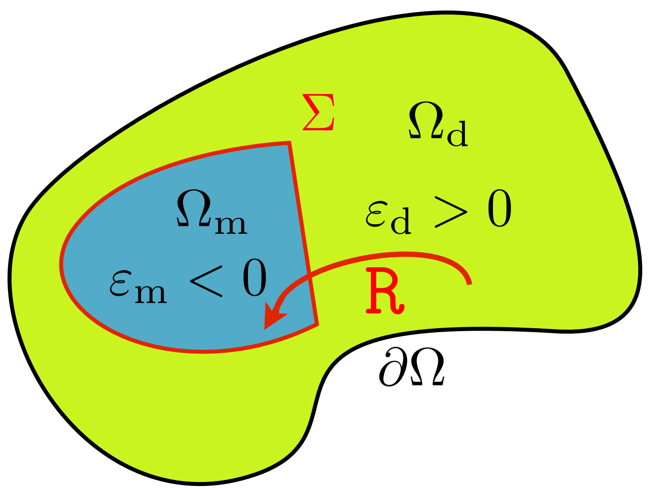

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$\mathtt{R}$ is a linear continuous operator from Ω_{d} into Ω_{m} such that $\mathtt{R}u|_\Sigma = u|_\Sigma$

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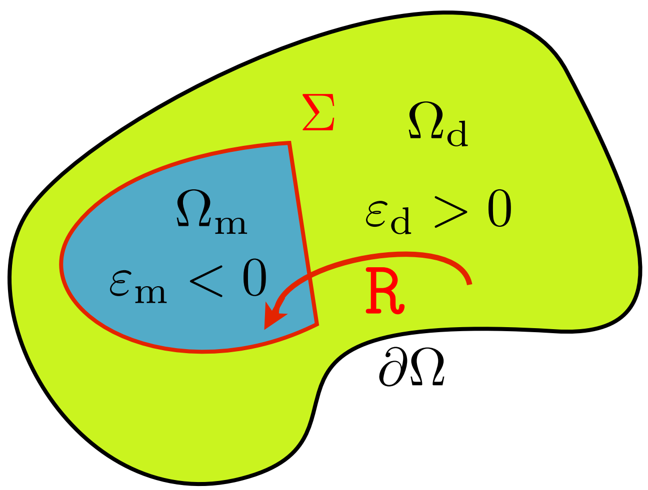

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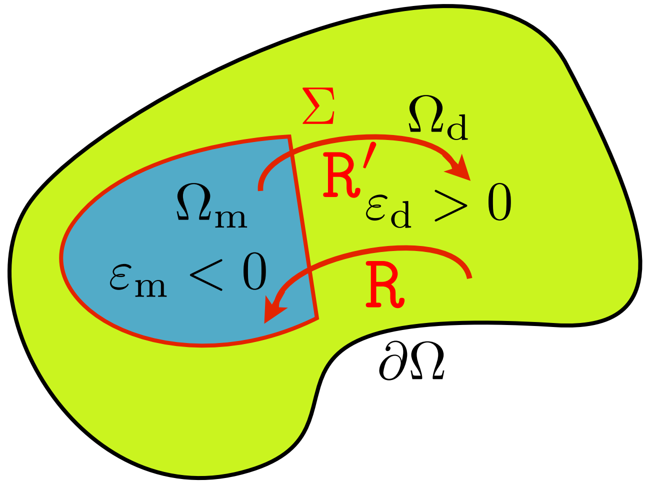

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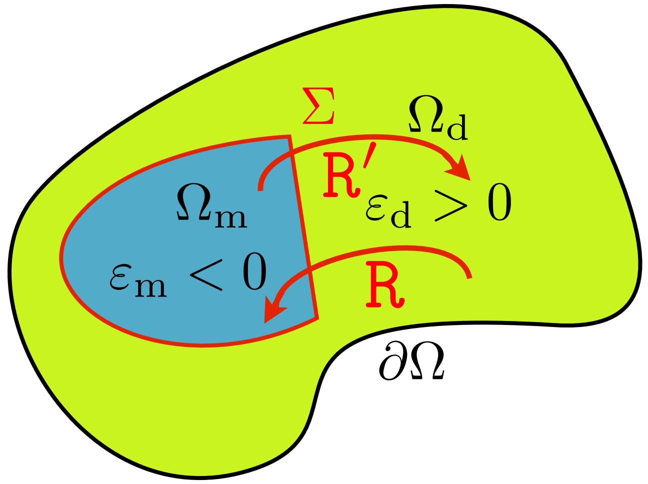

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Theorem. The form is $\mathtt{T}$-coercive if $\kappa_\varepsilon \notin [-\|\mathtt{R}'\|^2; -1/\|\mathtt{R}\|^2]$

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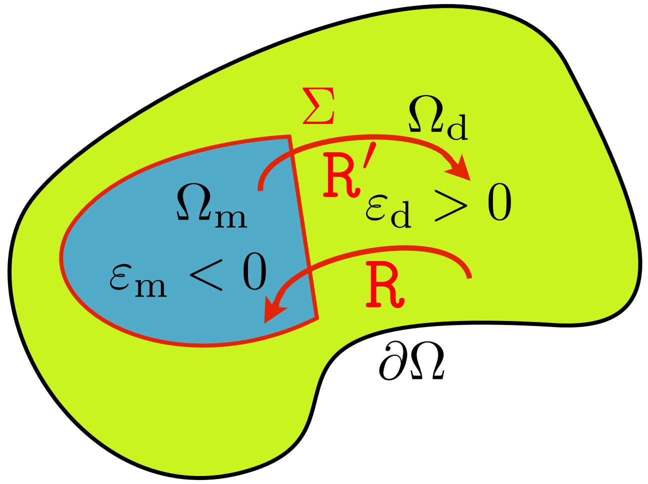

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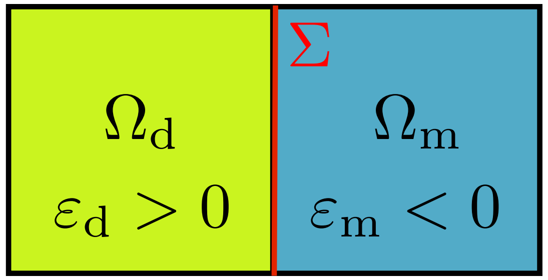
Next : build operators $\mathtt{R}$, $\mathtt{R}'$ minimizing the interval. To do so we use elementary geometrical transforms (symmetries, angular dilations, ...).

$$\boxed{\mathtt{R}u(x) = u(\mathcal{R}(x))}$$

Some examples

For a symmetric domain (w.r.t. Σ) :



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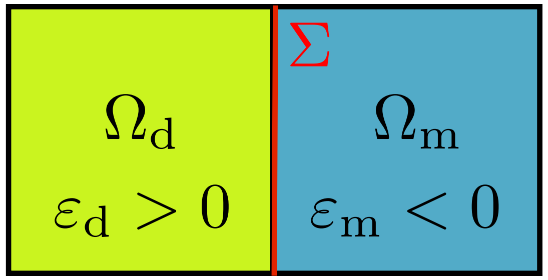

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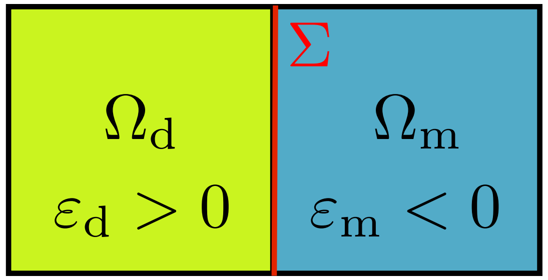

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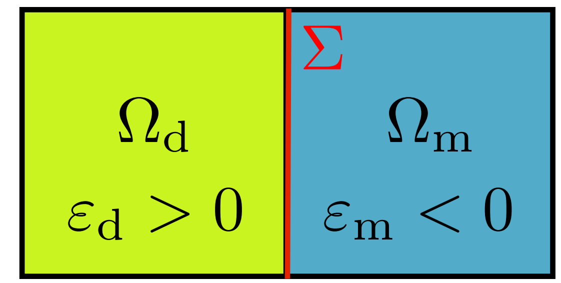
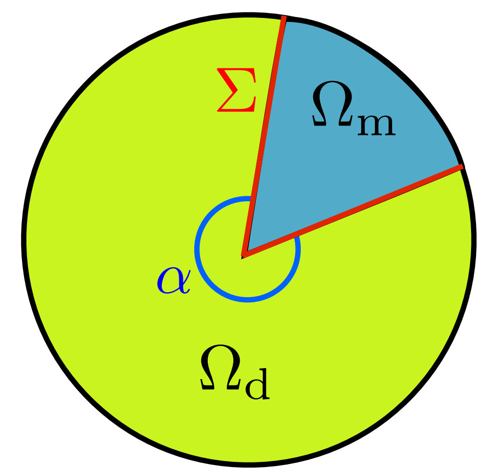


For an angular sector of aperture α:



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

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For a symmetric domain (w.r.t. Σ) :

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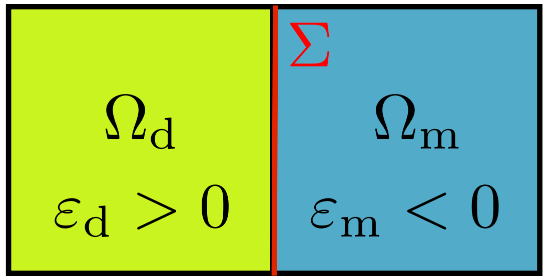

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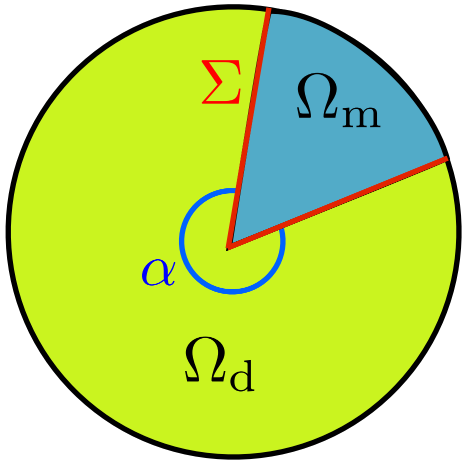

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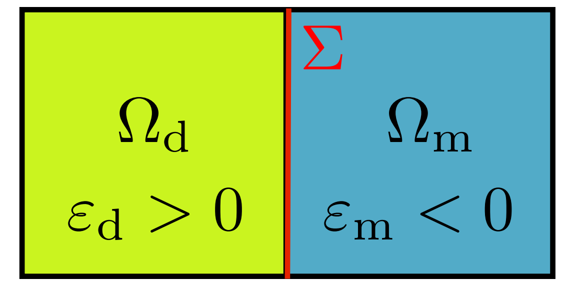

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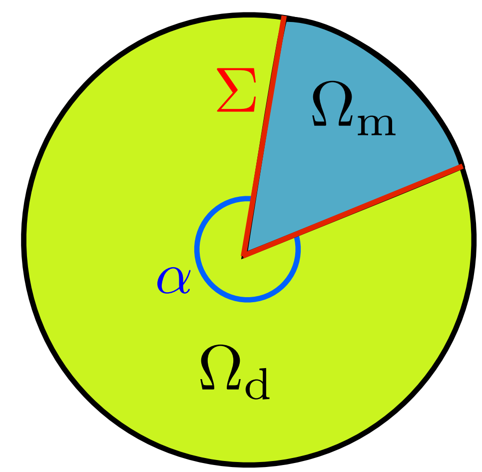

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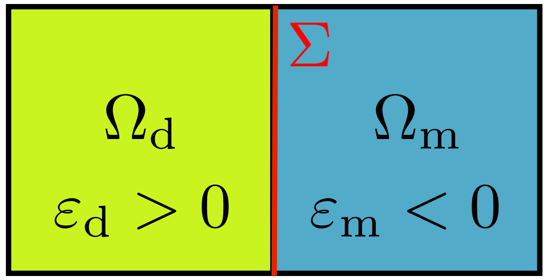

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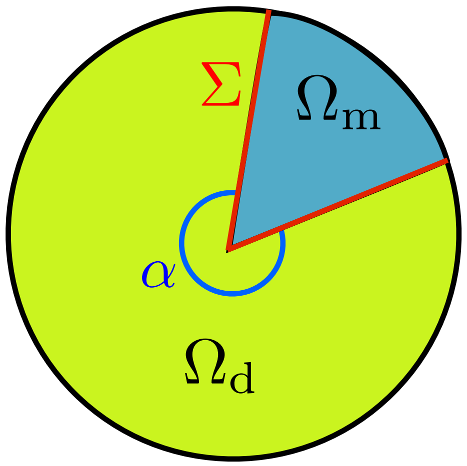

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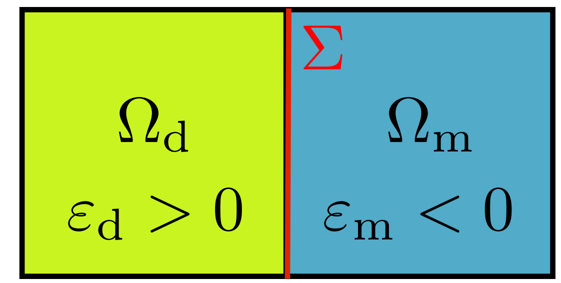

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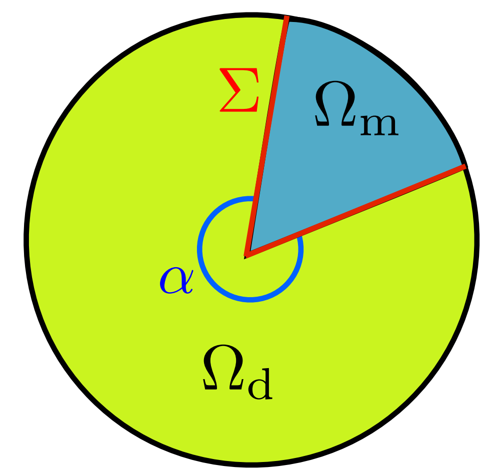

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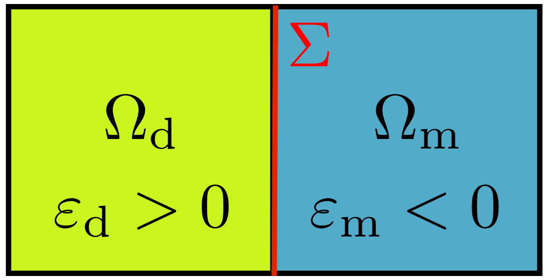

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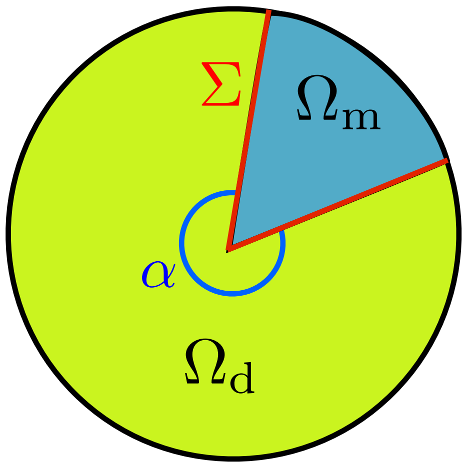

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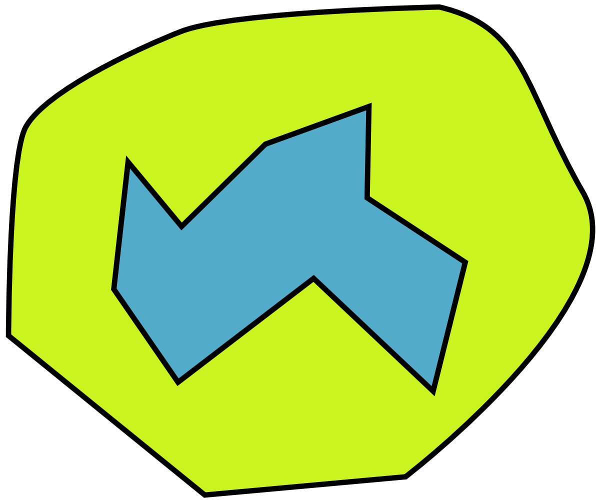
Case of a polygonal interface

For a polygonal interface, one simply use locally the two previous cases.



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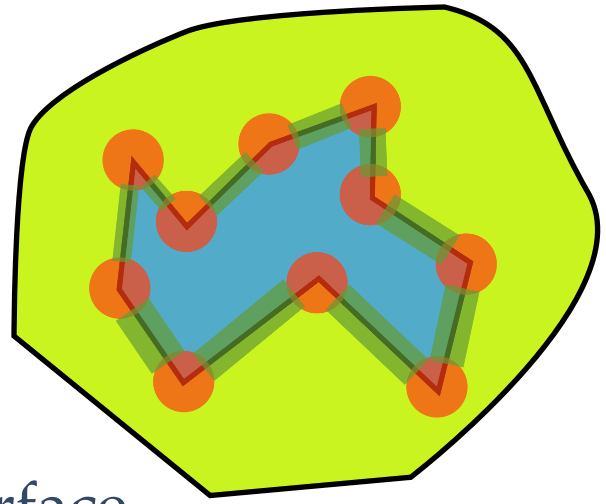

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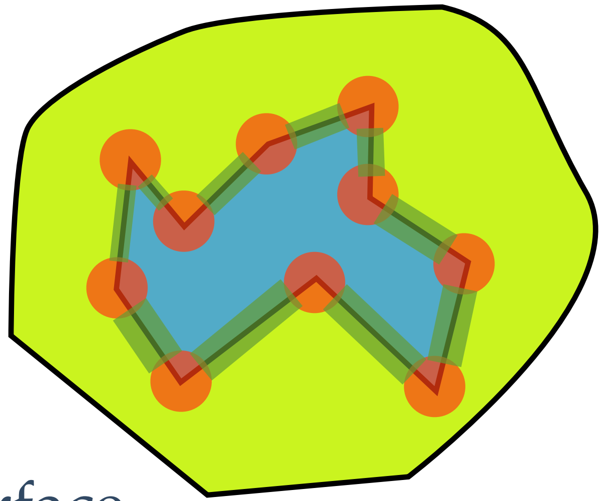

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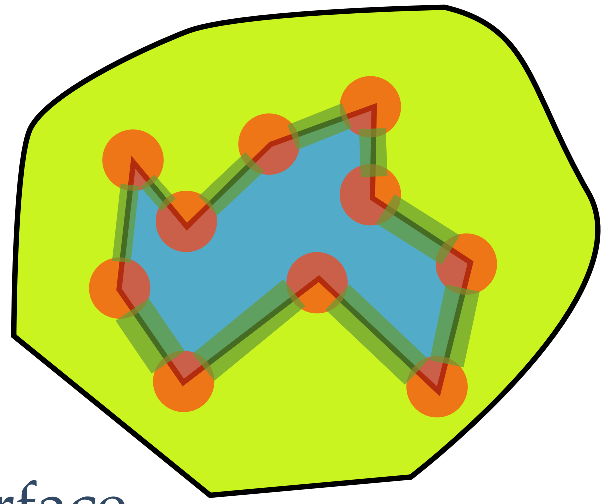

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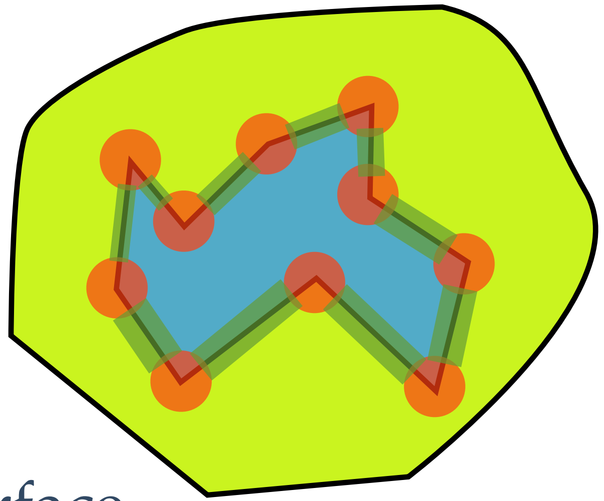

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What about the discretization ?

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Chesnel, Ciarlet (2013).

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Consider the same degree of approximation from each side of Σ .
Then $\mathtt{T}(V^h) \subset V^h$ corresponds to a simple condition on the mesh.

Chesnel, Ciarlet (2013).

Conformity for simple cases

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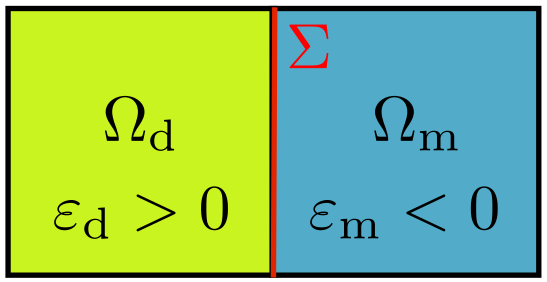

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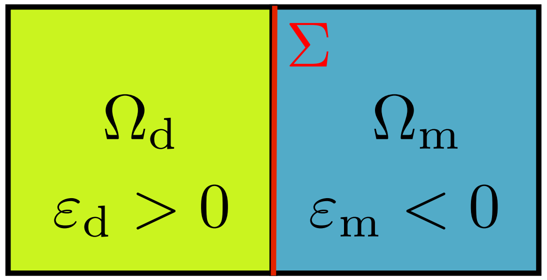

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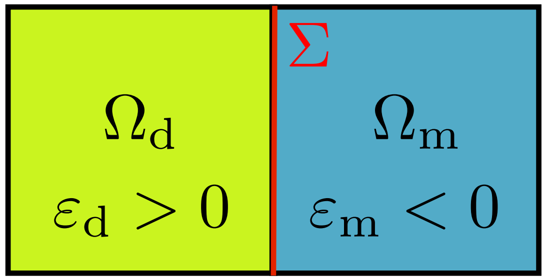

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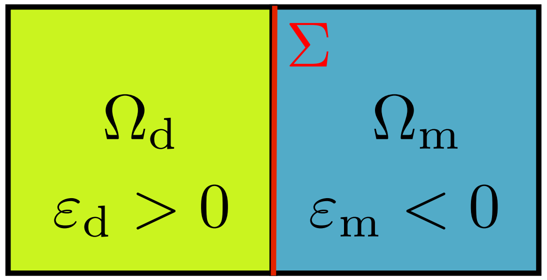

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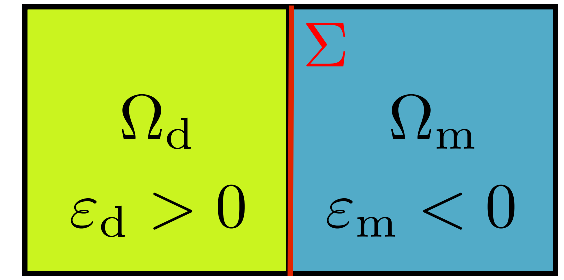

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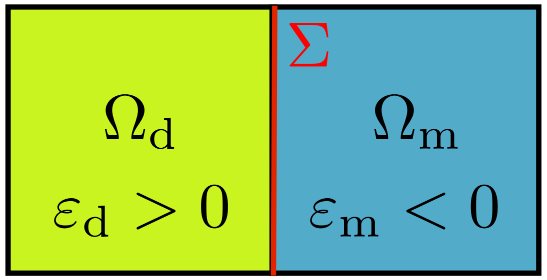

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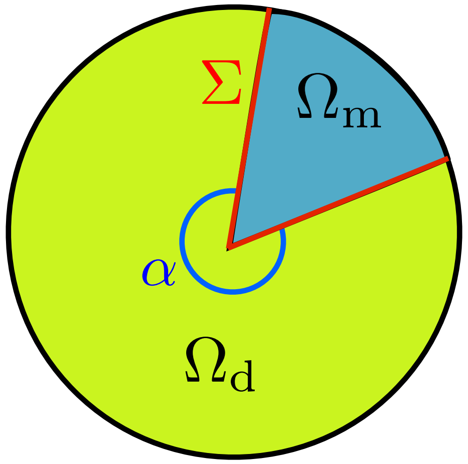
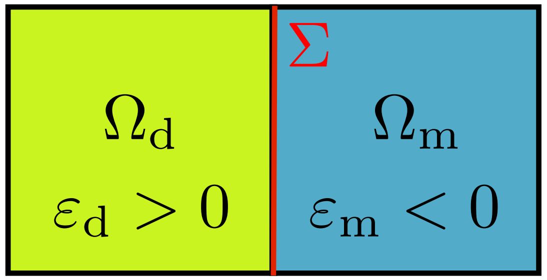


Unfortunately with the considered operators $\mathtt{T}(V^h) \not\subset V^h$
because angular dilations do not respect the polynomial
nature of the basic functions...

Conformity for simple cases

For a symmetric domain (w.r.t. Σ) :

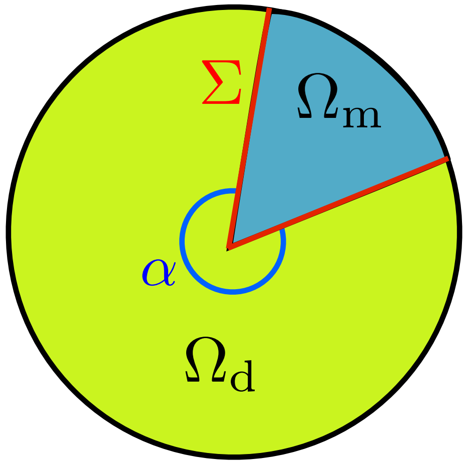


If the mesh is symmetric, then $\mathtt{T}(V^h) = V^h$.

If $\kappa_\varepsilon \neq -1$, and if the mesh is symmetric, then FE convergence.

We say that the mesh is T-conform.
One can also apply locally this conformity in the neighborhood of the interface.
We say that the mesh is locally T-conform.

For an angular sector of aperture α:

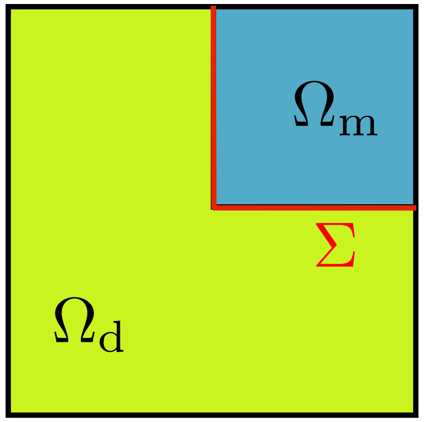


Unfortunately with the considered operators $\mathtt{T}(V^h) \not\subset V^h$ because angular dilations do not respect the polynomial nature of the basic functions...

Can we find other optimal operators $\mathtt{R}$ satisfying this $\mathtt{T}$-conformity ?

The corners's problem

Consider the particular case of a right angle.



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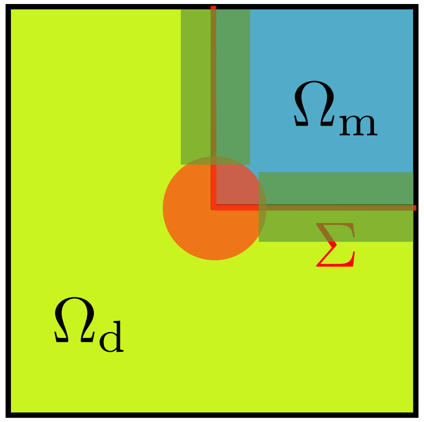

Bonnet-Ben Dhia, Chesnel, Ciarlet (2012).

$$\mathtt{T}u = \begin{cases} u_{\mathrm{d}} & \text{in } \Omega_{\mathrm{d}} \\ -u_{\mathrm{m}} + 2\sum_p \chi_p \mathtt{R_p} u_{\mathrm{d}} & \text{in } \Omega_{\mathrm{m}} \end{cases}$$

The problem is Fredholm iff $\kappa_\varepsilon \notin I_c := [-3; -1/3]$.

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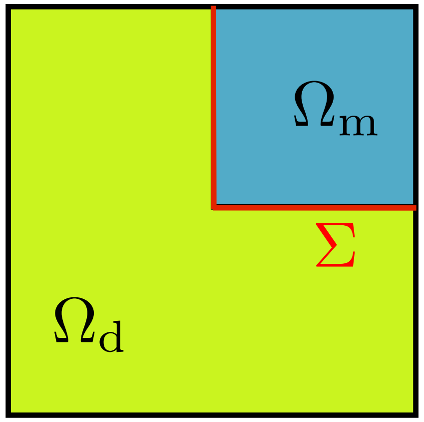
Another optimal operator $\mathtt{T}$ based on symmetries has been proposed.

Nicaise, Venel (2011).



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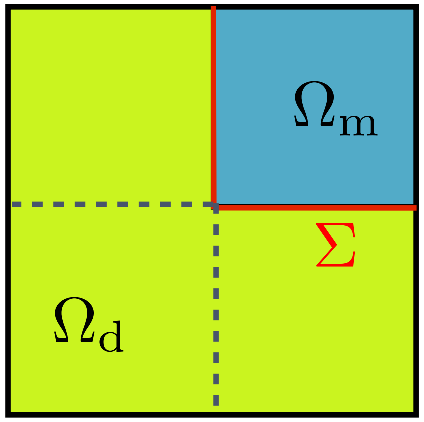

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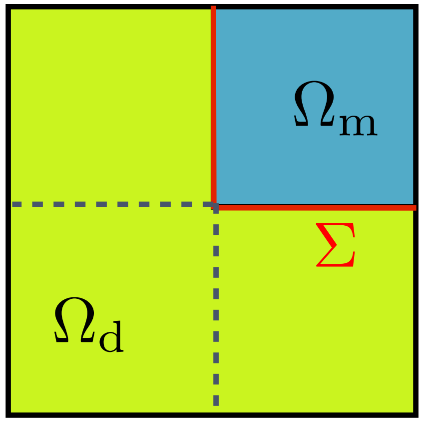

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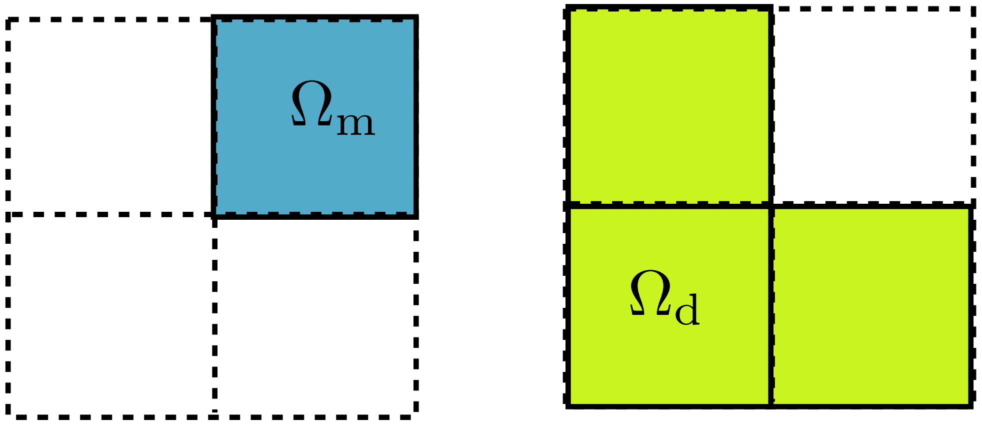

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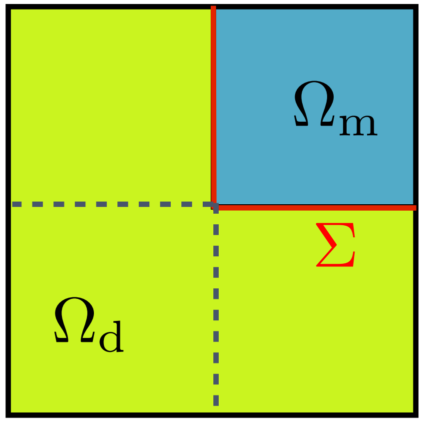

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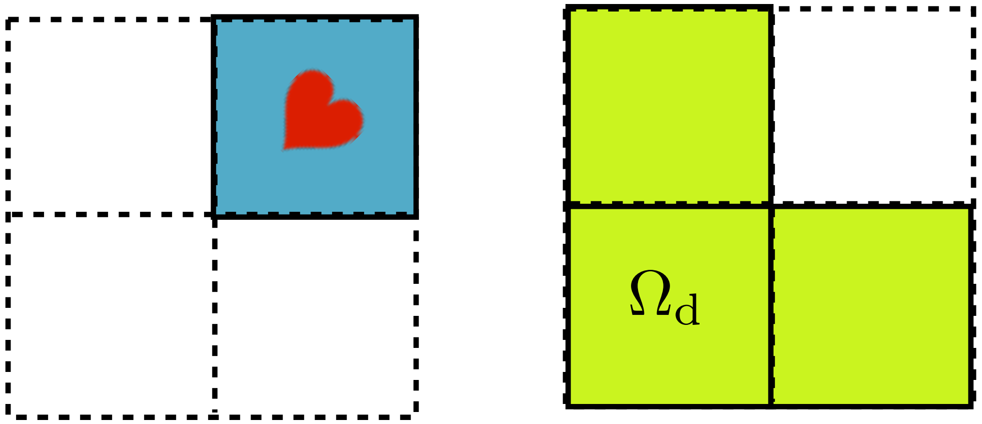

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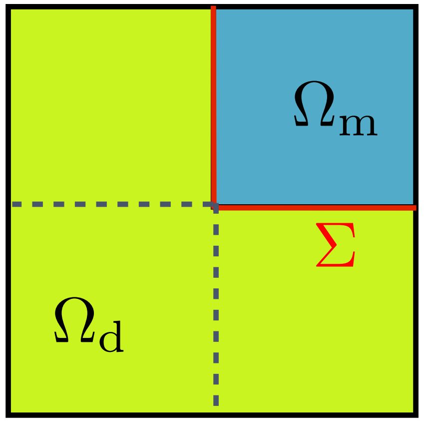

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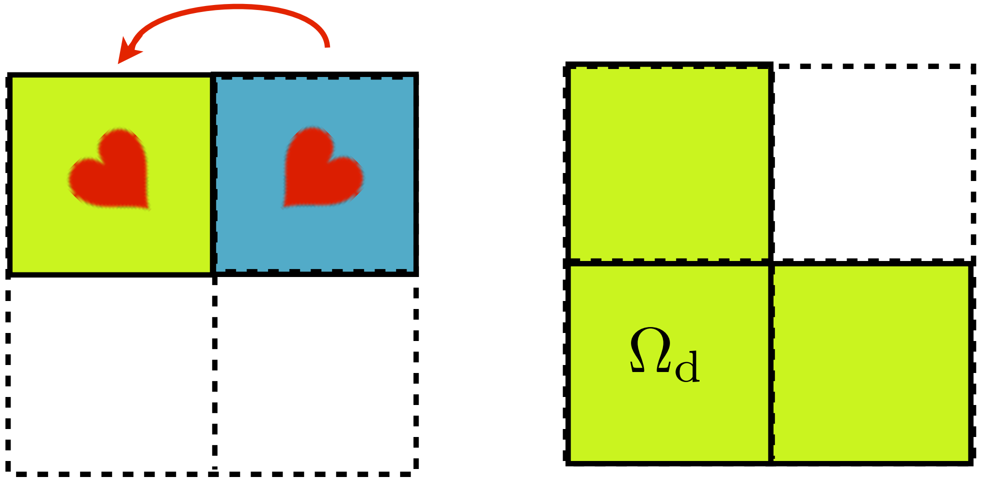

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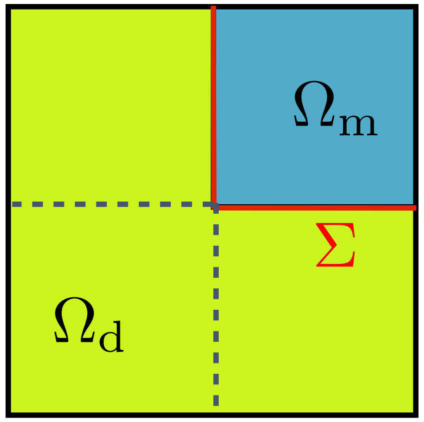

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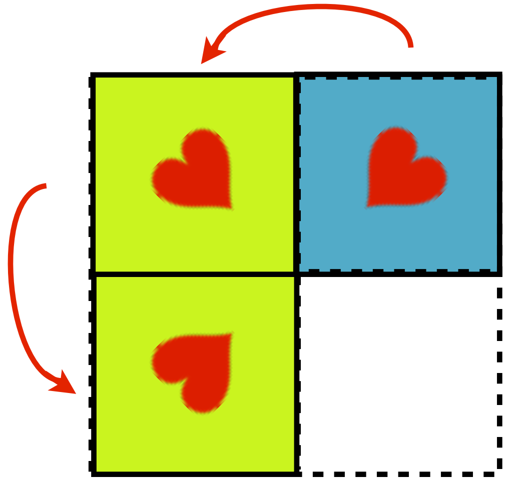

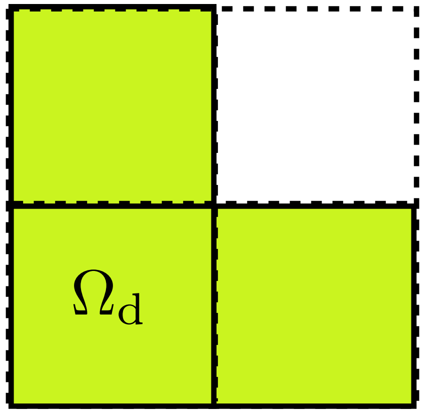

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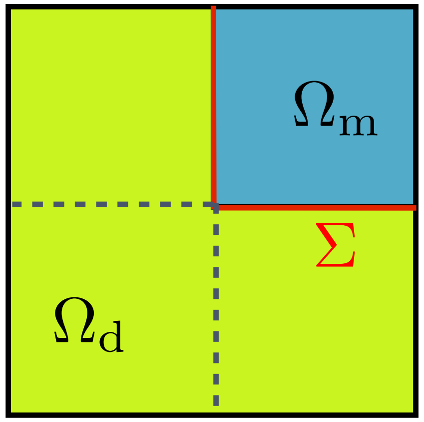

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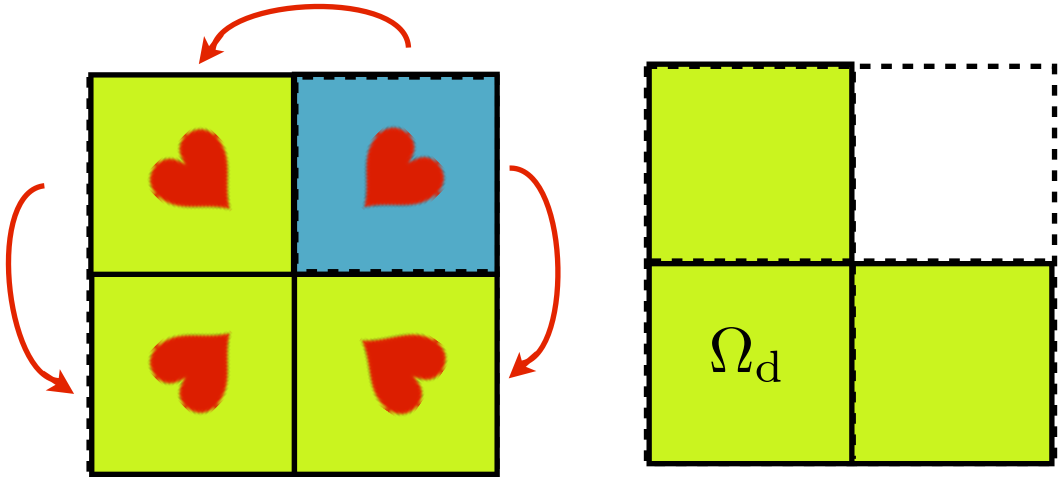

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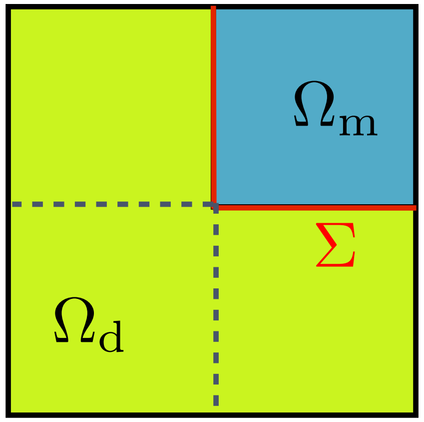

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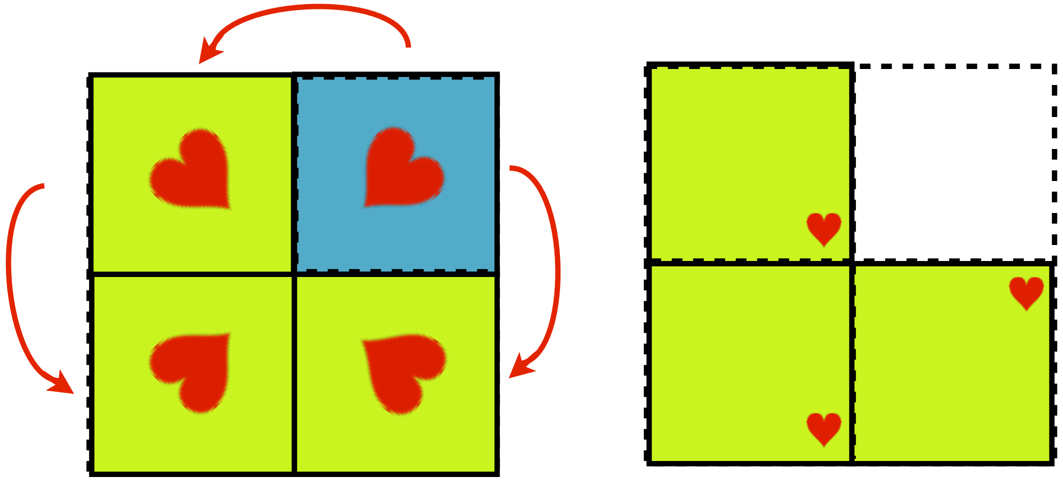

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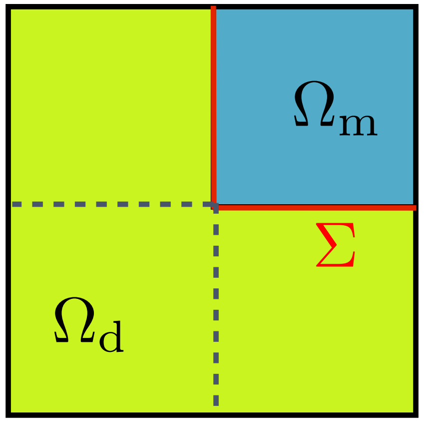

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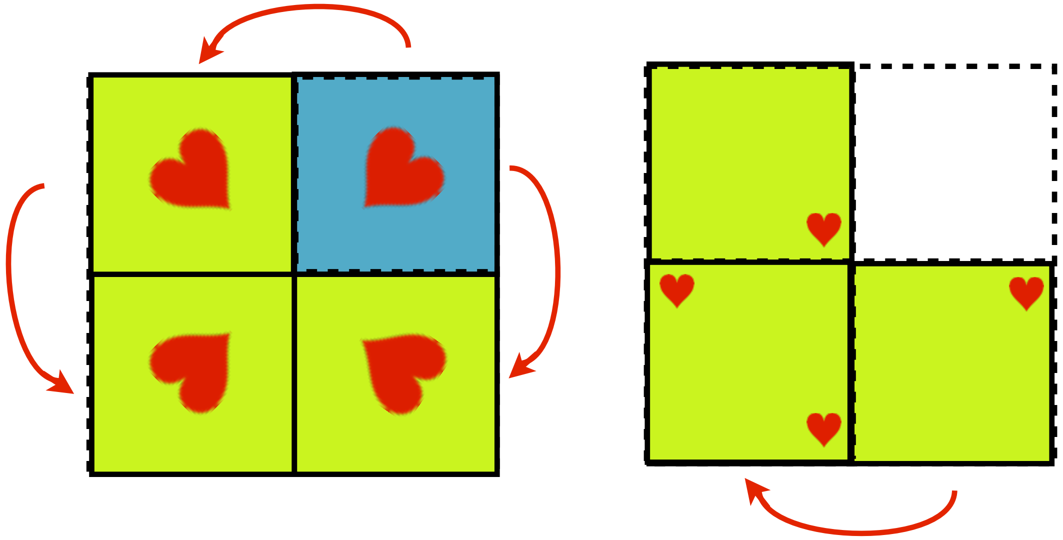

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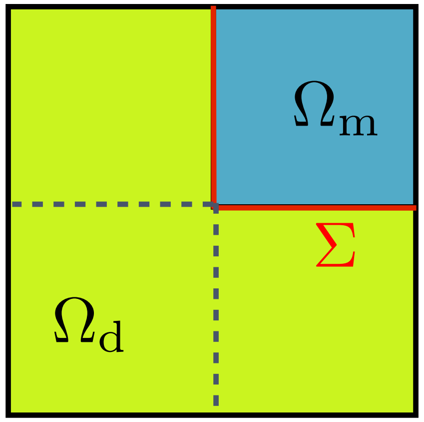

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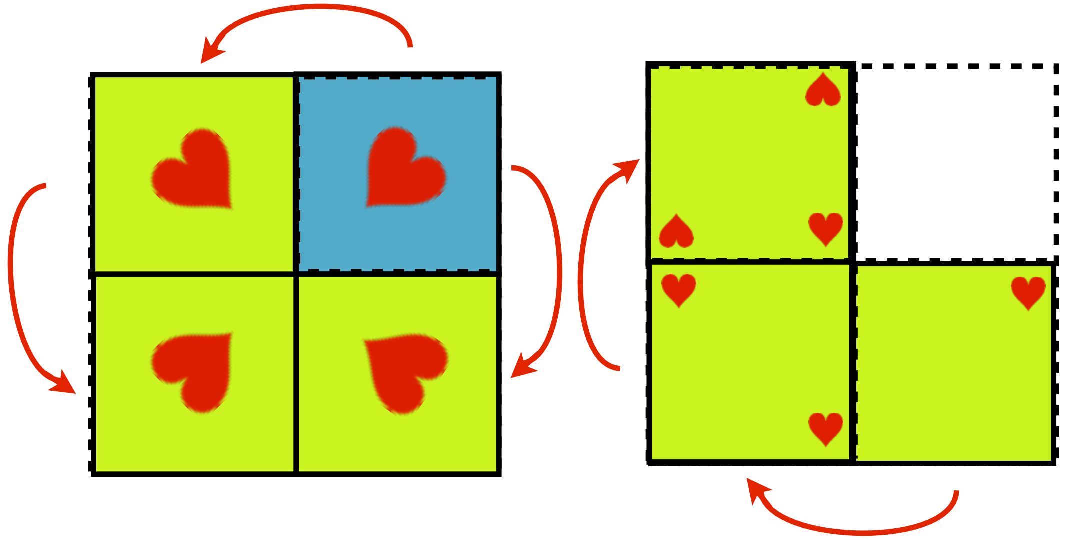

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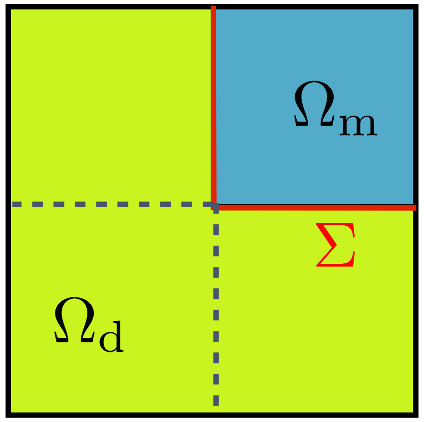

Nicaise, Venel (2011).

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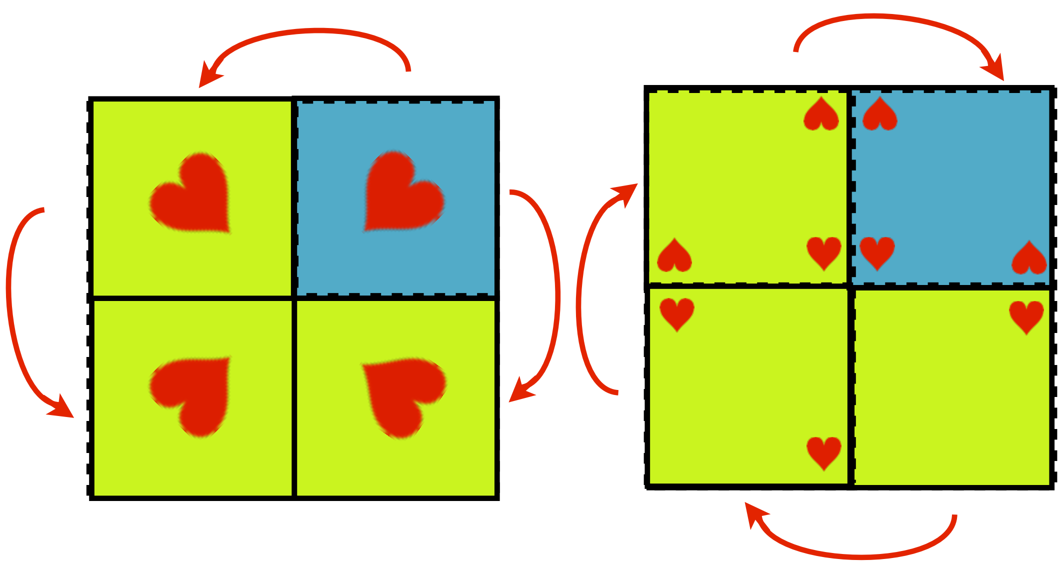
R is based on axial symmetries.



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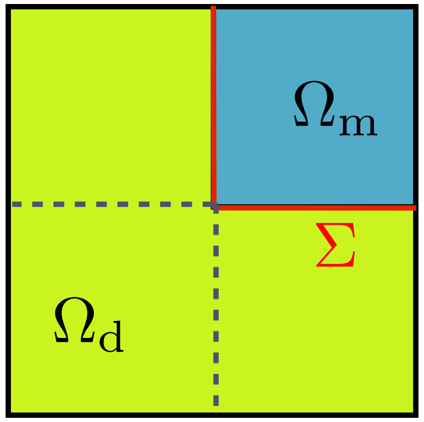

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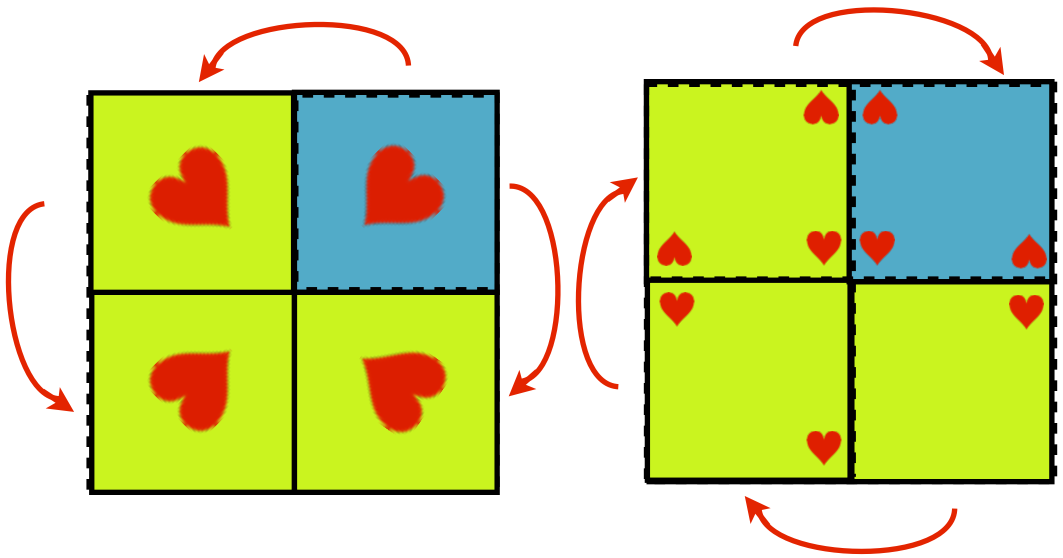

$$\|\mathtt{R}\|^2 = \|\mathtt{R}'\|^2 = 3$$

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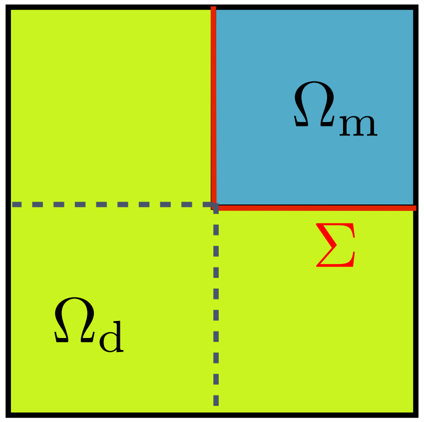

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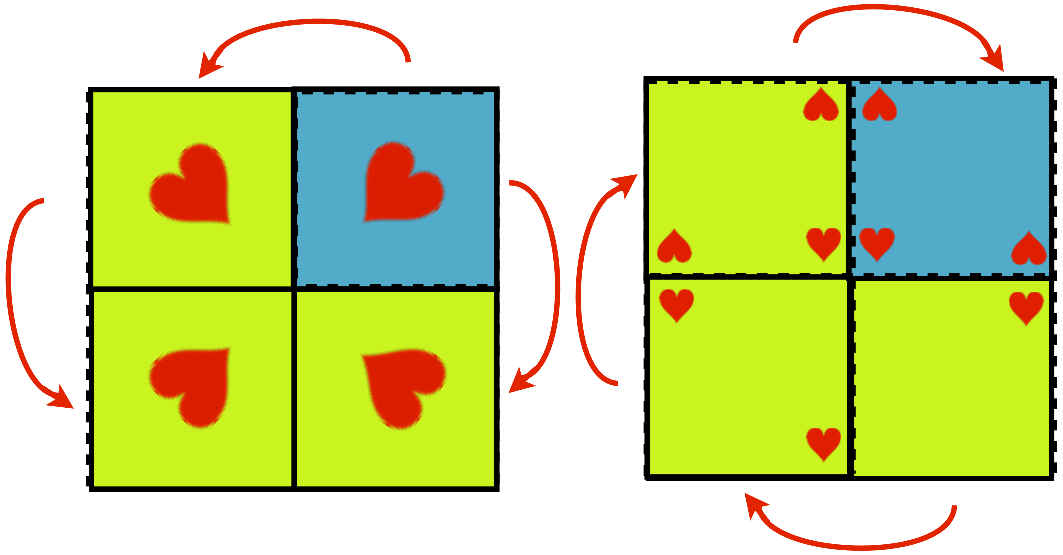

$$\|\mathtt{R}\|^2 = \|\mathtt{R}'\|^2 = 3$$

If the mesh is symmetric with respect to the two axes, then $\mathtt{T}(V^h) \subset V^h$.

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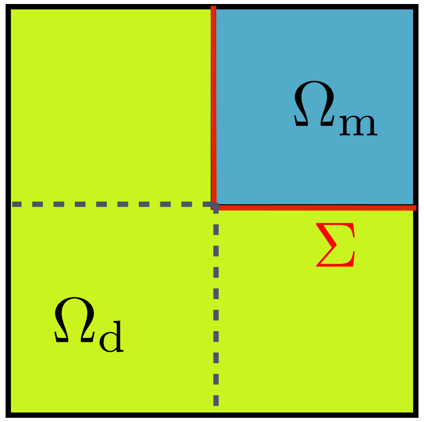

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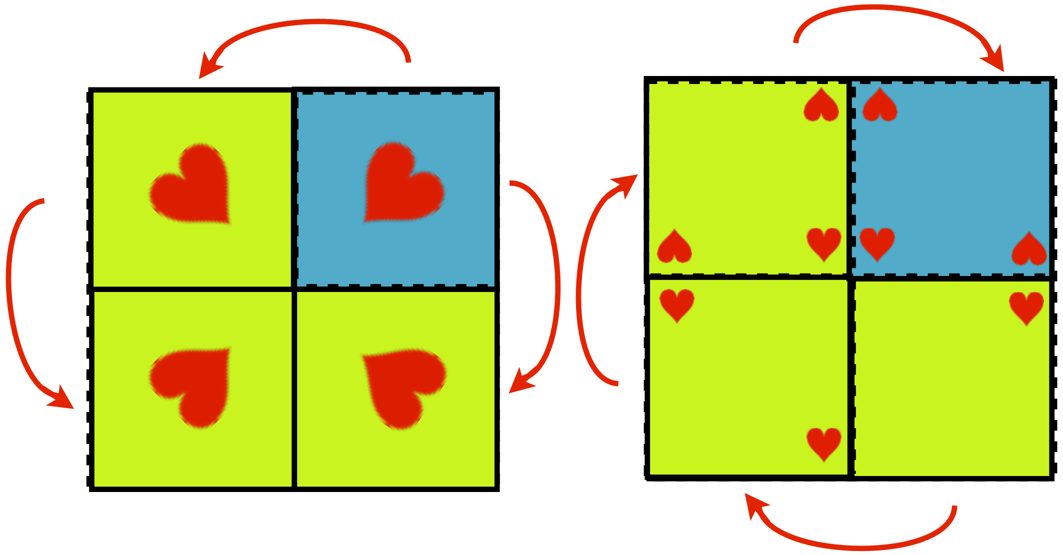


$$\|\mathtt{R}\|^2 = \|\mathtt{R}'\|^2 = 3$$

If the mesh is symmetric with respect to the two axes, then $\mathtt{T}(V^h) \subset V^h$.

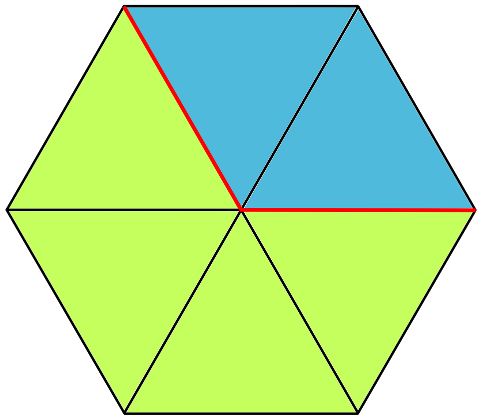
Idea : generalize these isometry-based operators $\mathtt{R}$ for any angle.

Bonnet-Ben Dhia, C., Ciarlet in preparation.

Folding operators and tillings rules

One can generalize this folding method using symmetry-based and rotation-based operators.

Example of a folding operator from Ω_{m} to Ω_{d} for an angle $\alpha = \dfrac{4\pi}{3}$.



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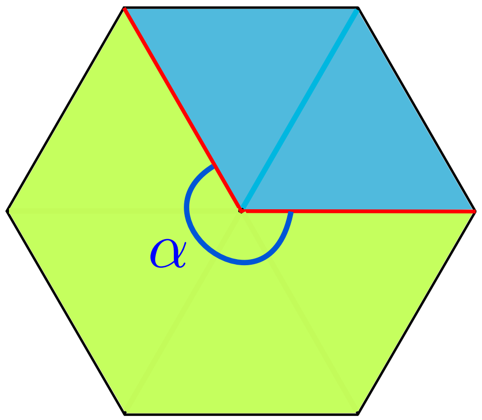

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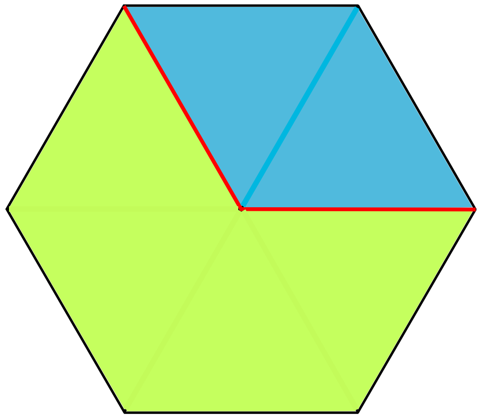

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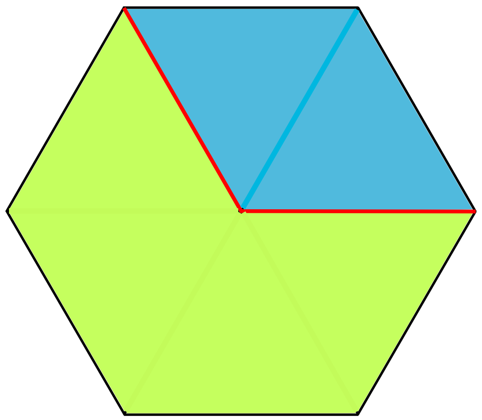

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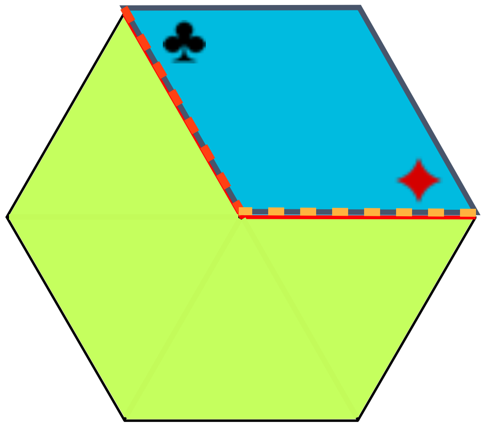

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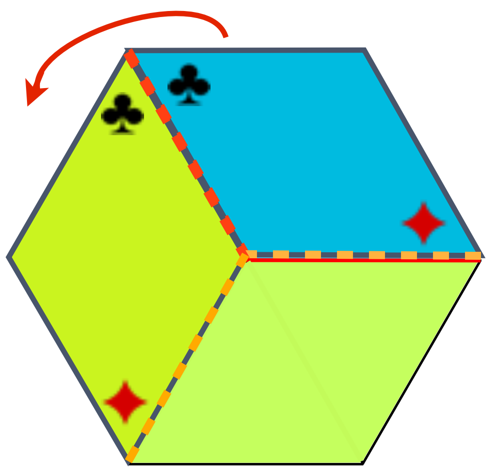

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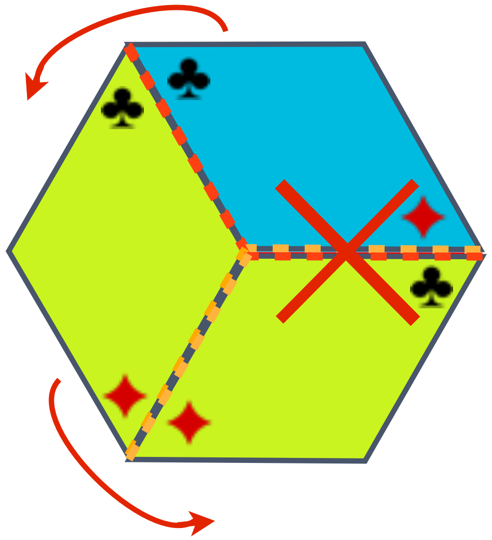

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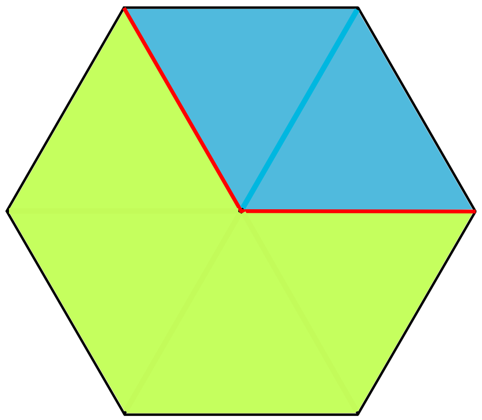

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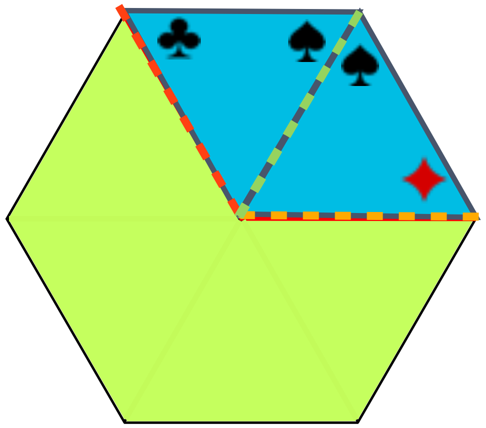

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Example of a folding operator from $\Omega_{\rm m}$ to $\Omega_{\rm d}$ for an angle $\alpha = \dfrac{4\pi}{3}$.

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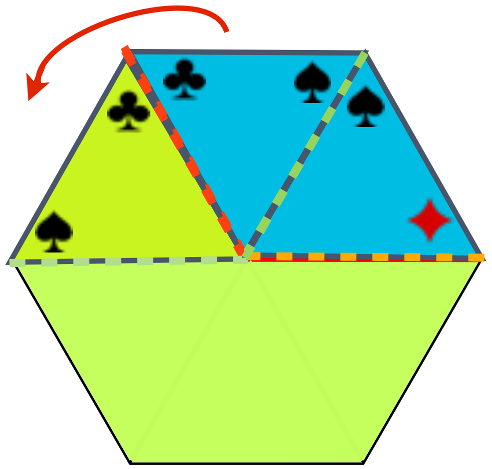

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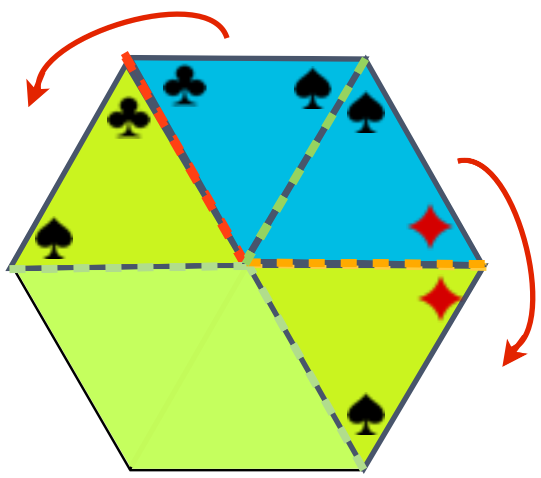

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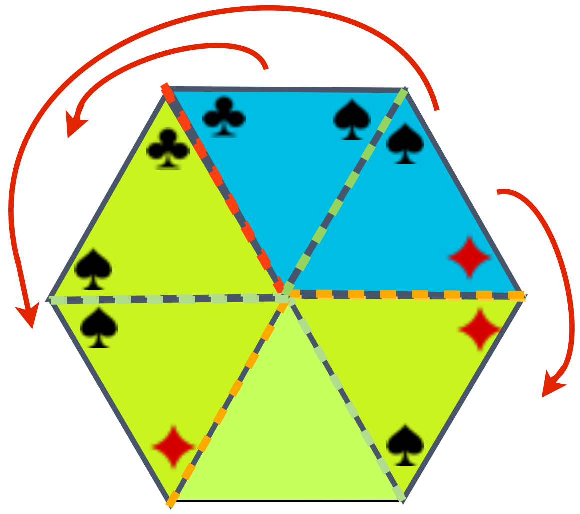

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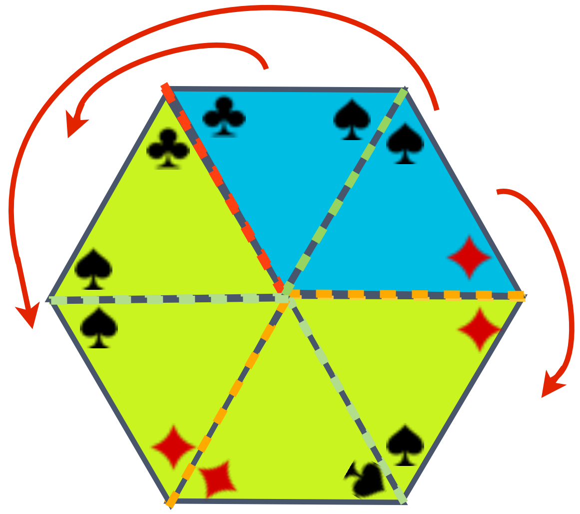

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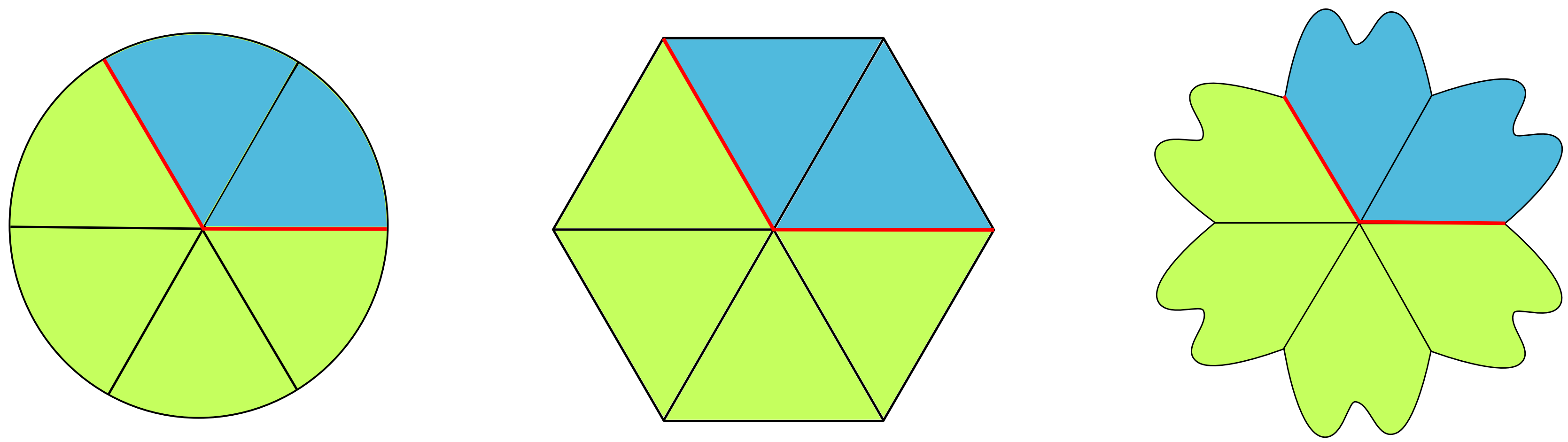

Once the pattern is chosen, for any form, one builds the T-conforming mesh by duplicating the pattern by symmetries.

Folding operators and tillings rules

One can generalize this folding method using symmetry-based and rotation-based operators.

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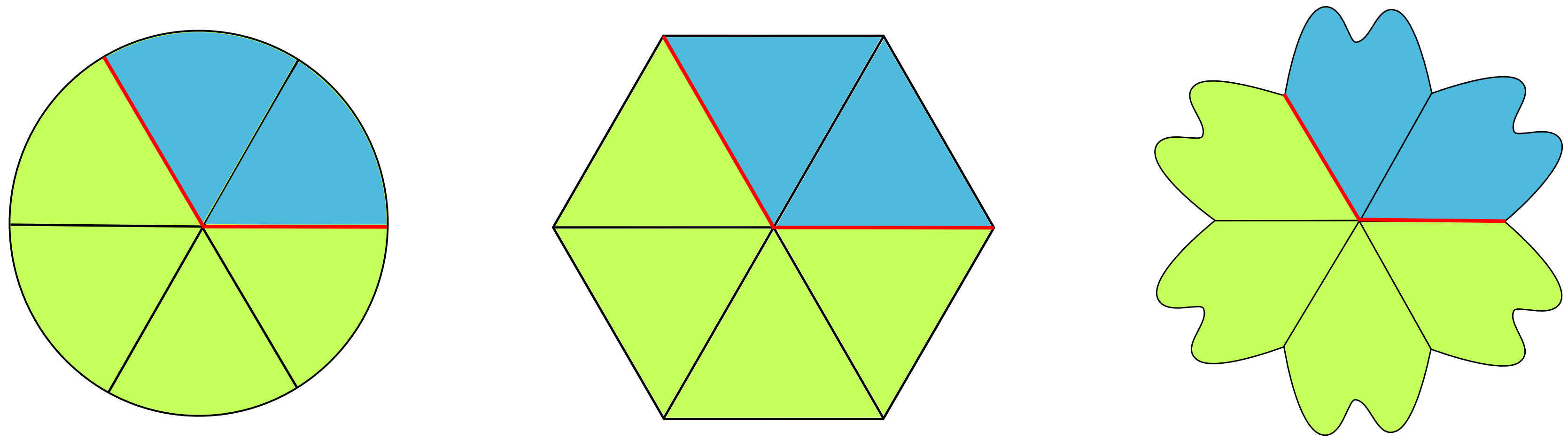

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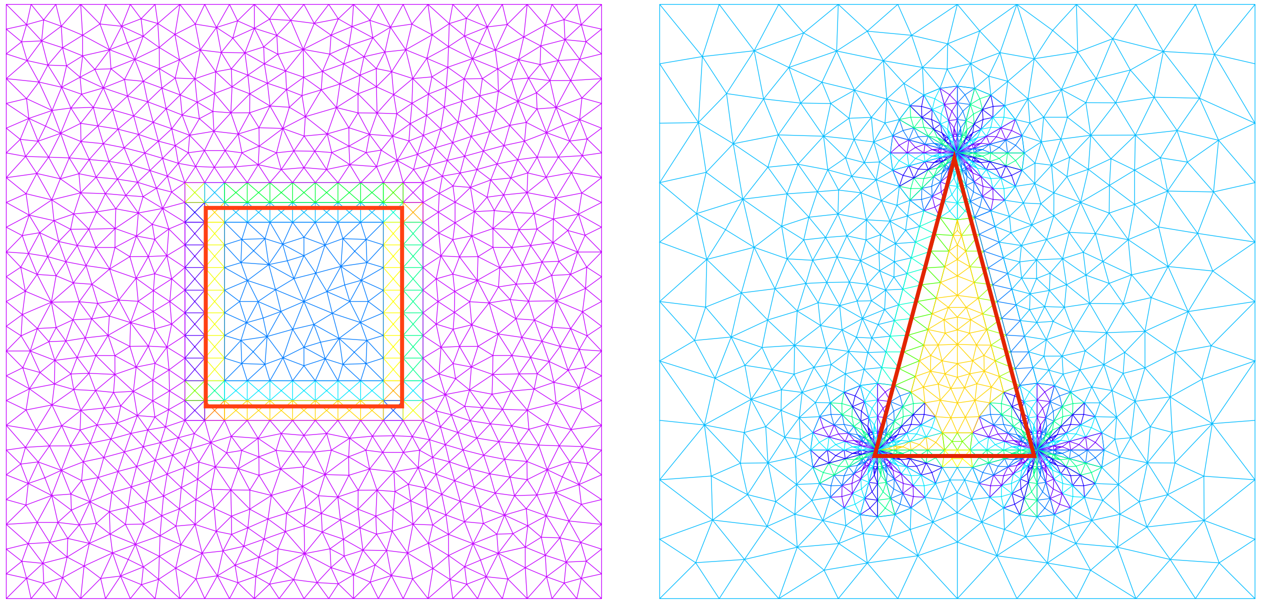

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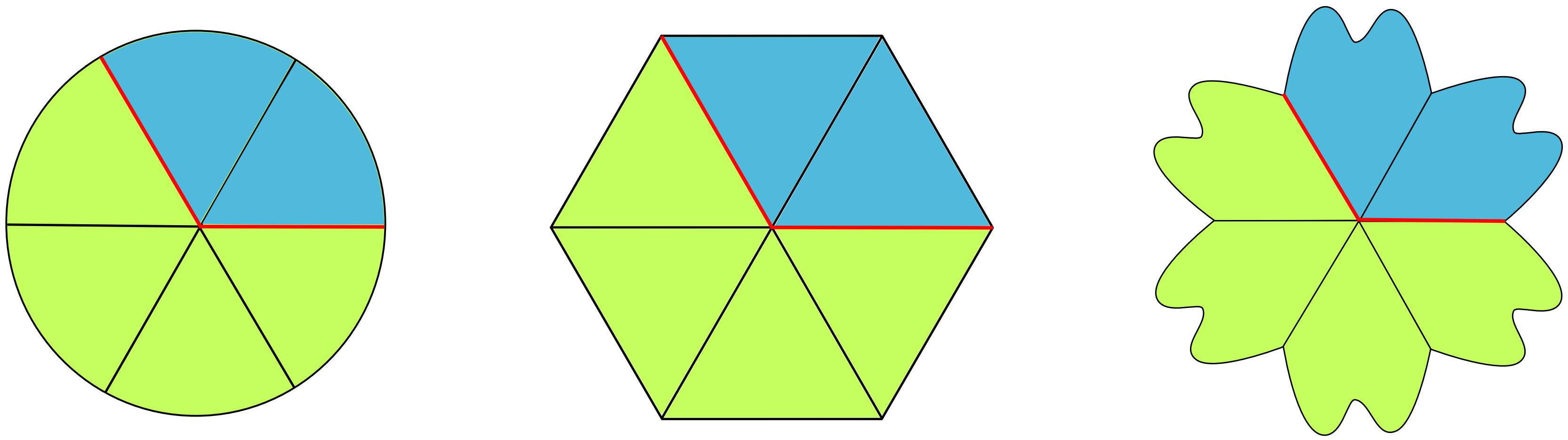

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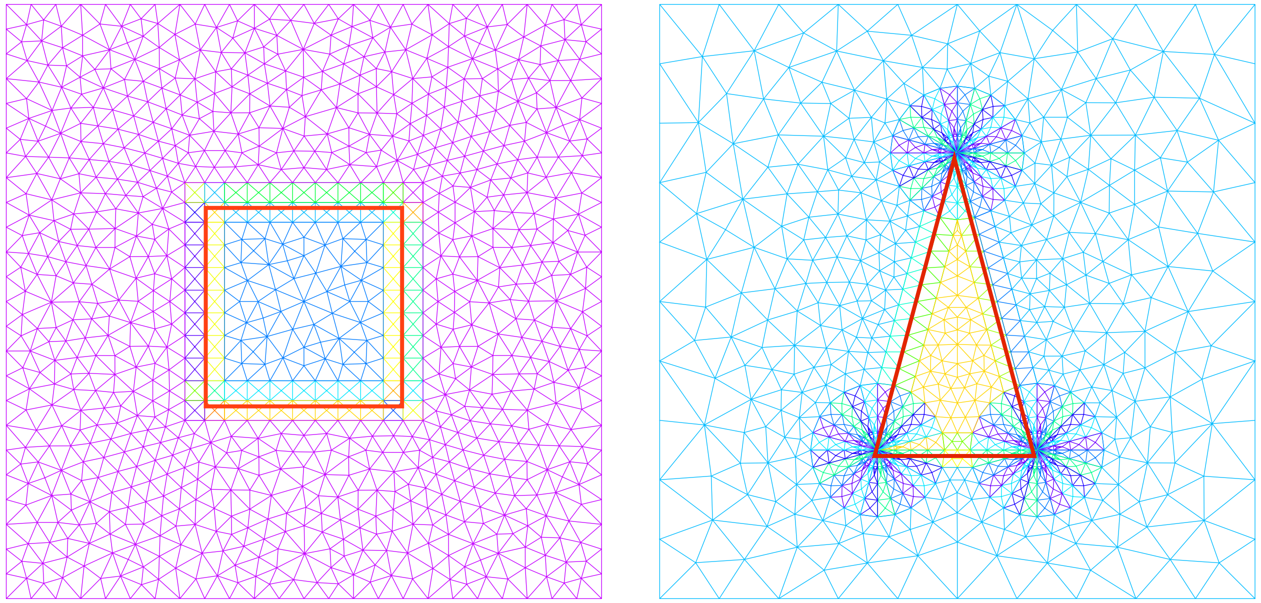

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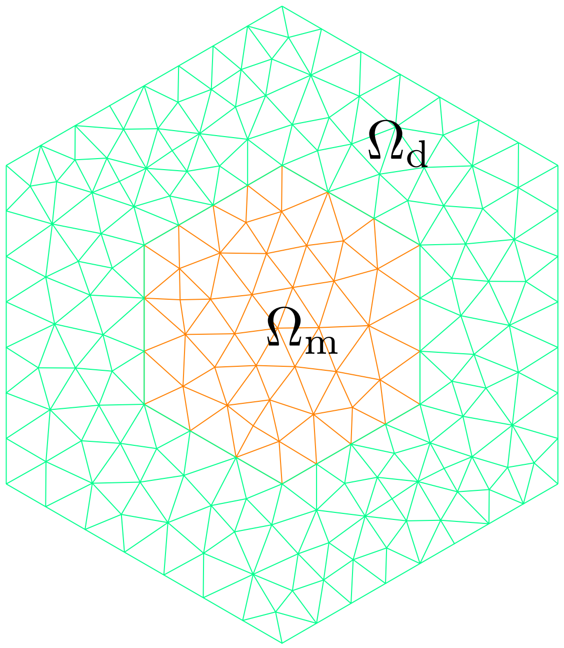
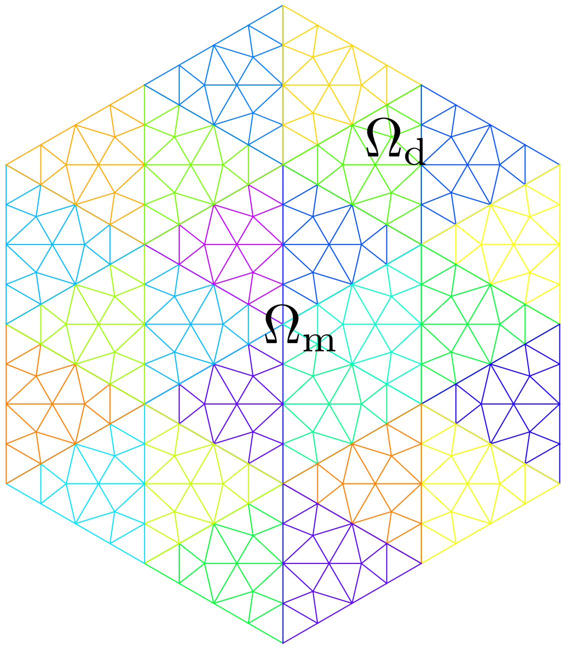
Theorem. For any angle $\alpha \in 2\pi\mathbb{Q}$, if the mesh is locally built as a duplicated pattern by symmetries, then $\mathtt{T}(V^h) \subset V^h$.

Application to the eigenvalue problem

Find $(u,\lambda) \in H^1_0(\Omega) \setminus \{0\} \times \mathbb{C}$ such that:
$-\operatorname{div}(\varepsilon^{-1}\nabla u) = \lambda \mu u \quad \text{in } \Omega.$



standard mesh



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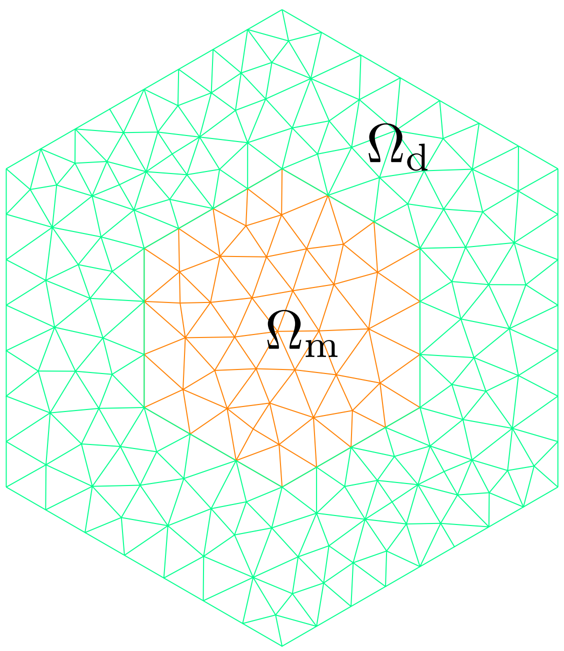

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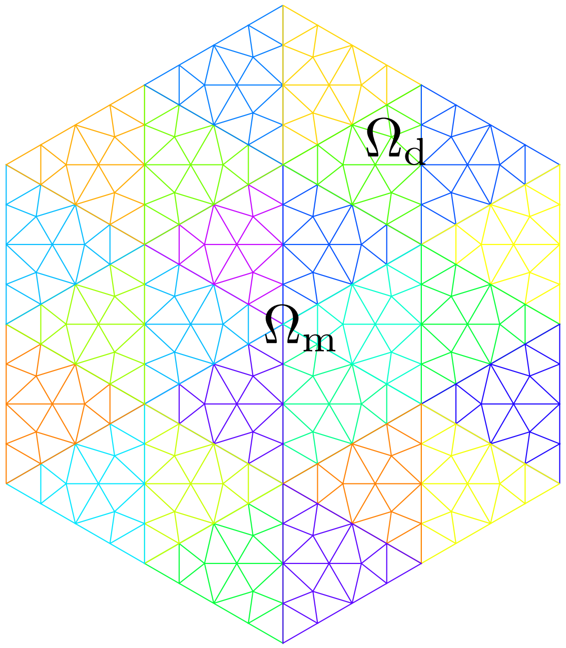

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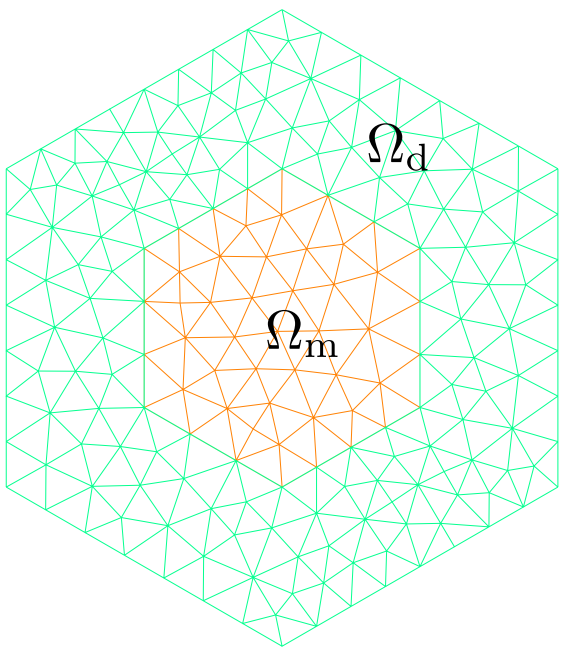

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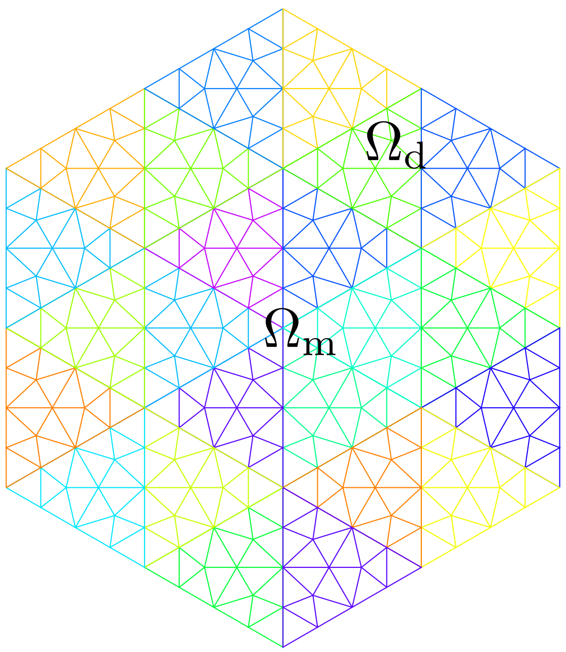

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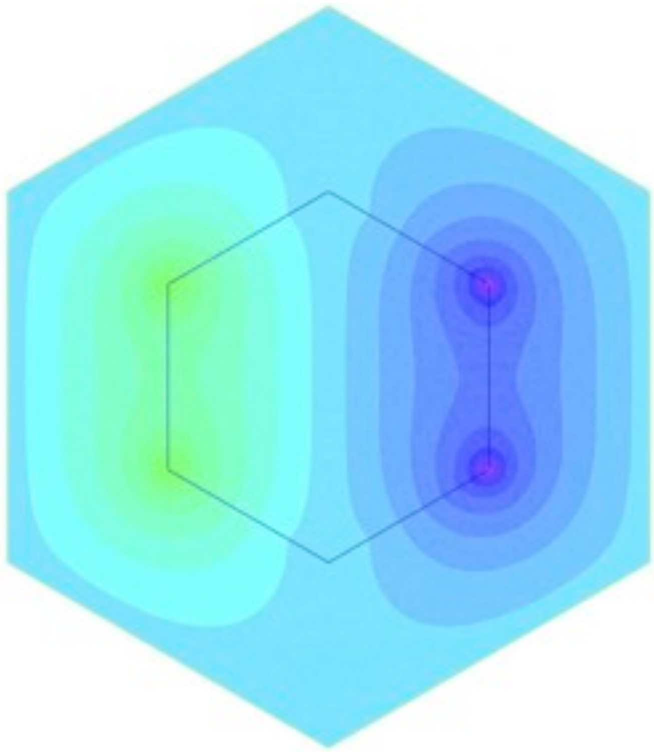
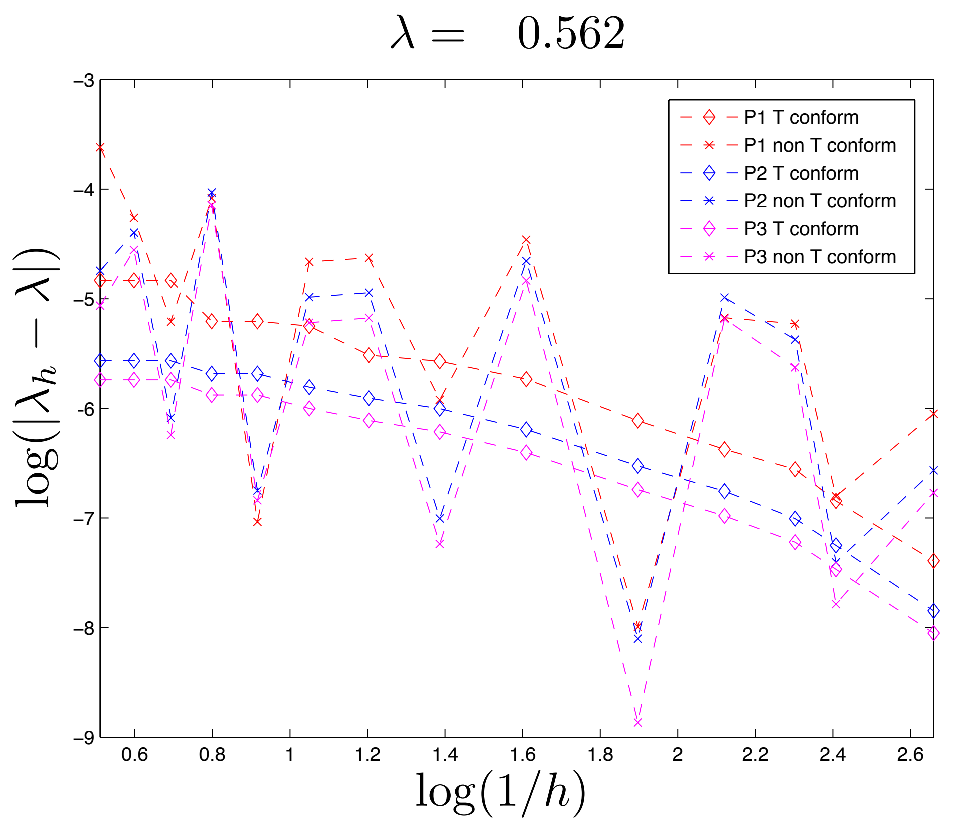
For a positive eigenvalue:





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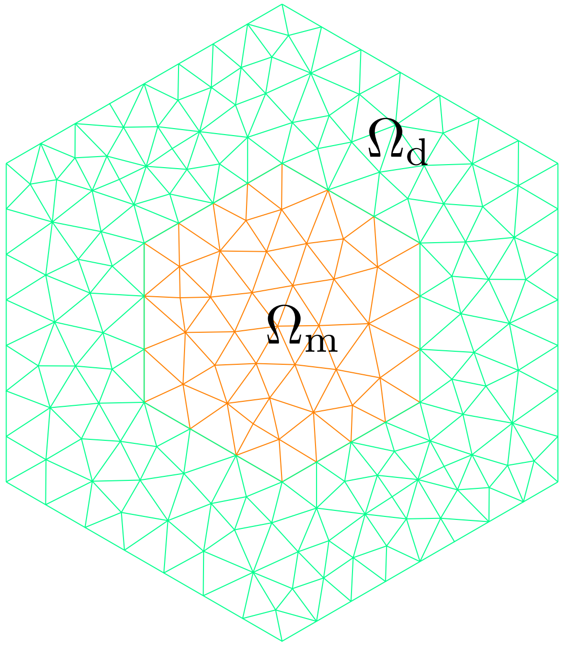

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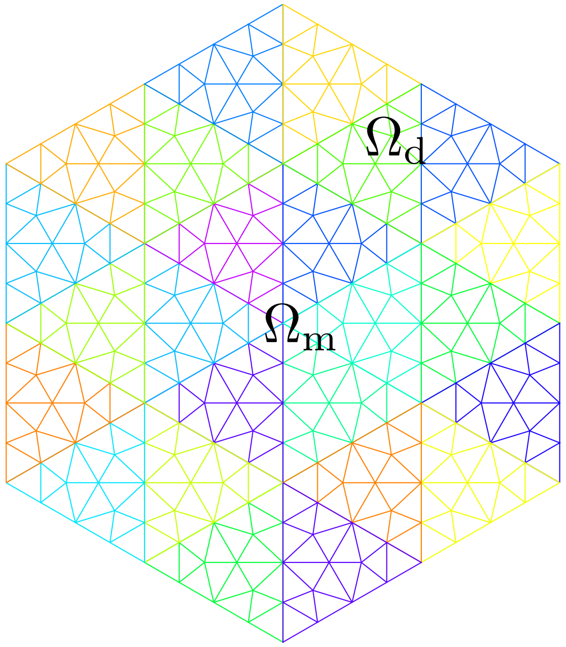

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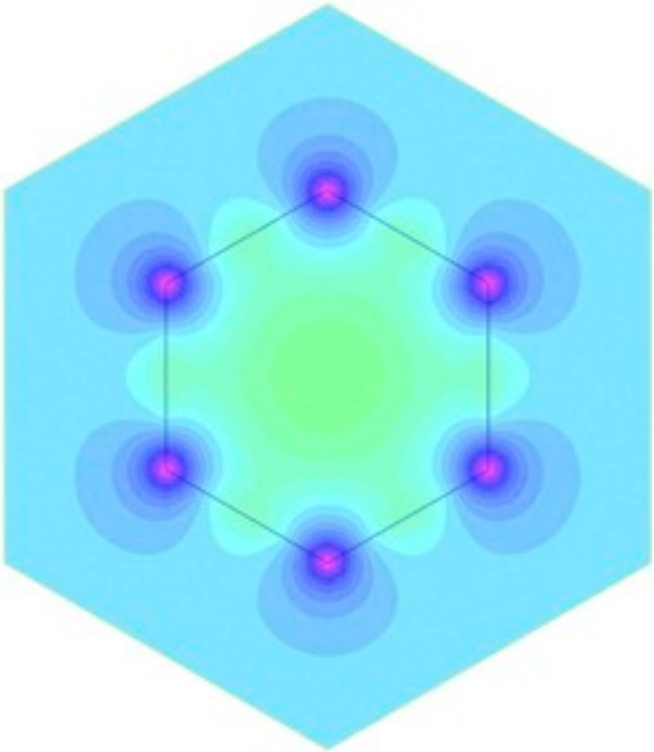
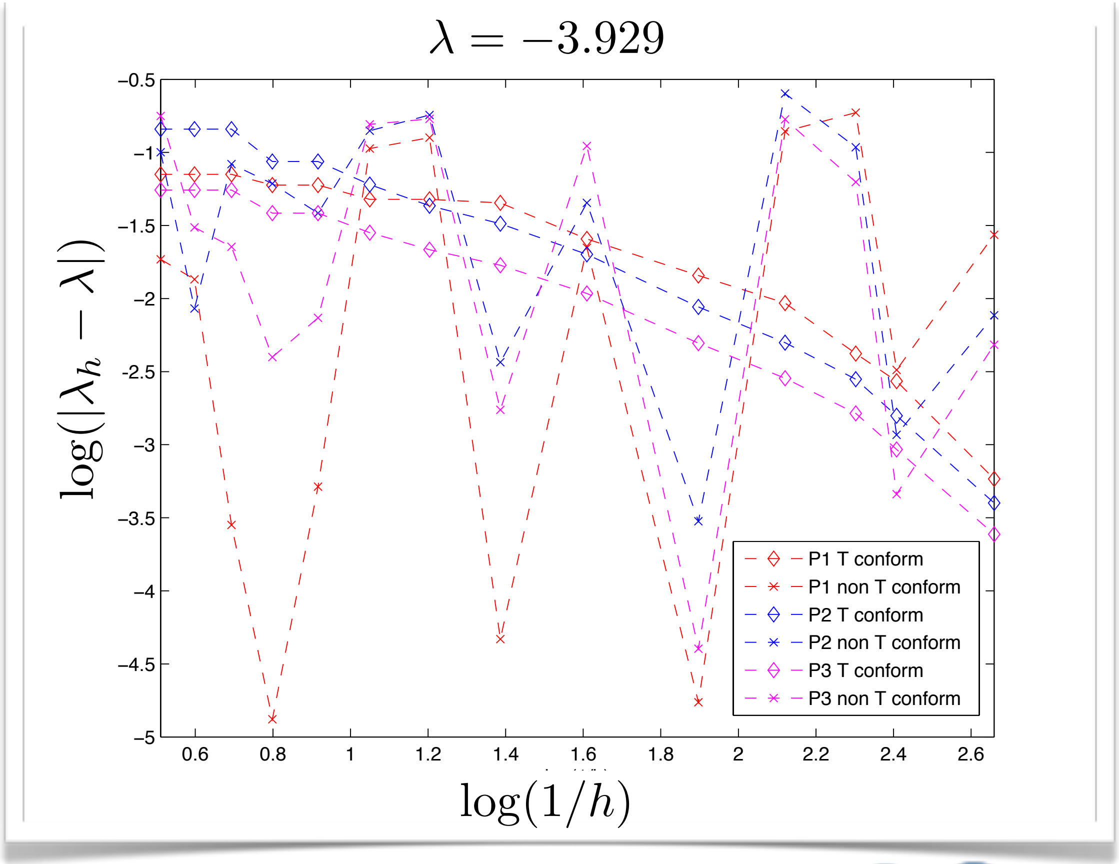


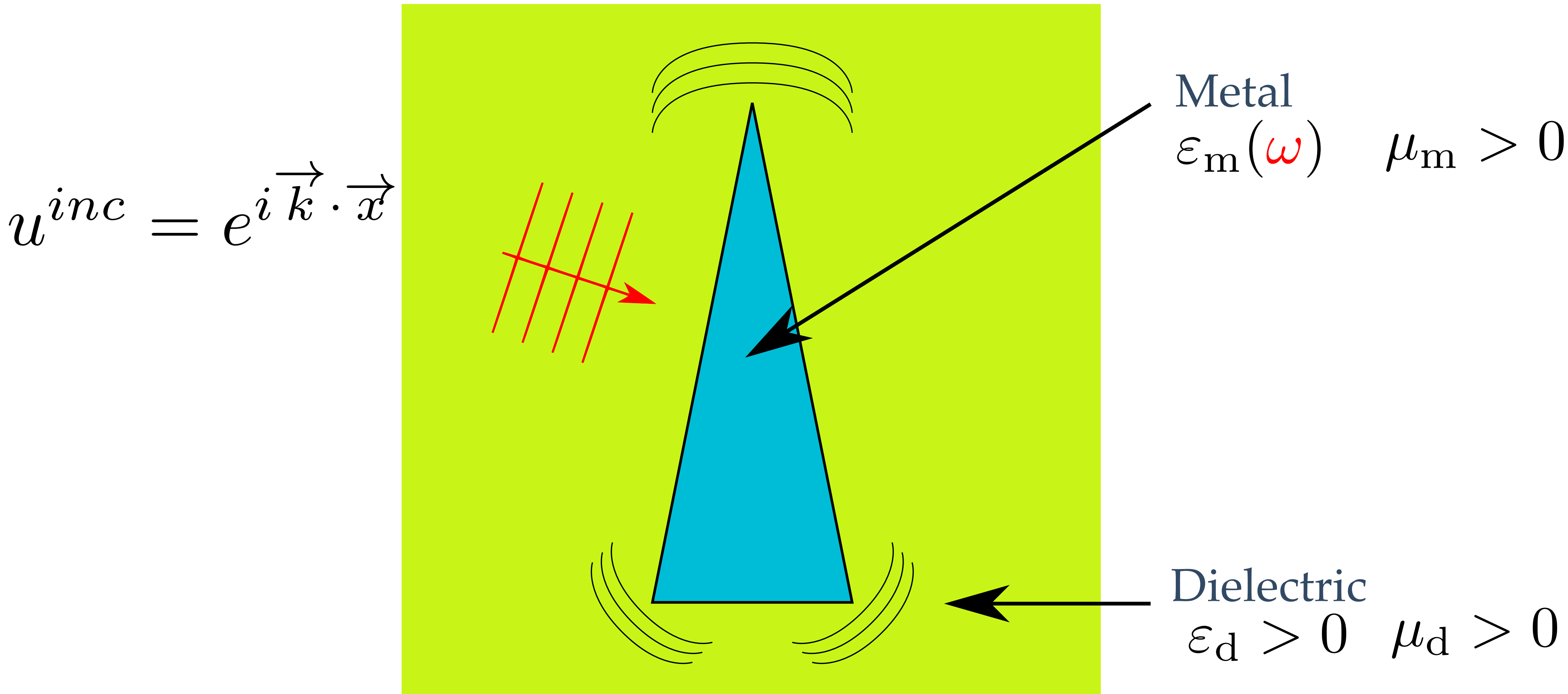


Outline

- Part II: scattering problem with sign-changing coefficients

Motivations

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



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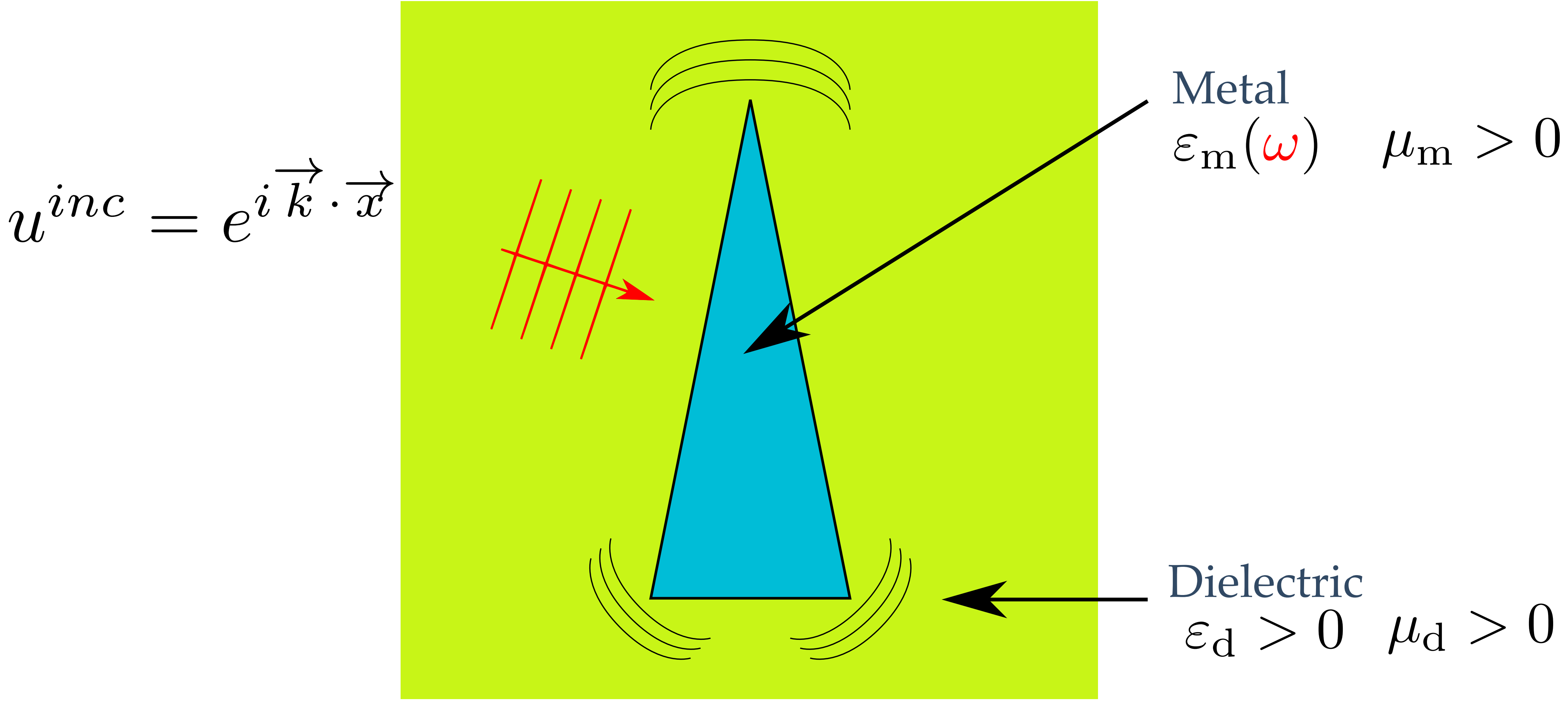

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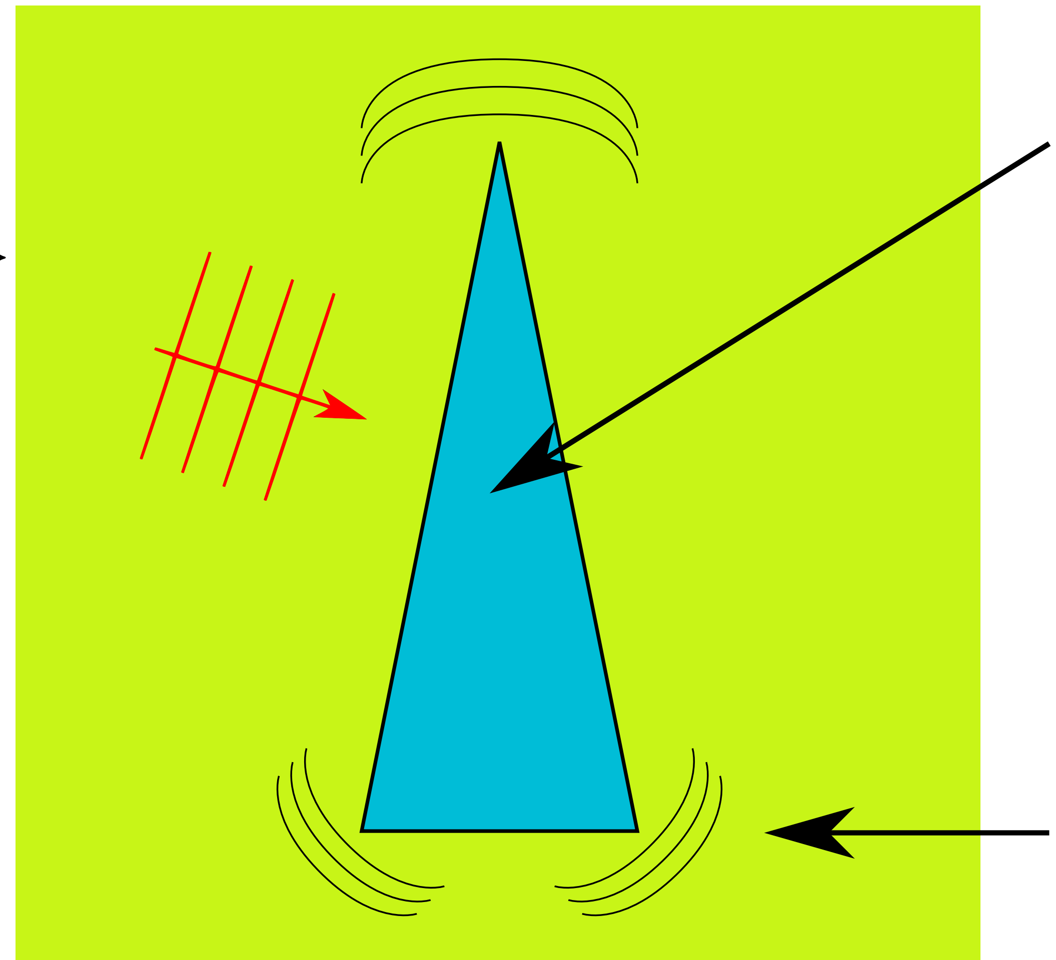
$$u^{inc} = e^{i\overrightarrow{k}\cdot\overrightarrow{x}}$$



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

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

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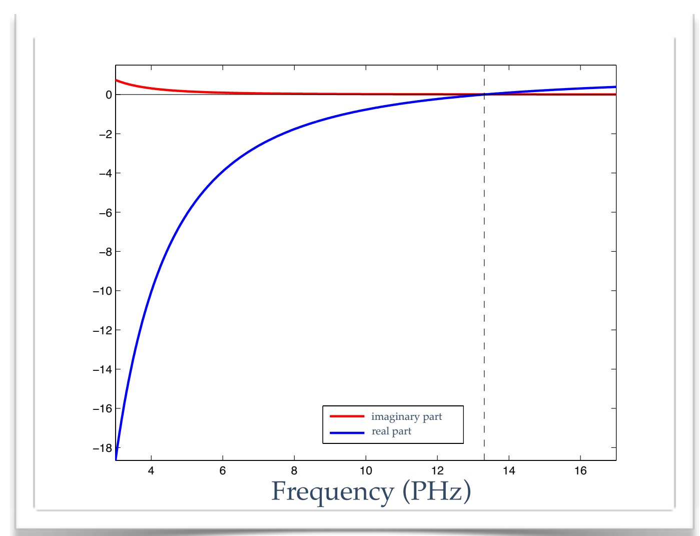

Time-harmonic equations for the TM polarization

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

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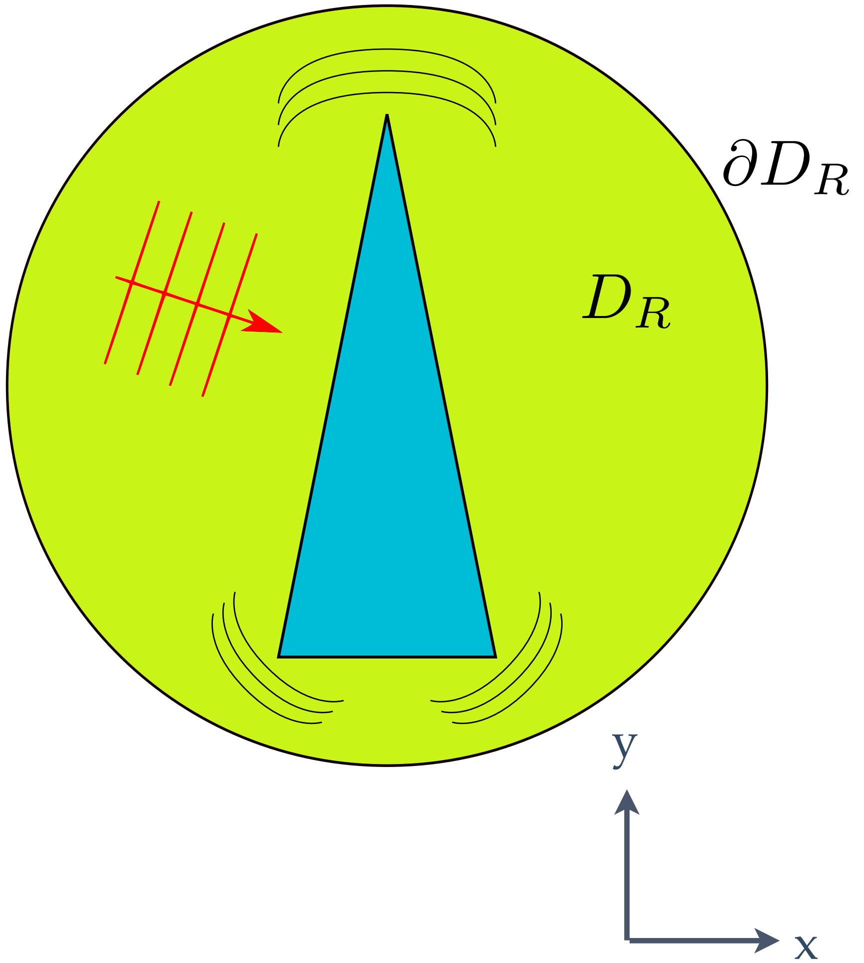
- Radiation condition at finite distance

Work at a chosen frequency.



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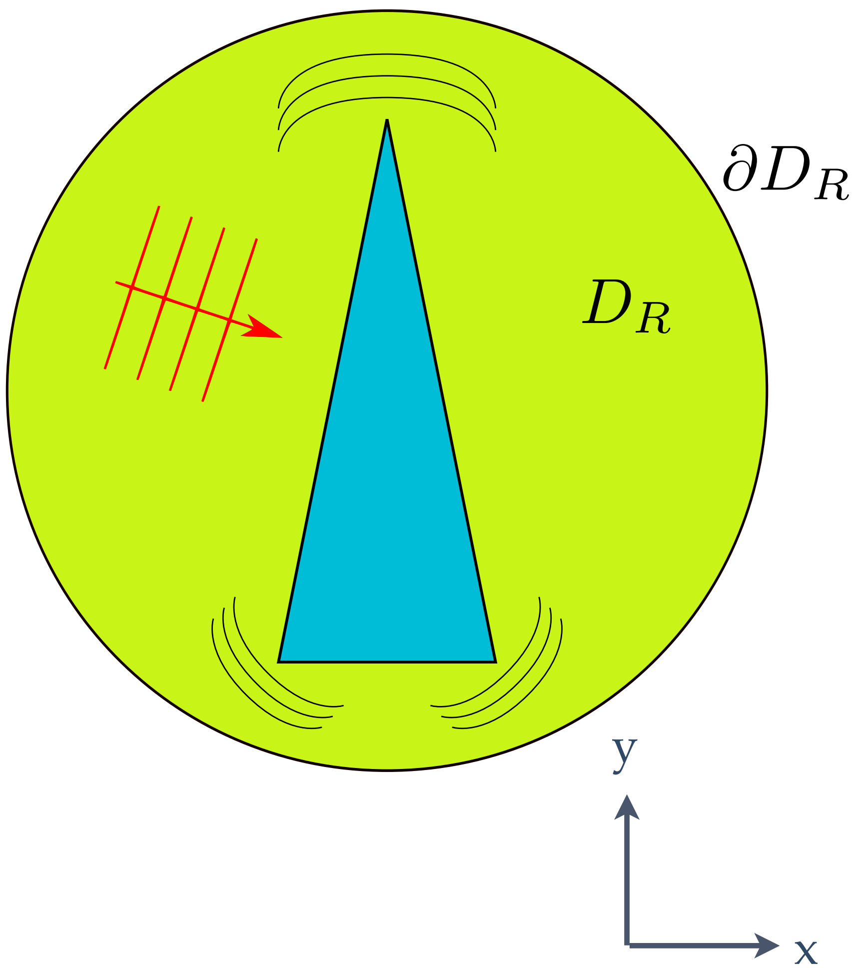

Work at a chosen frequency.

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

Numerical illustrations

We computed the total field for a triangular silver inclusion embedded in vacuum. We use Finite Element of order 2, with a plane wave of incidence $-\pi/12$.

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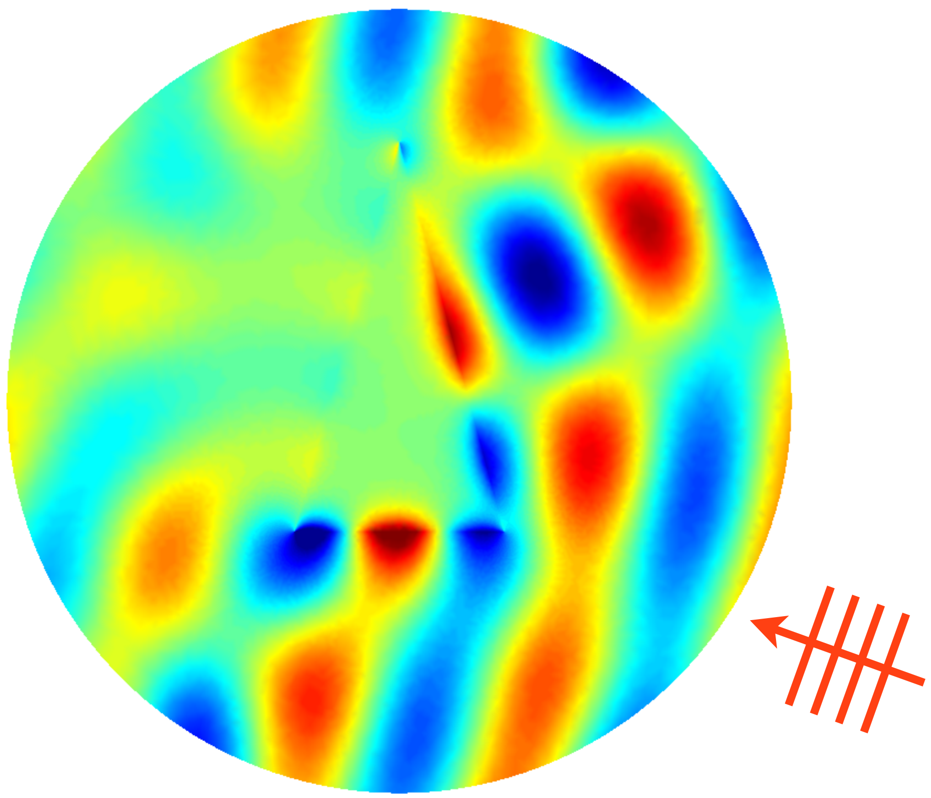

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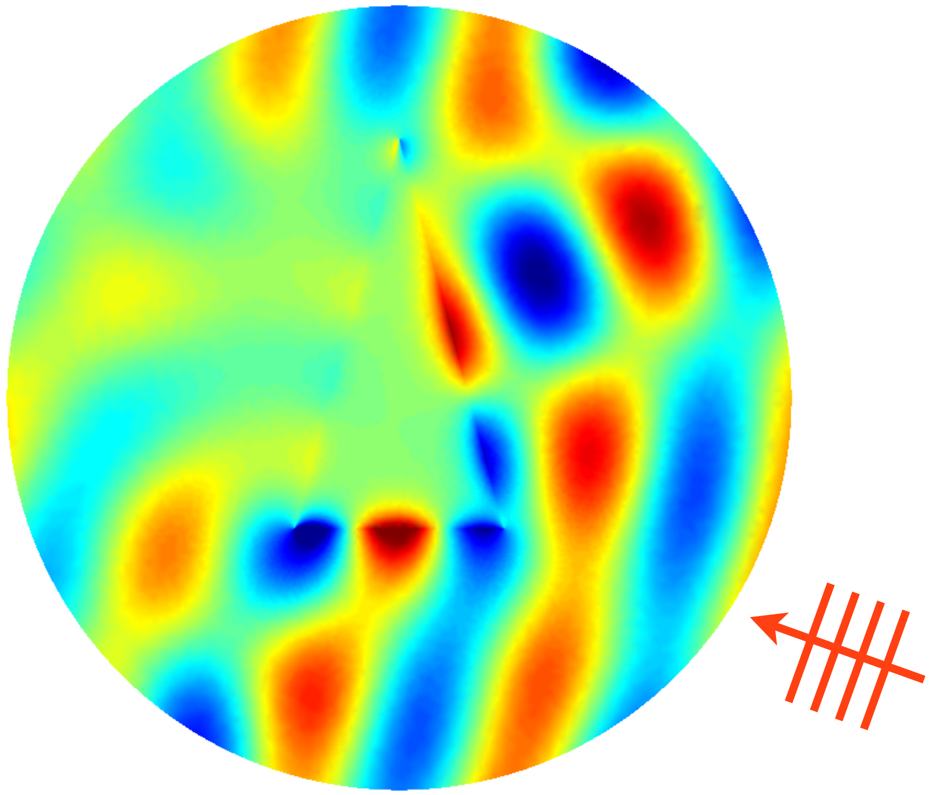

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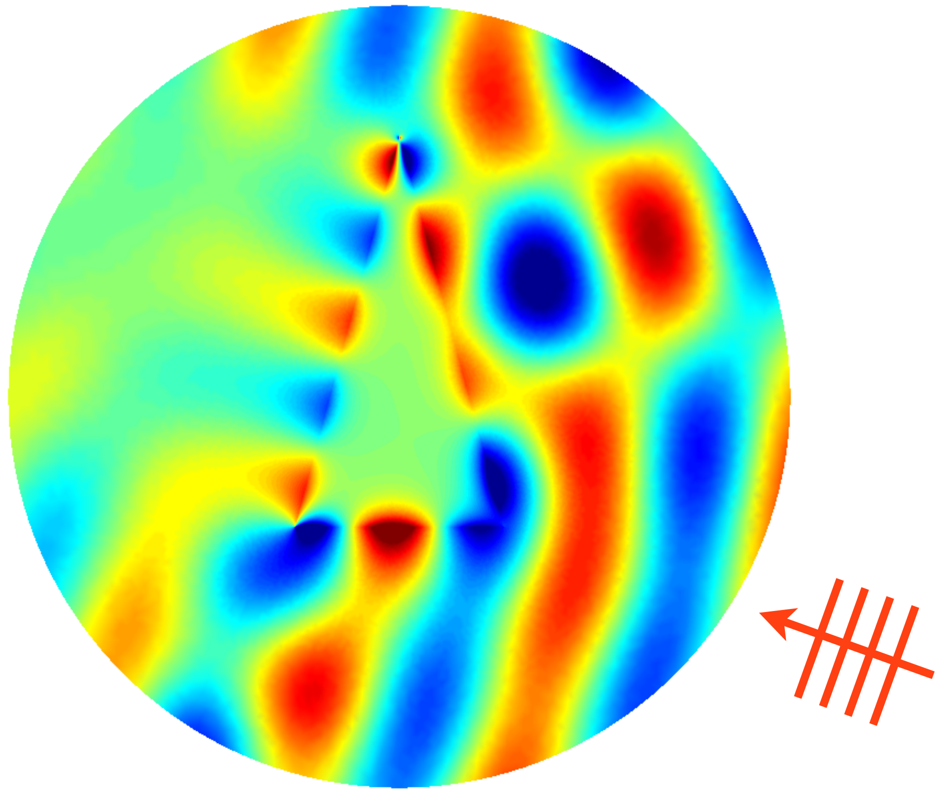

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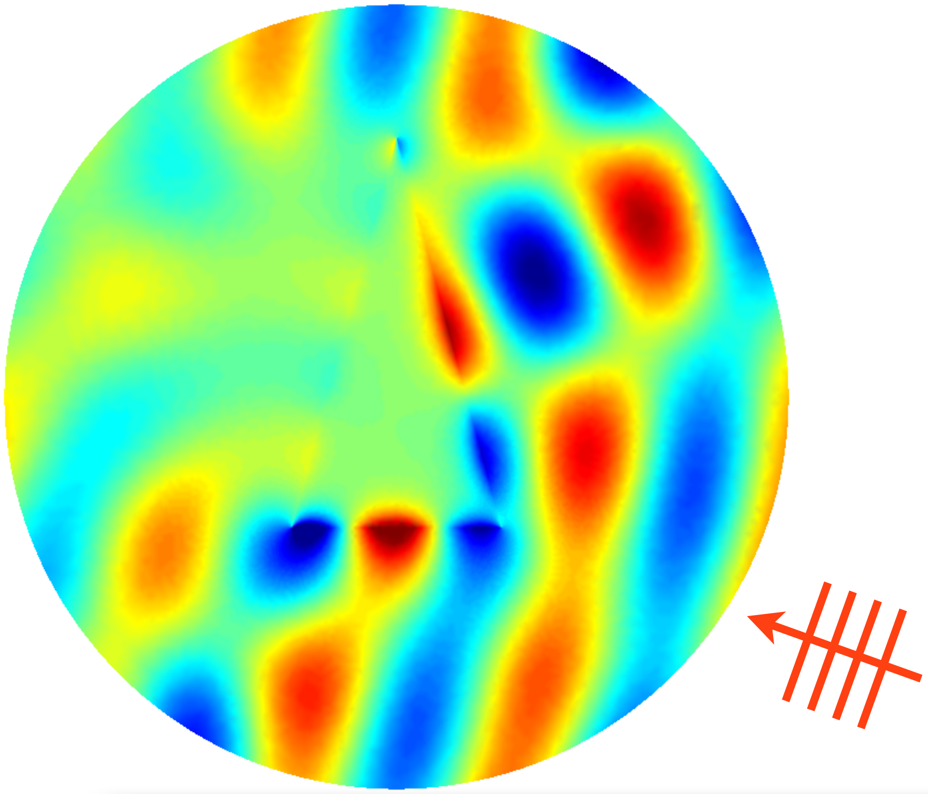

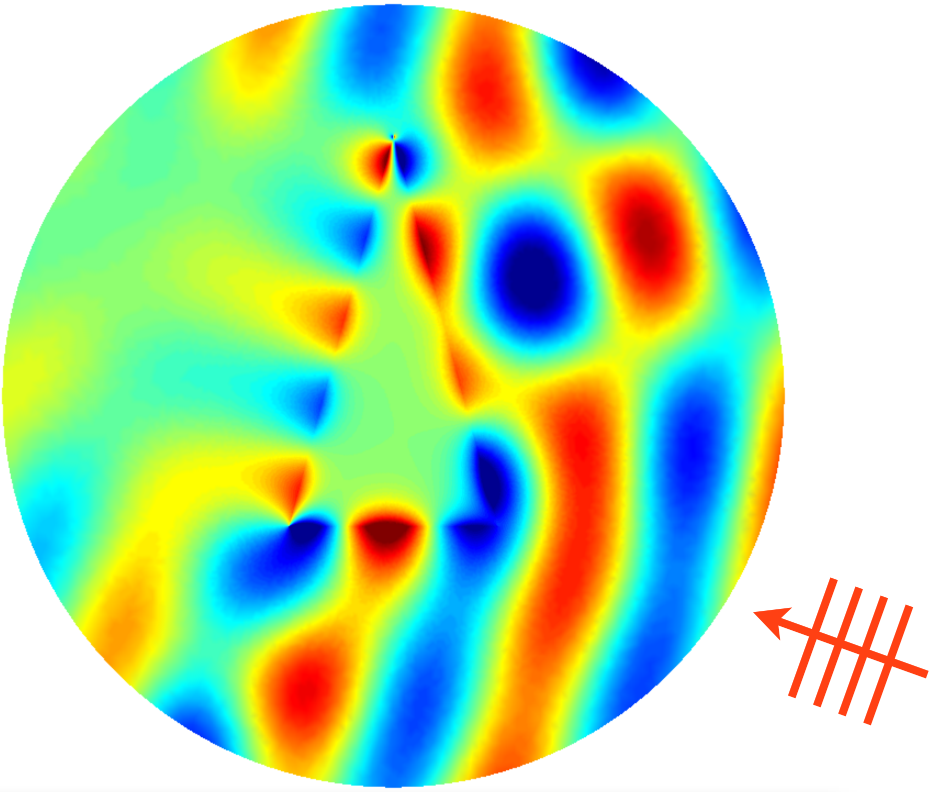

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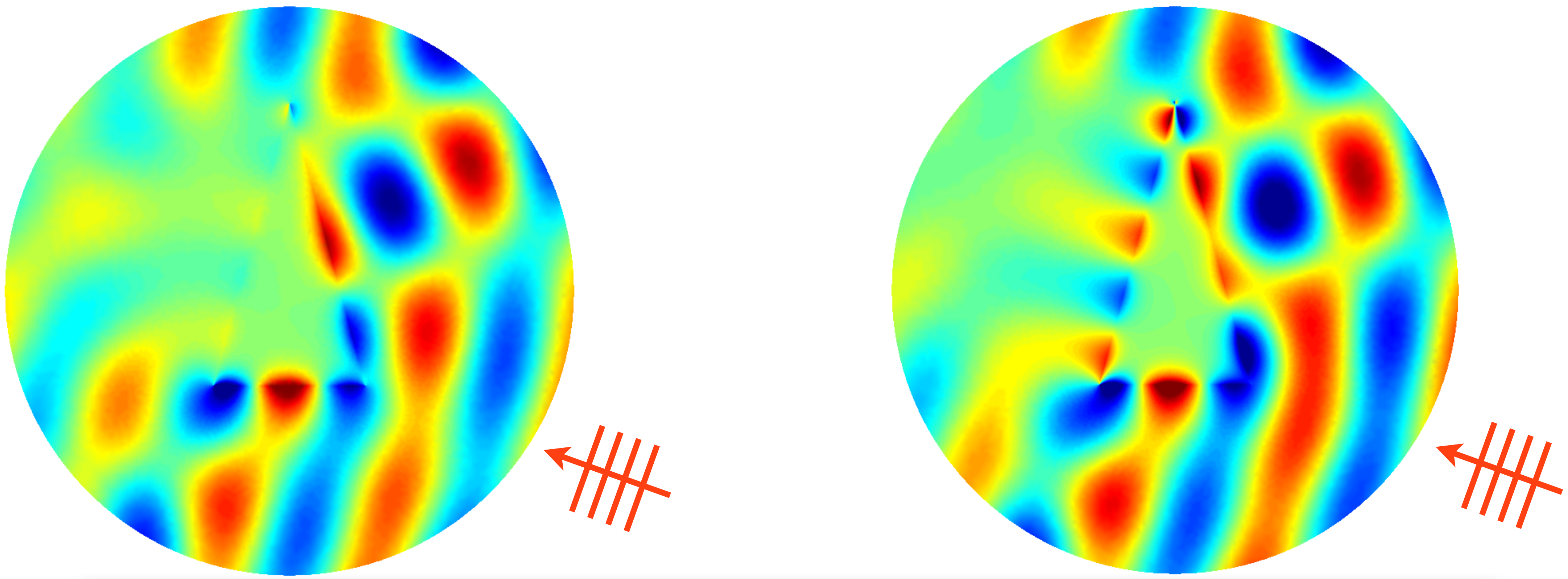

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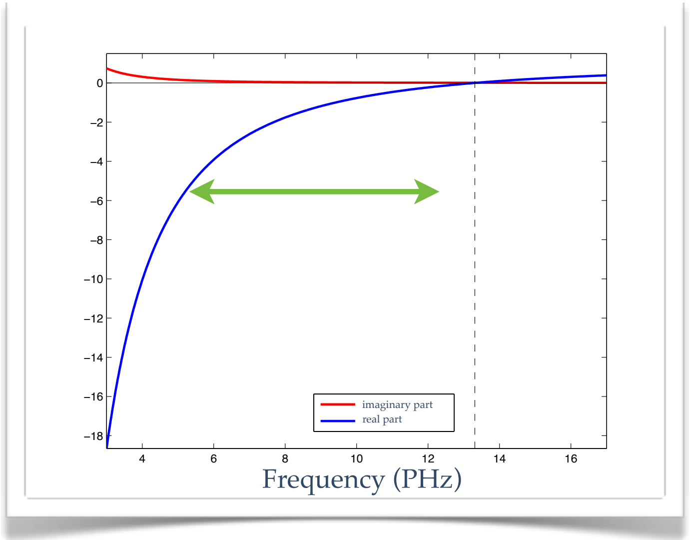
To understand the reasons of such instabilities and how to avoid them, we study a **limit problem by neglecting dissipation.**

The dissipationless Drude's model

At optical frequencies one can neglect dissipation so that the metal's permittivity follows the law:

$$\boxed{\varepsilon = \varepsilon^0(\omega) := 1 - \frac{\omega_p^2}{\omega^2} < 0}$$



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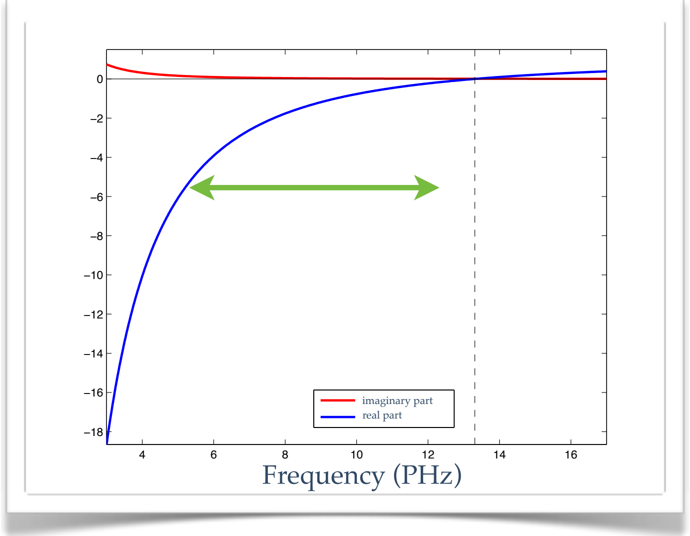

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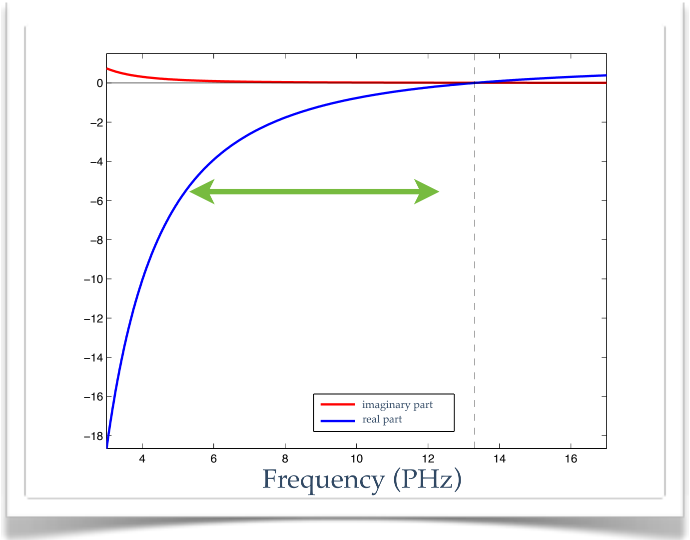

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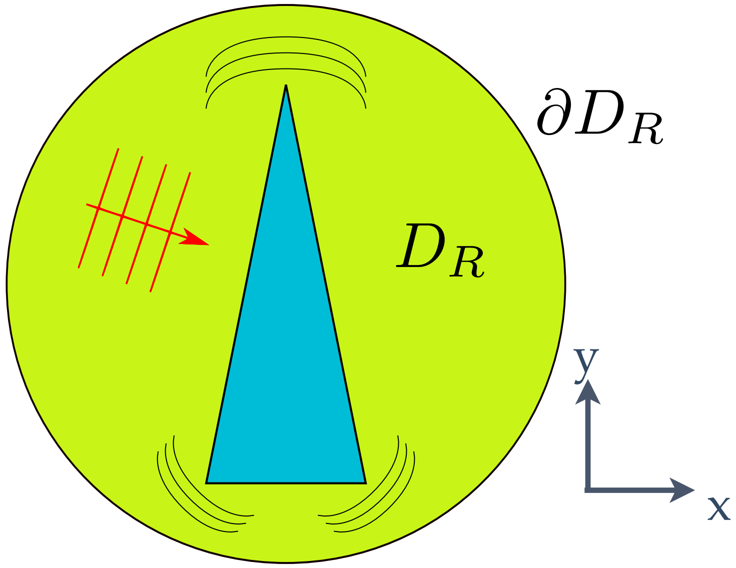

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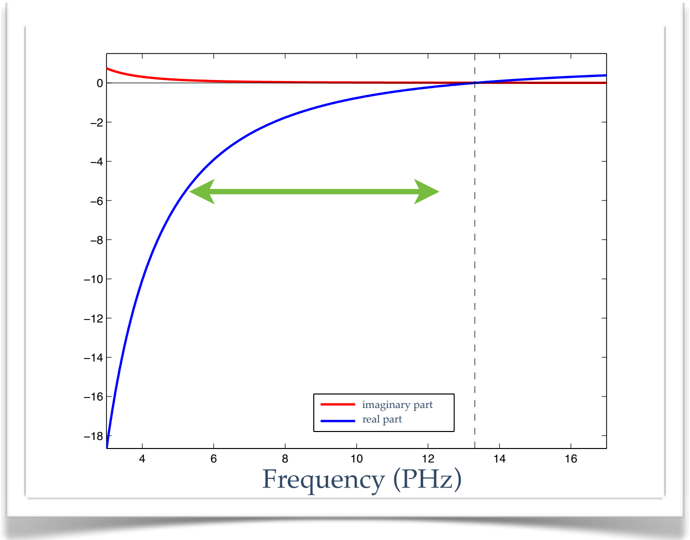

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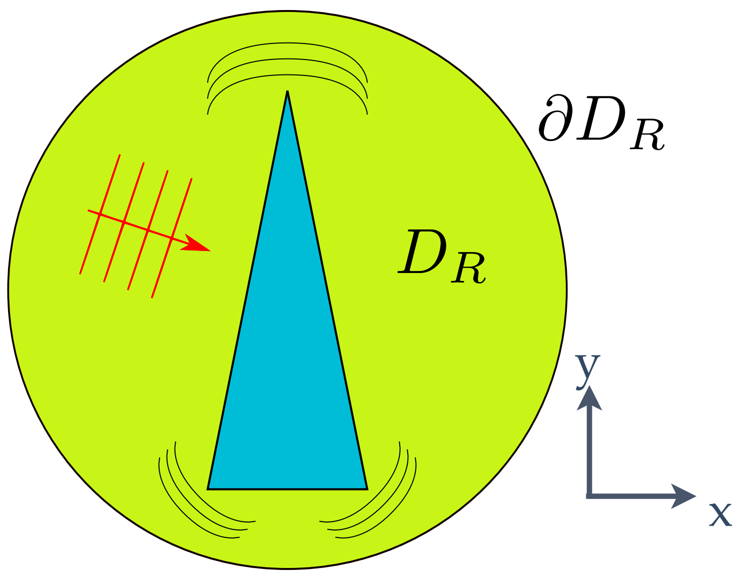

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-difficulties to prove existence and uniqueness of the solution
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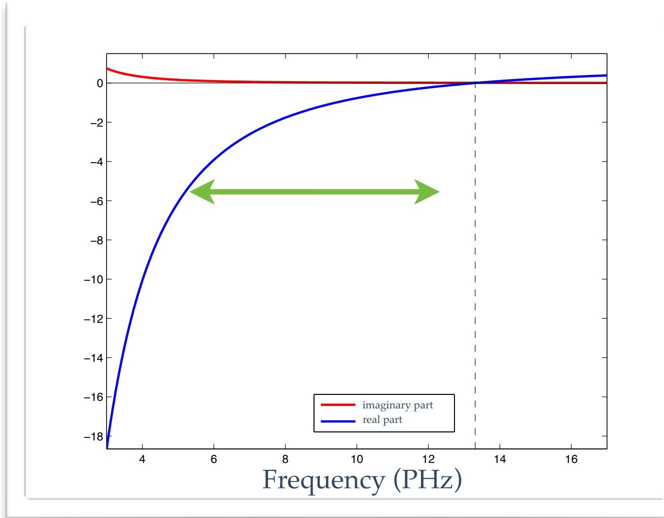

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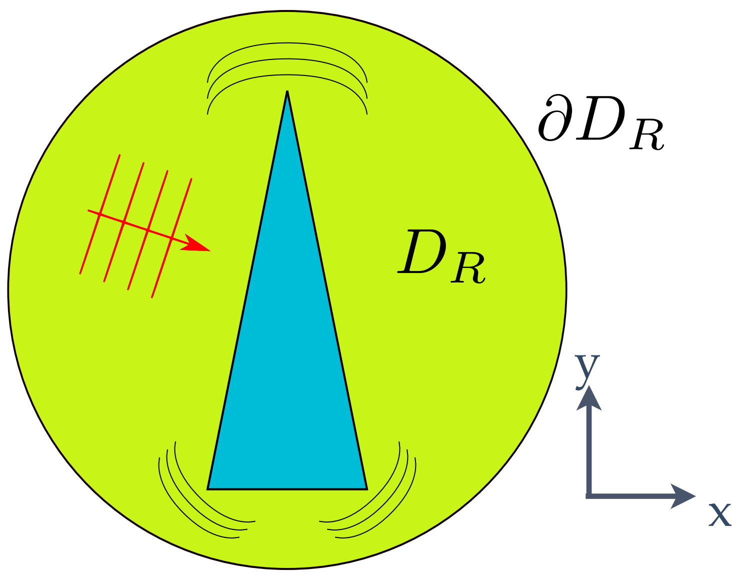

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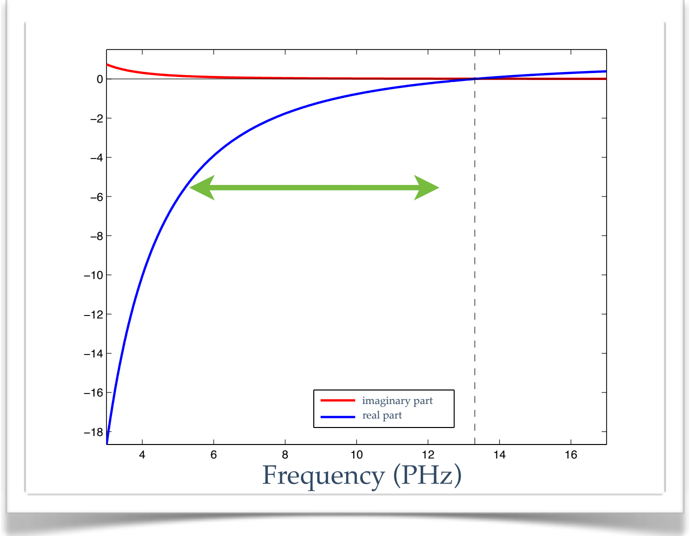

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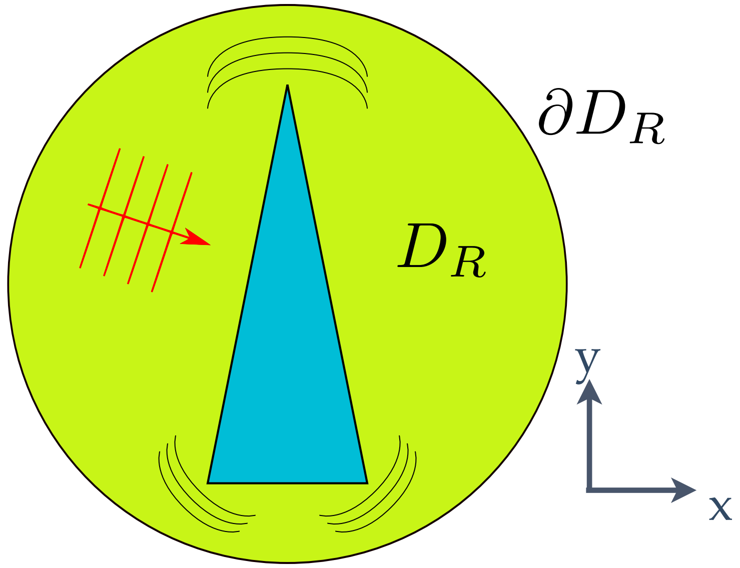

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For a contrast $\kappa_\varepsilon \in I_c$

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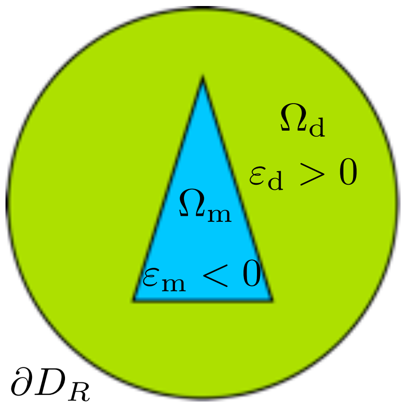

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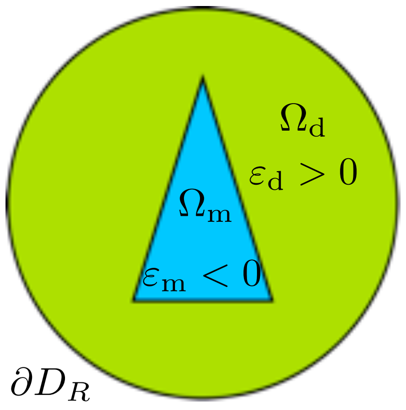
$\longrightarrow$

Find $u := u^{\text{inc}} + u^{\text{sac}} \in H^1(D_R)$ such that:

$$a(u,v) + c(u,v) = l(v), \quad \forall v \in H^1(D_R)$$

$$a(u,v) := \int_{D_R} \varepsilon^{-1}\nabla u \cdot \overline{\nabla v}\, d\mathbf{x},$$



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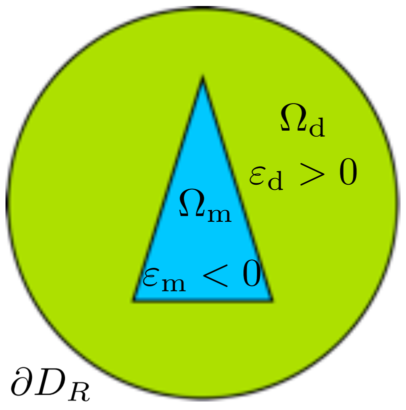

In that case the form a is not T-coercive !

Can we still compute the total field with finite elements ?

For a contrast $\kappa_\varepsilon \in I_c$

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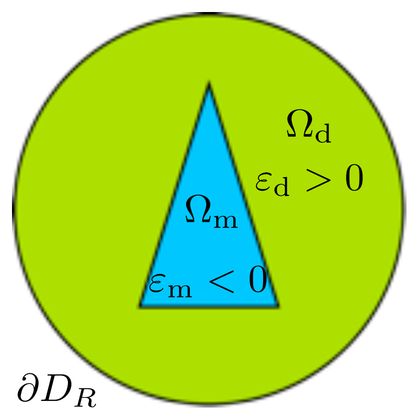

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Can we still compute the total field with finite elements ?

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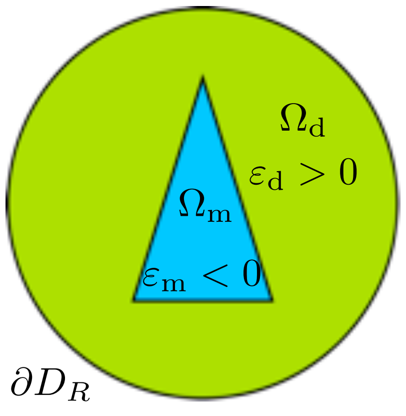

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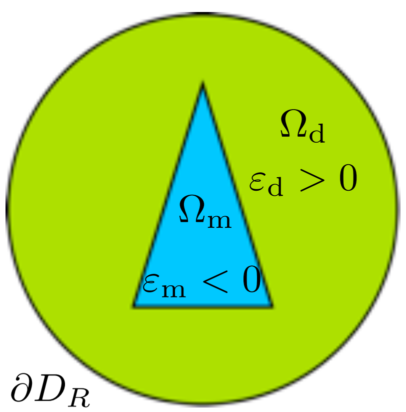

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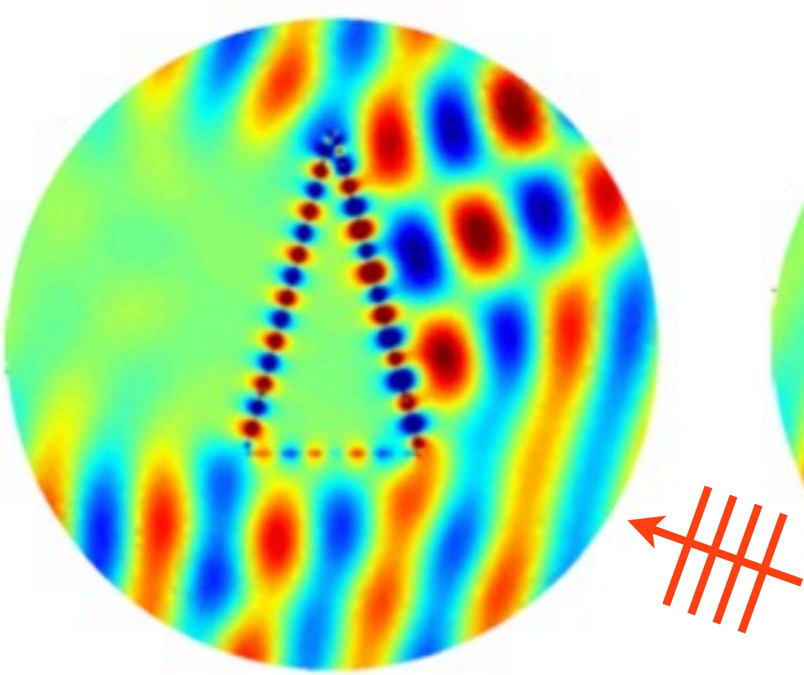
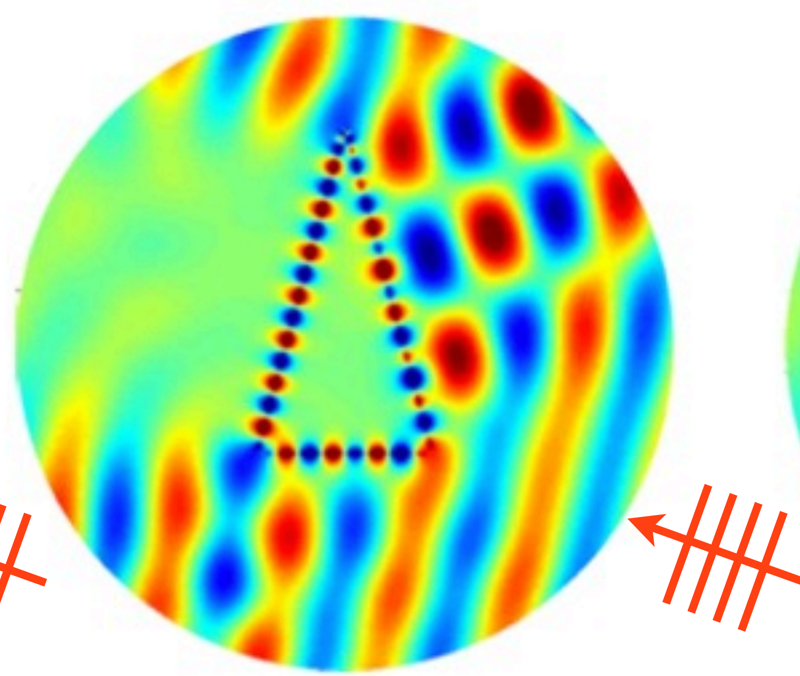
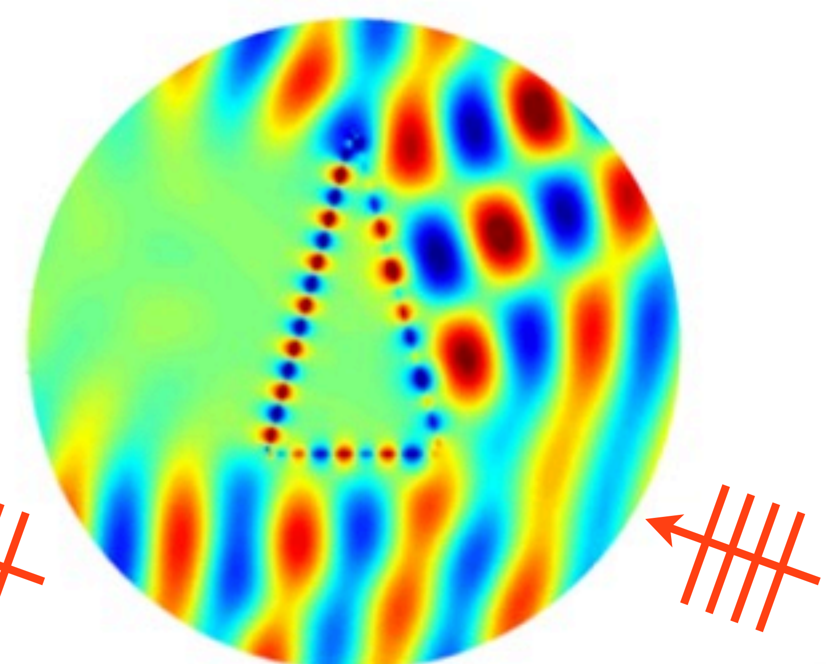


coarse mesh



intermediate mesh



refined mesh

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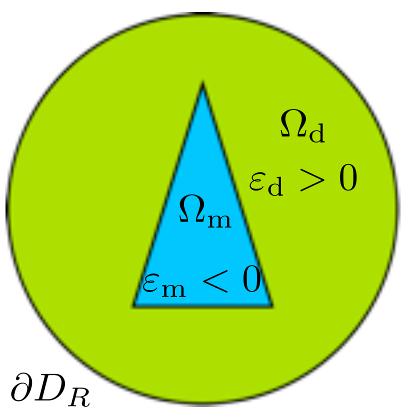

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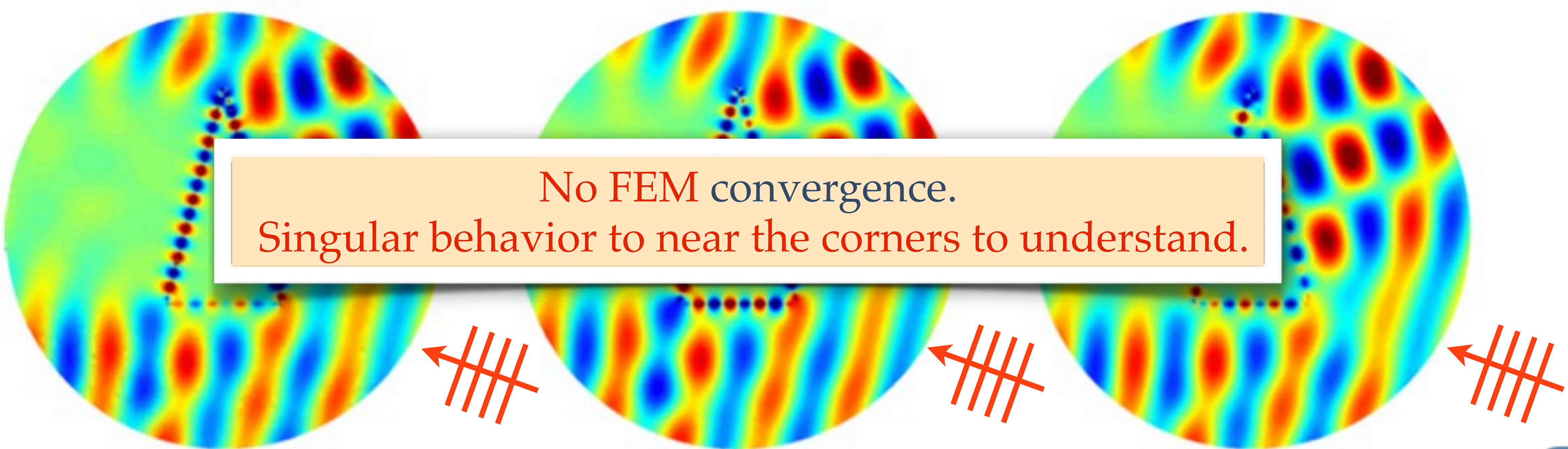


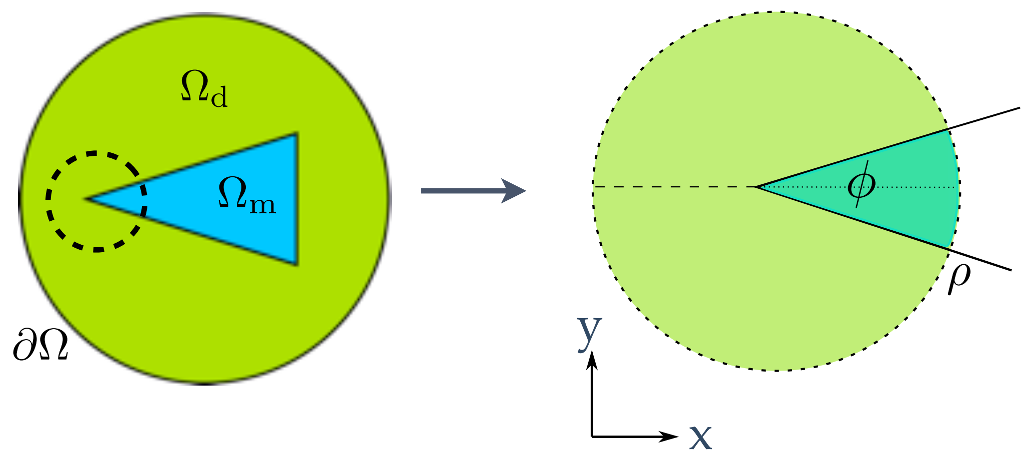
No FEM convergence.

Singular behavior to near the corners to understand.

coarse mesh intermediate mesh refined mesh

Analysis of the singularities at the corners

For simplicity, we consider only one corner.



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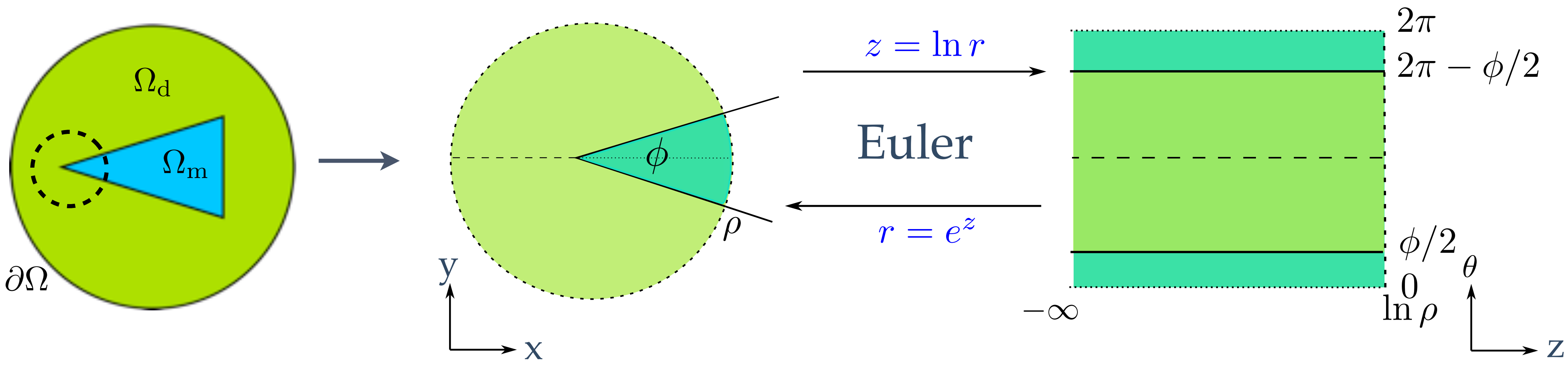

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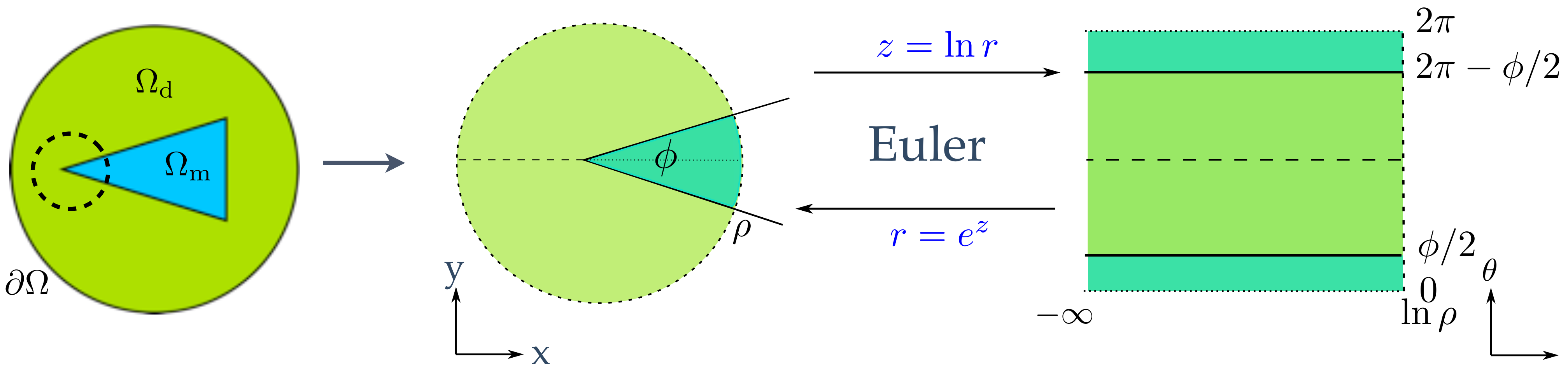

Limit behaviour a the corner

Behaviour at infinity in the strip

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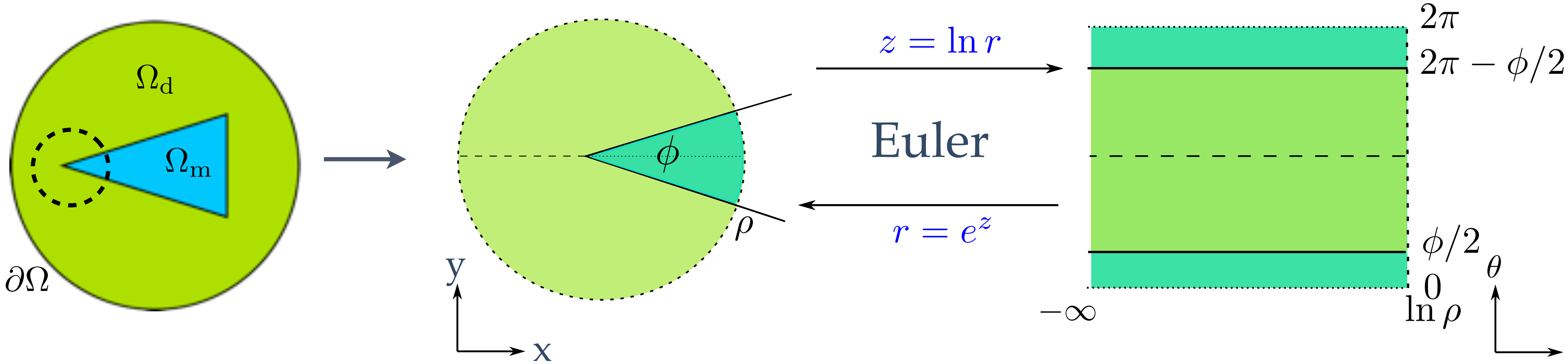

Limit behaviour a the corner

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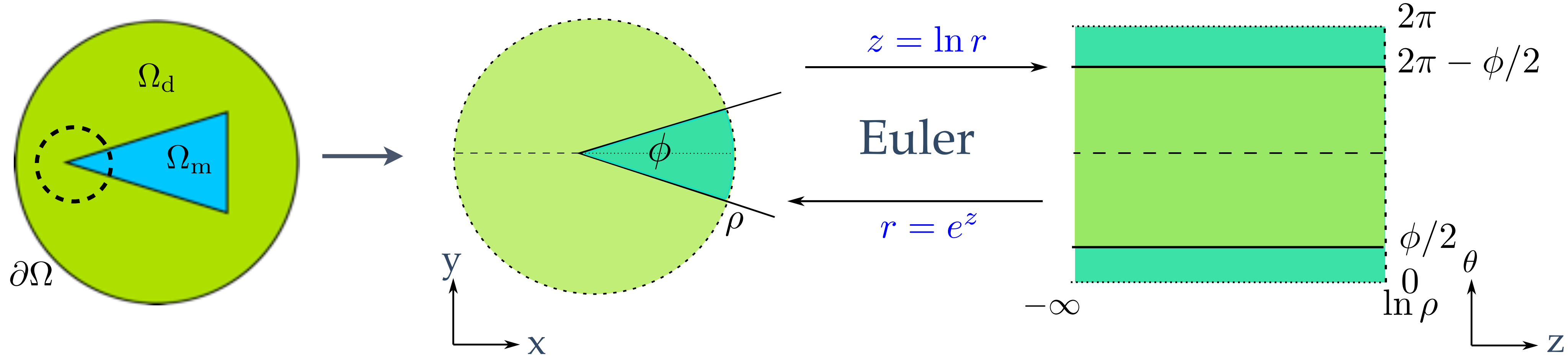

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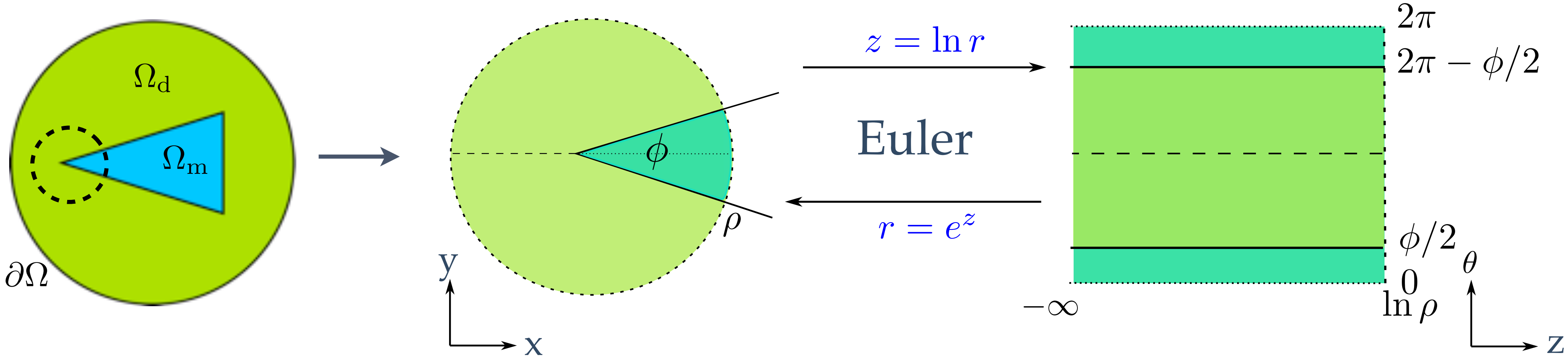

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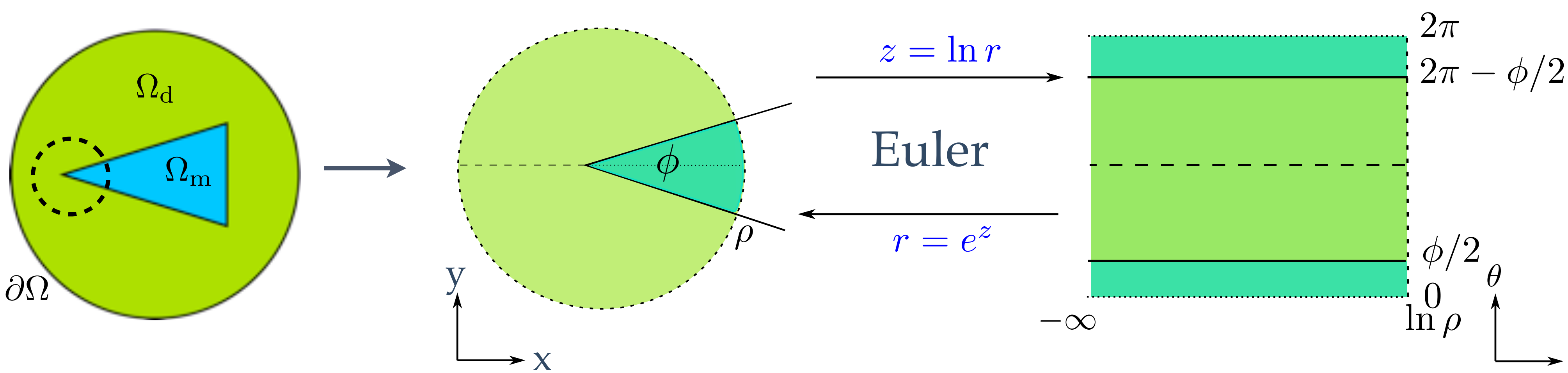

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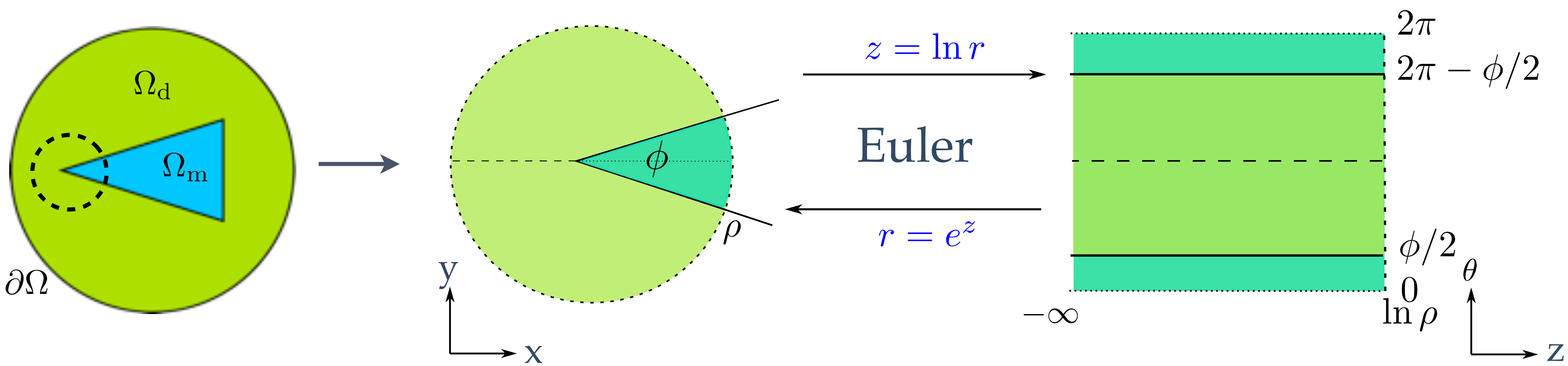

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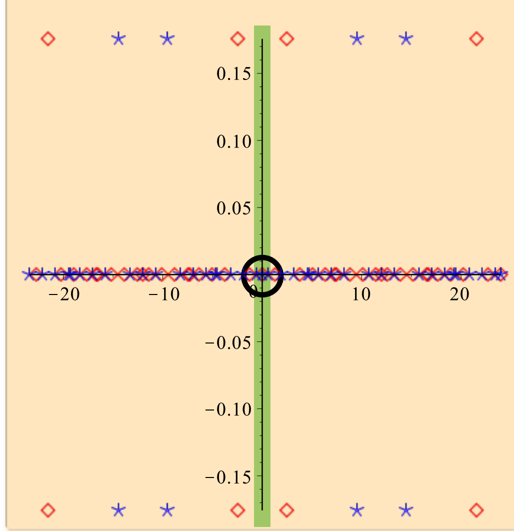
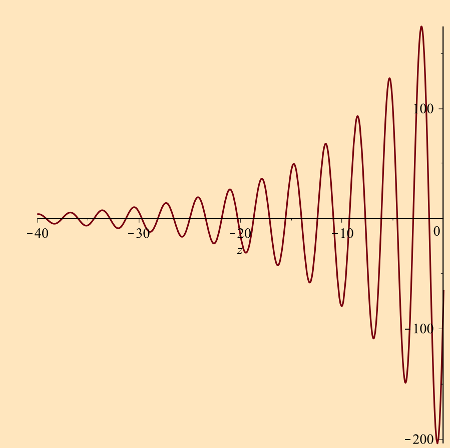
$\boxed{\kappa_\varepsilon \notin I_c}$

The modes are evanescent

$\Re e(\lambda) > 0,\ \forall \lambda \neq 0$





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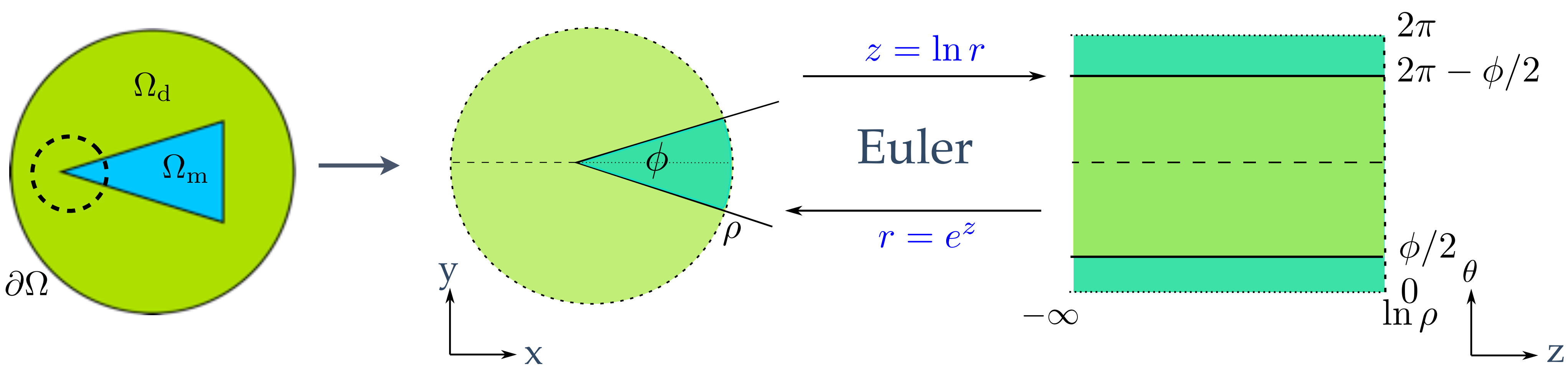

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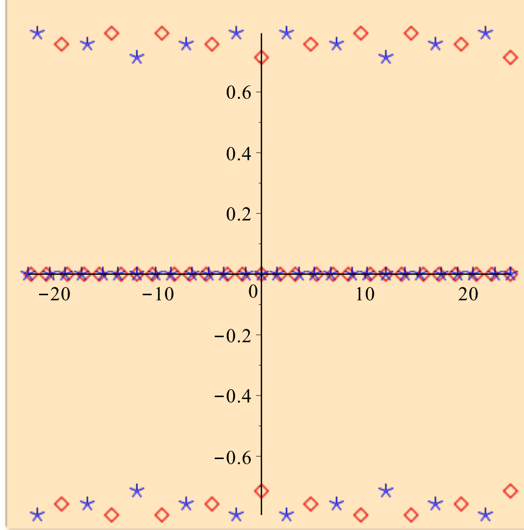
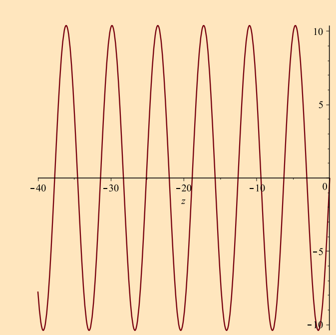
$s(z,\theta) = e^{i\eta z}\phi(\theta)$





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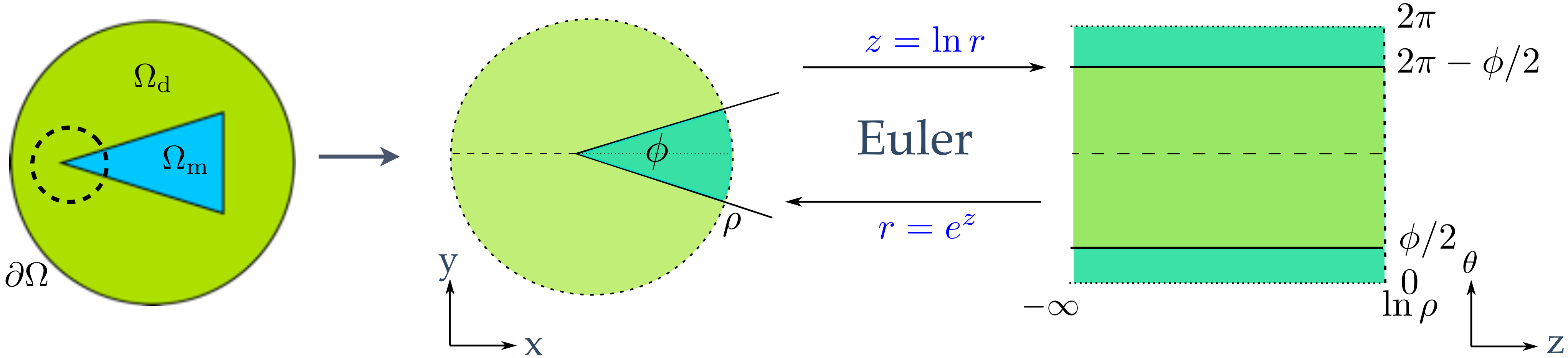

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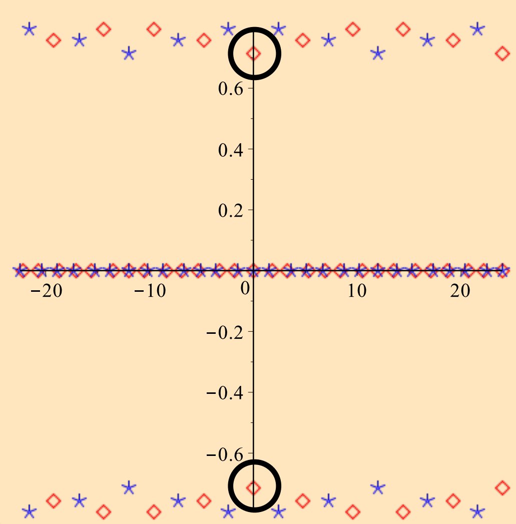

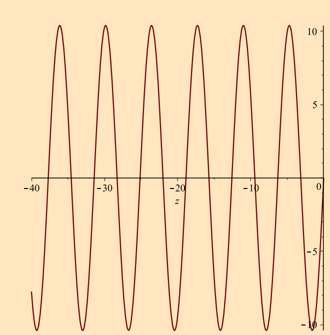

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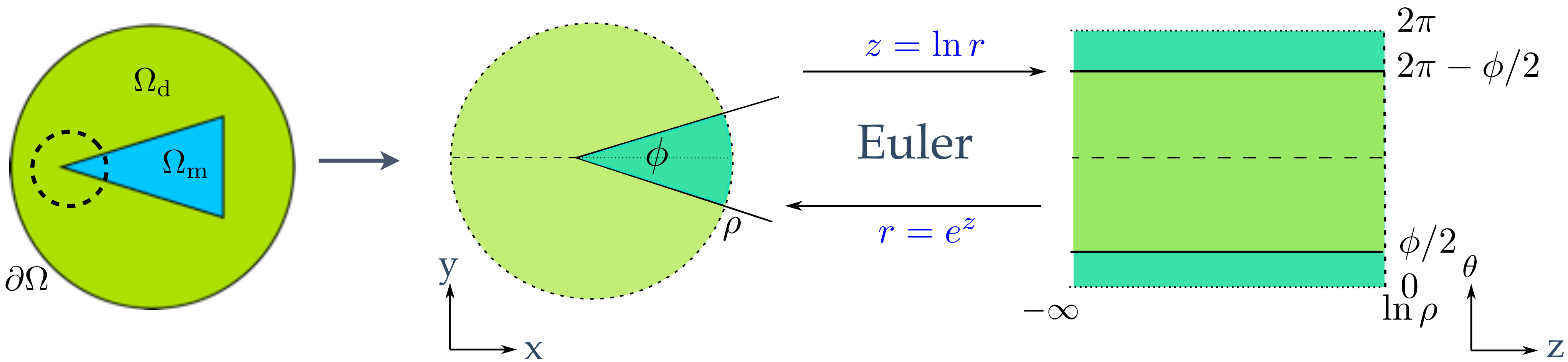

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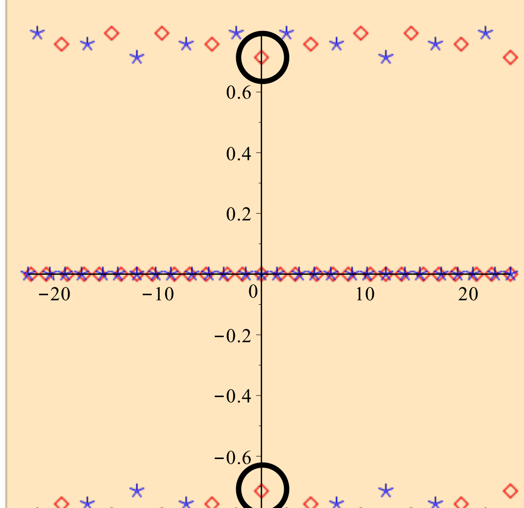

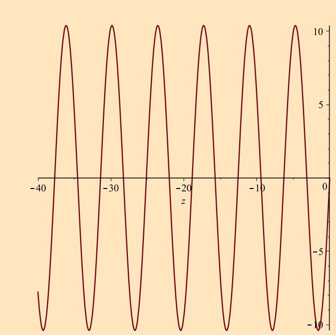

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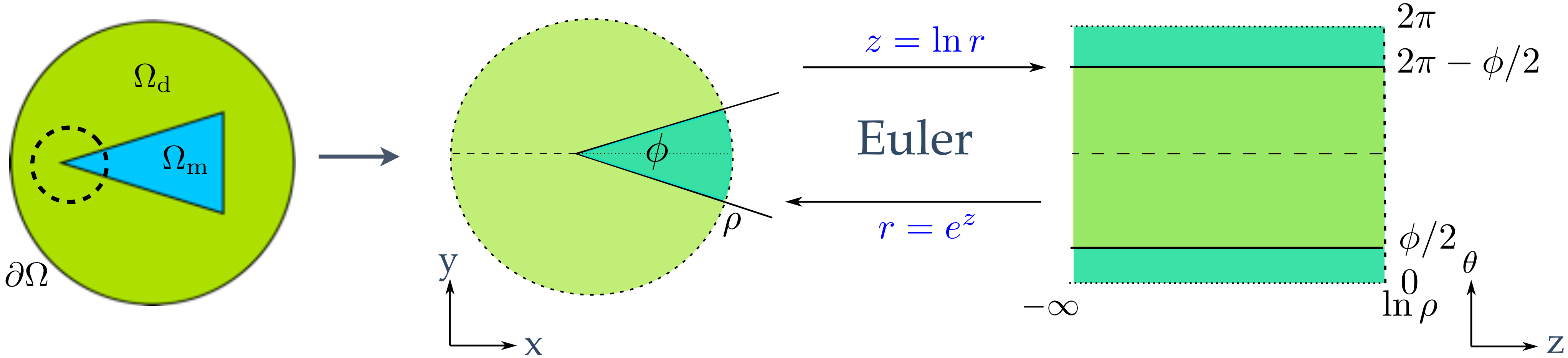

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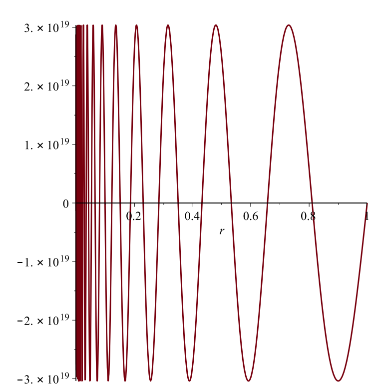

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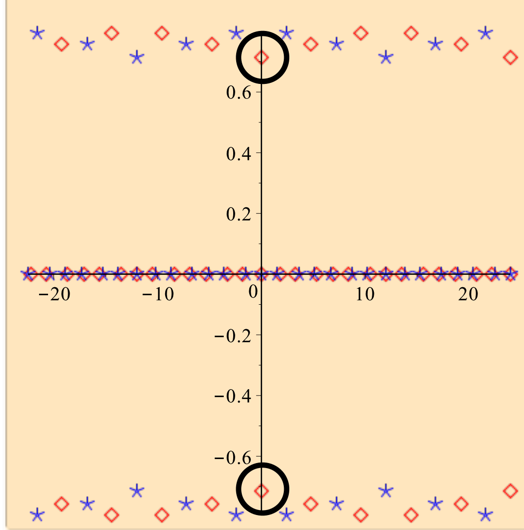

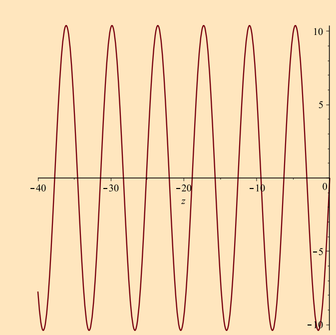

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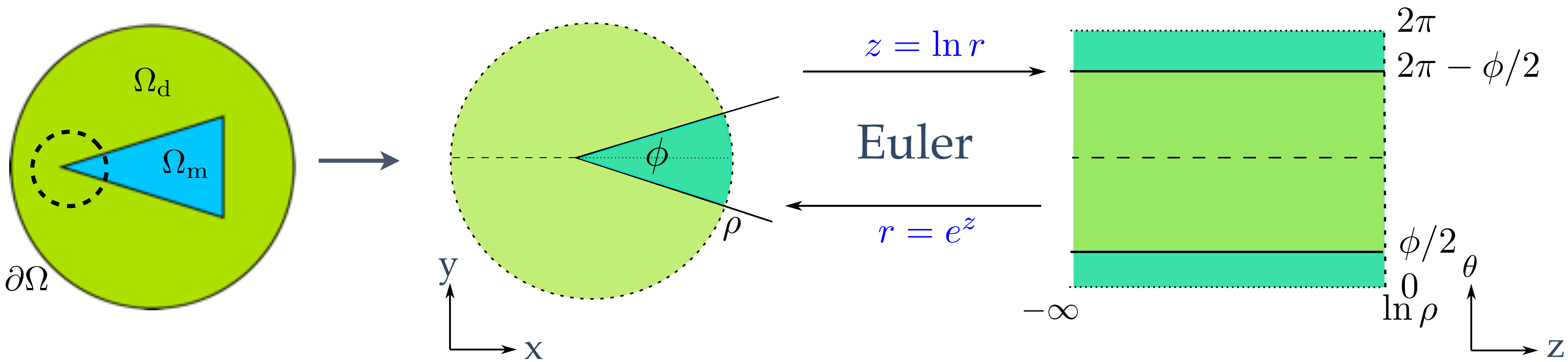

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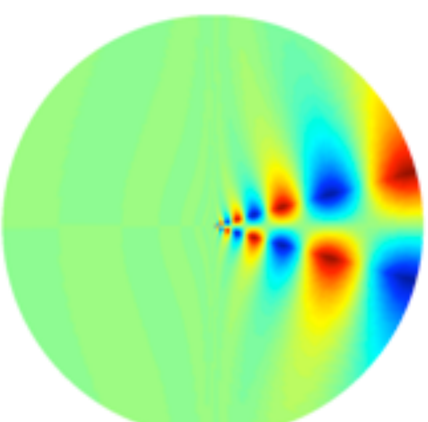

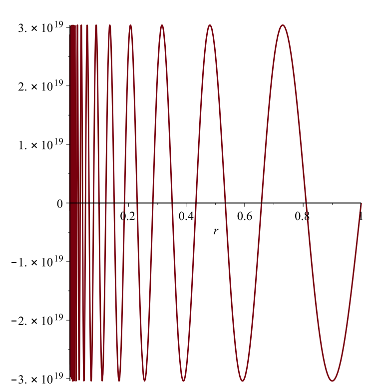

Black-hole wave.

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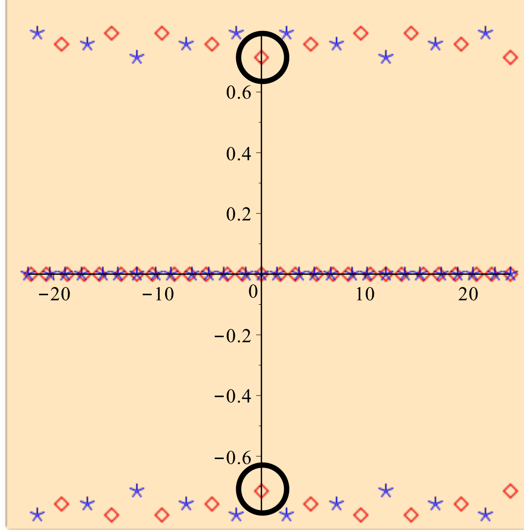
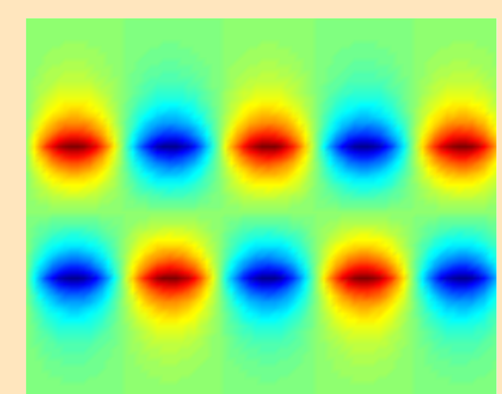
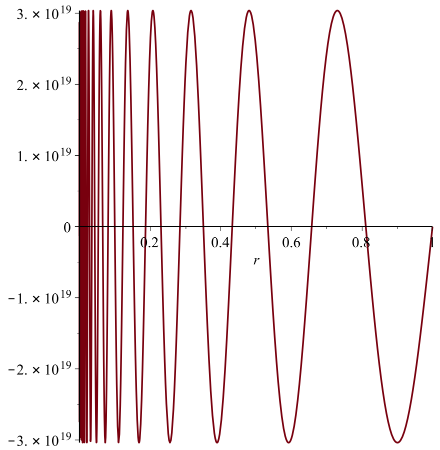




Black-hole waves and Fredholmness

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



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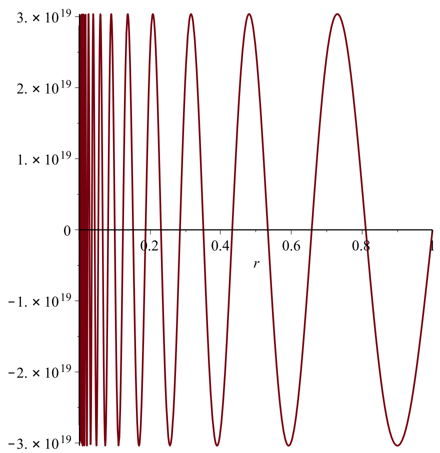

These black-hole waves are of infinite energy and strongly oscillating at the corners.

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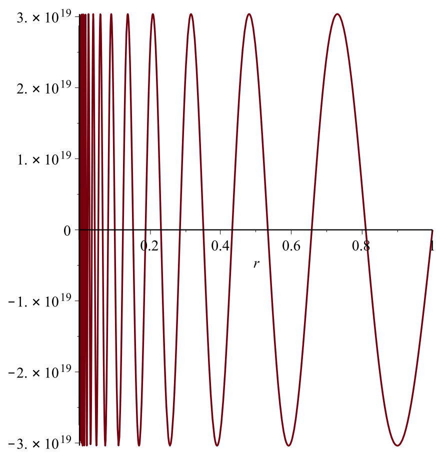

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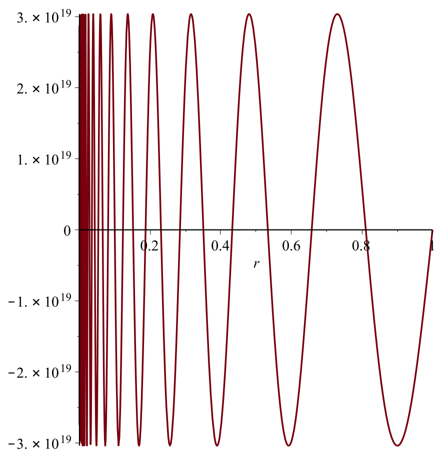

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Bonnet-Ben Dhia, C., Chesnel, Ciarlet submitted (2015).

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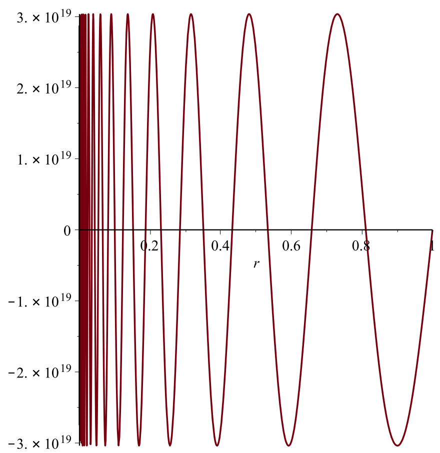

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Near the corners the solution decomposes as
$u = b^{+}s^{+} + b^{-}s^{-} + \tilde{u}, \quad \tilde{u} \in H^1(D_R),\ s^{\pm} \notin H^1(D_R),\ b^{\pm} \in \mathbb{C}$

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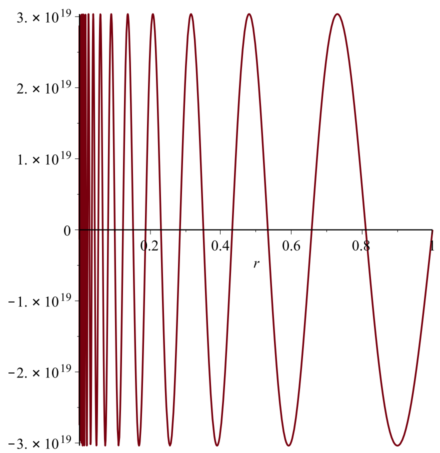

These black-hole waves are of infinite energy and strongly oscillating at the corners.
This is why standard FEM fail to approximate the solution: spurious reflexions appear.
However we need to take them into account to recover a well-posed formulation.

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

To get a unique solution, one needs to enforce a condition on $b^{\pm}$. How to proceed ?
By energy flux:

-one singularity carries energy absorbed by the corner
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Bonnet-Ben Dhia, C., Chesnel, Ciarlet submitted (2015).

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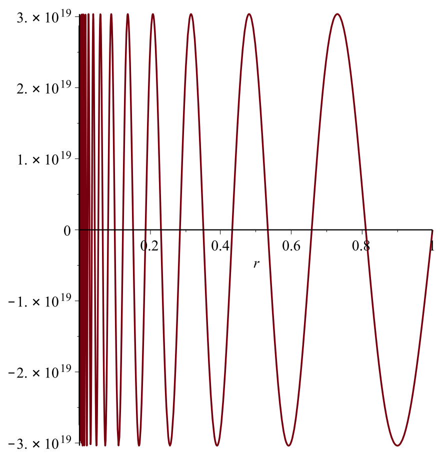

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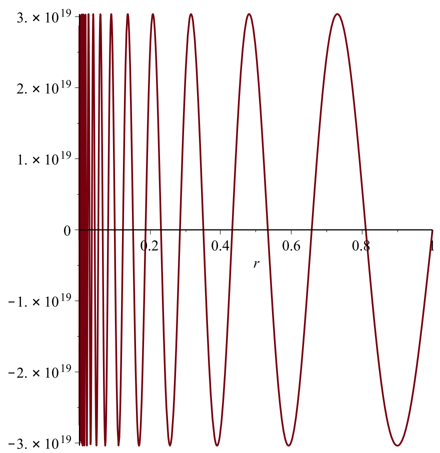

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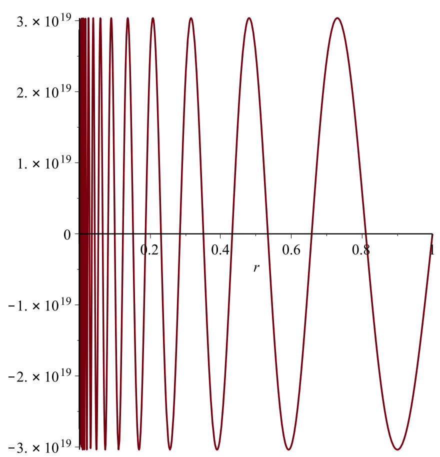

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How to proceed numerically to select the good singularity ?

Perfectly Matched Layers (PMLs)

PMLs enable to artificially bound the strip while making the propagative modes become evanescent.

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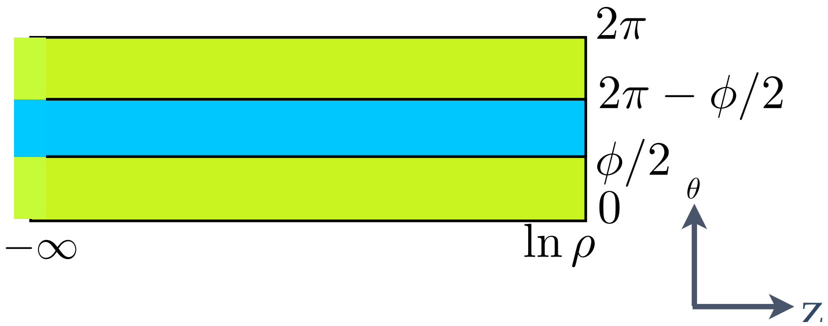

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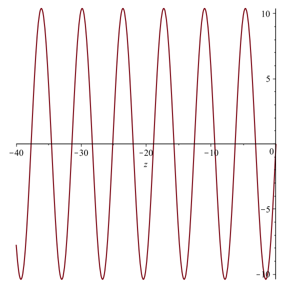

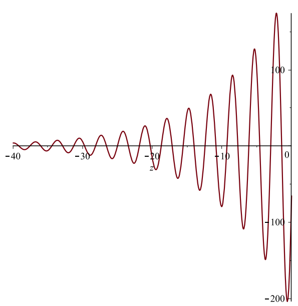

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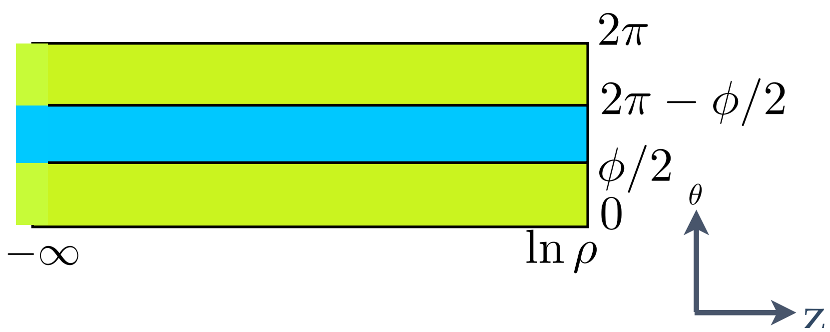

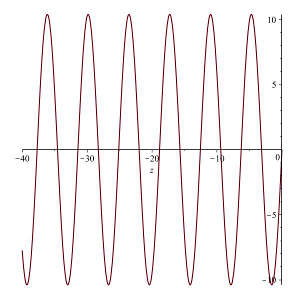

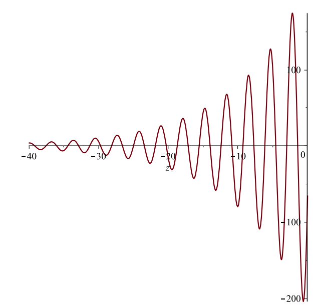

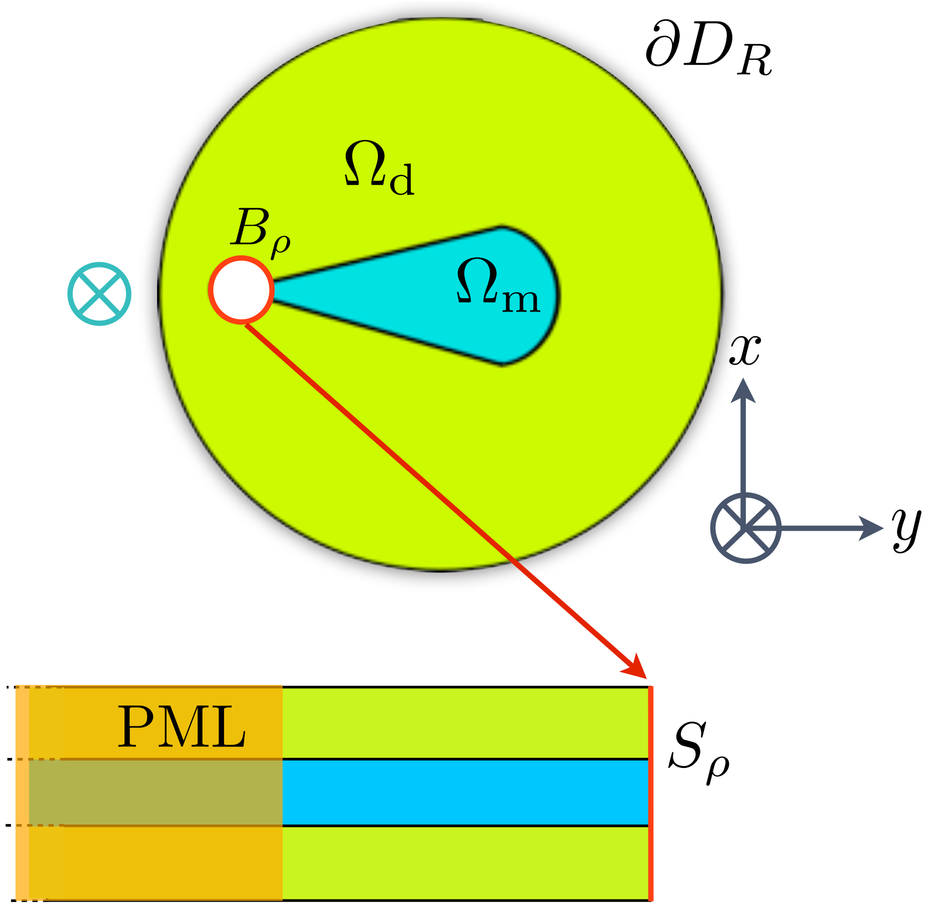

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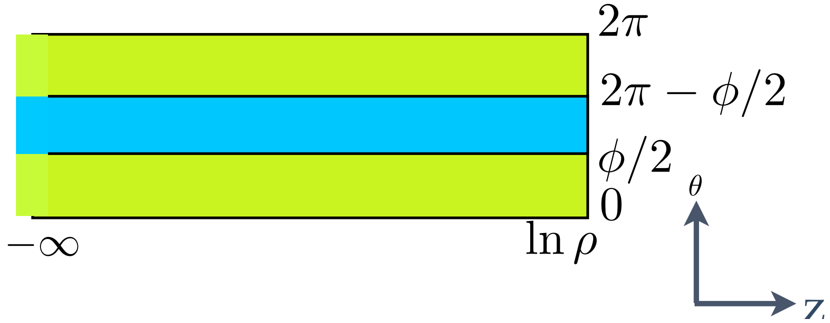

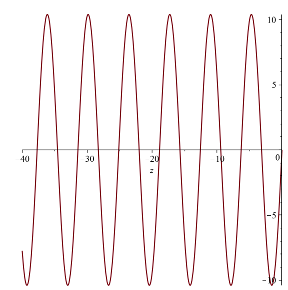

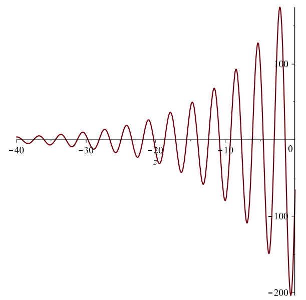

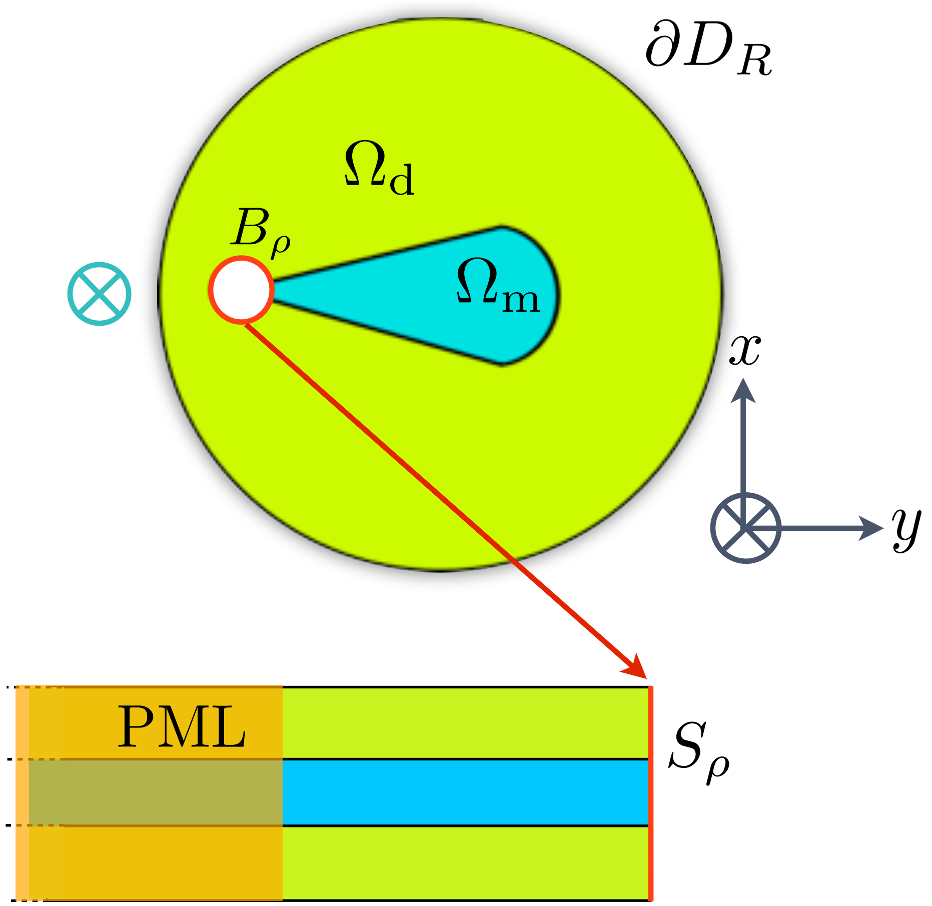

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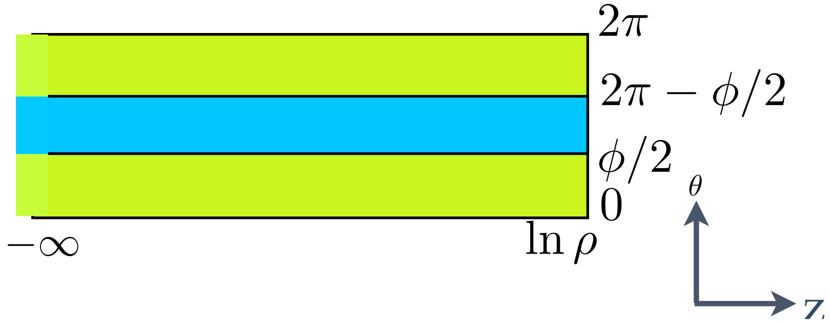

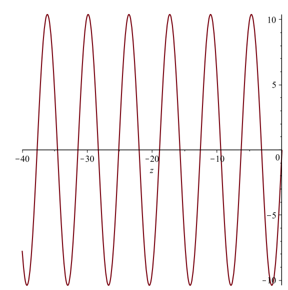

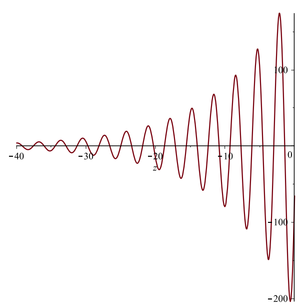

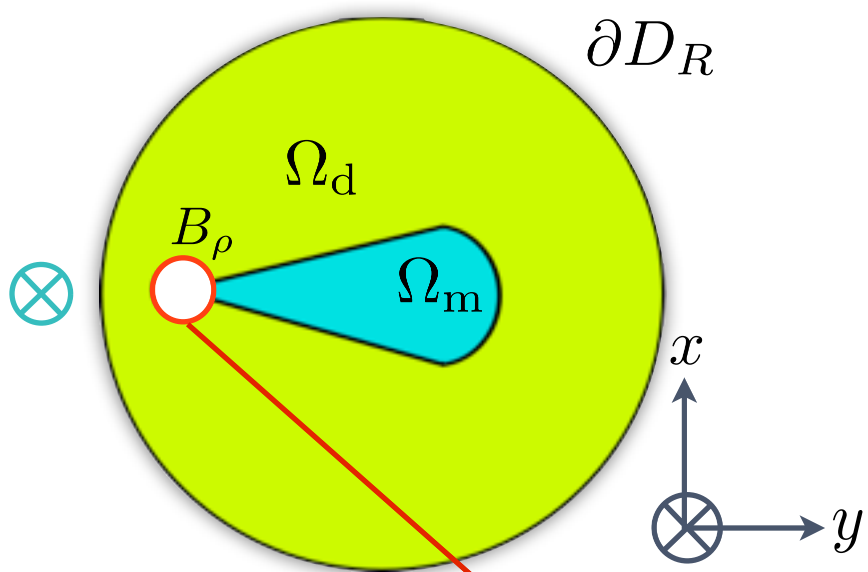

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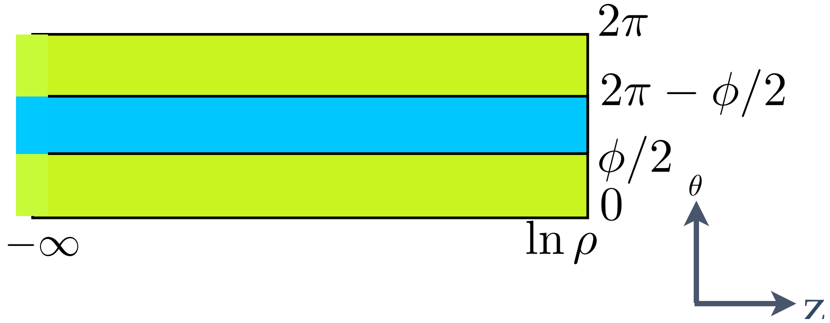

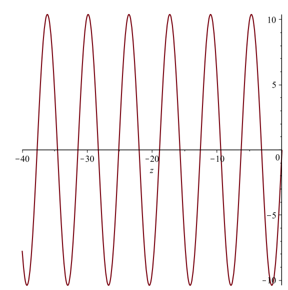

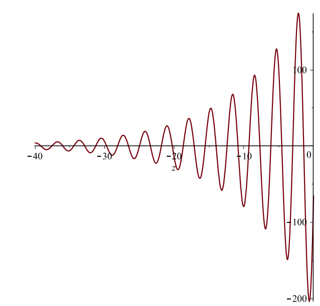

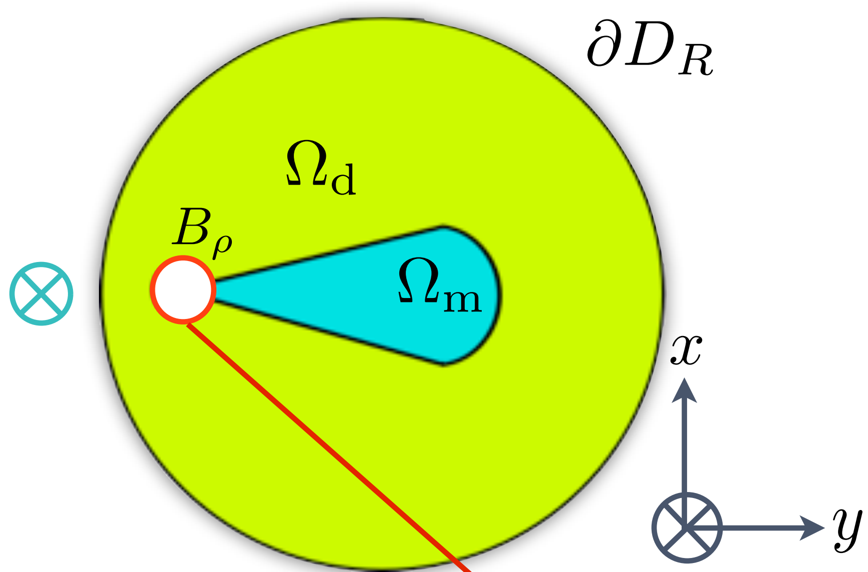

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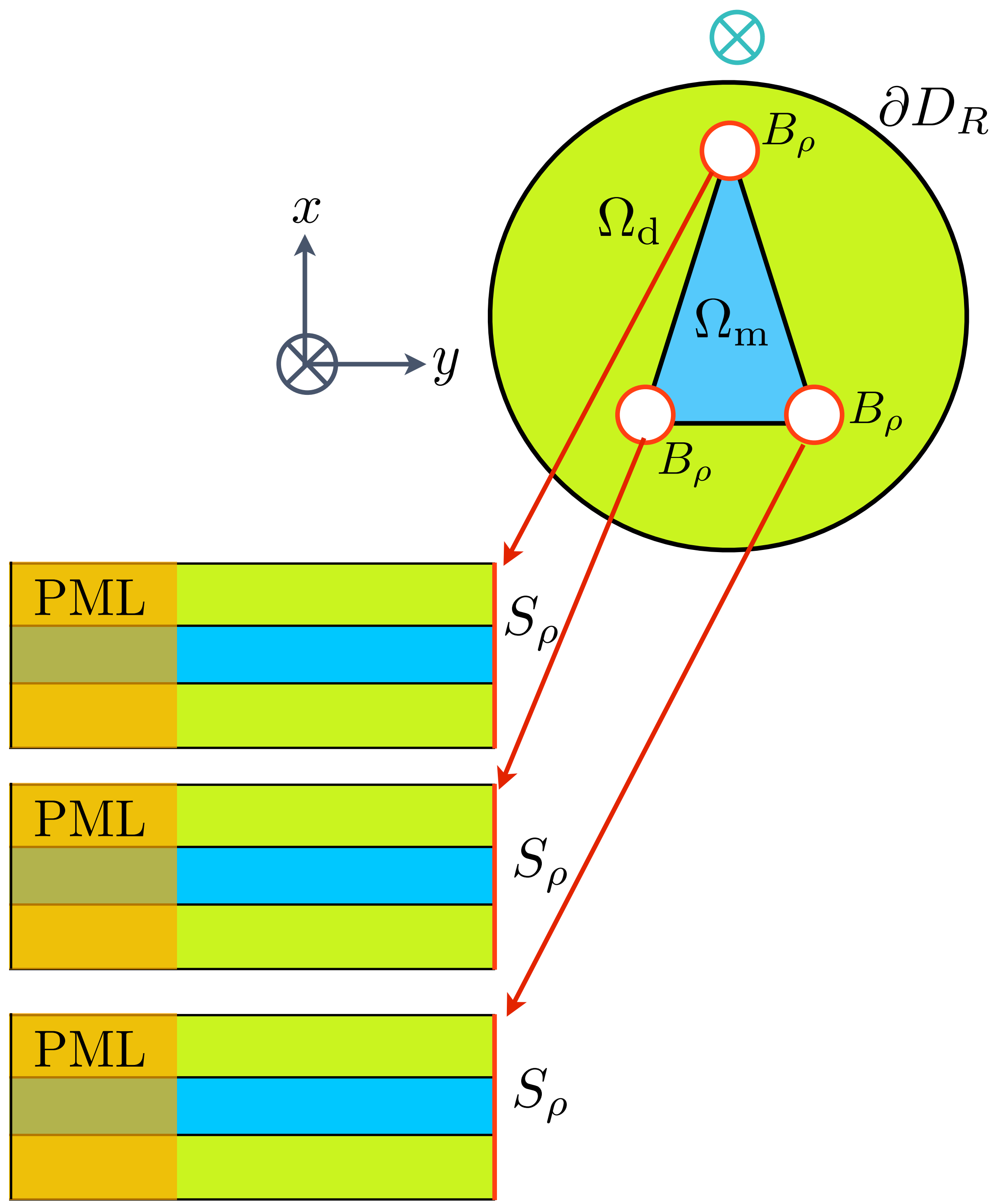
Neumann condition due to the constant mode

With several corners



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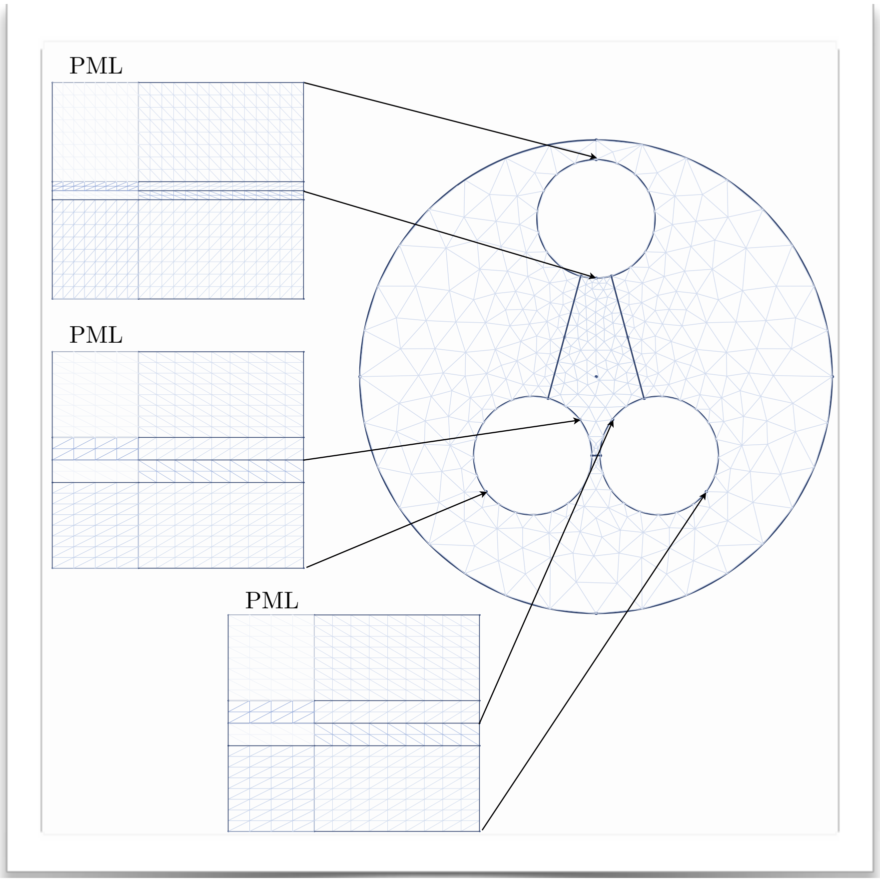

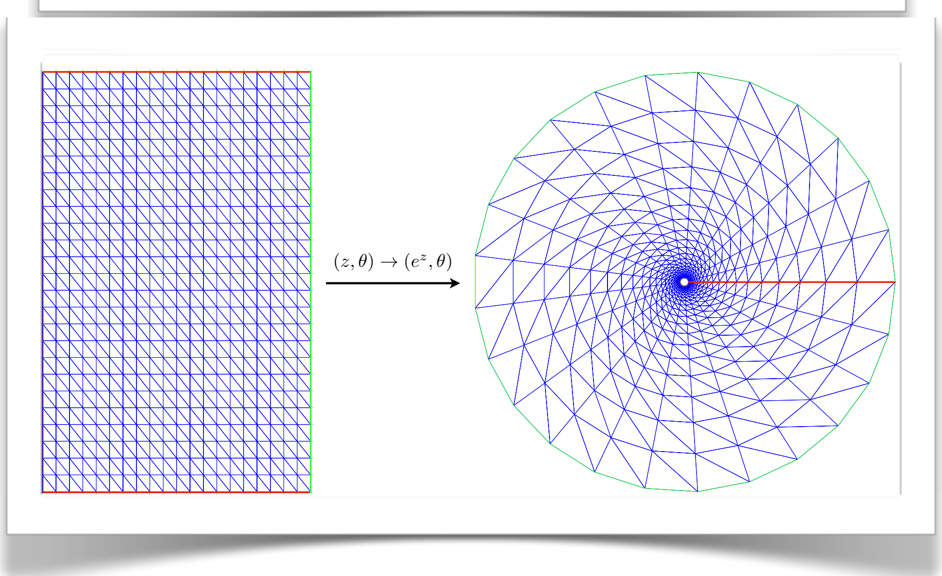

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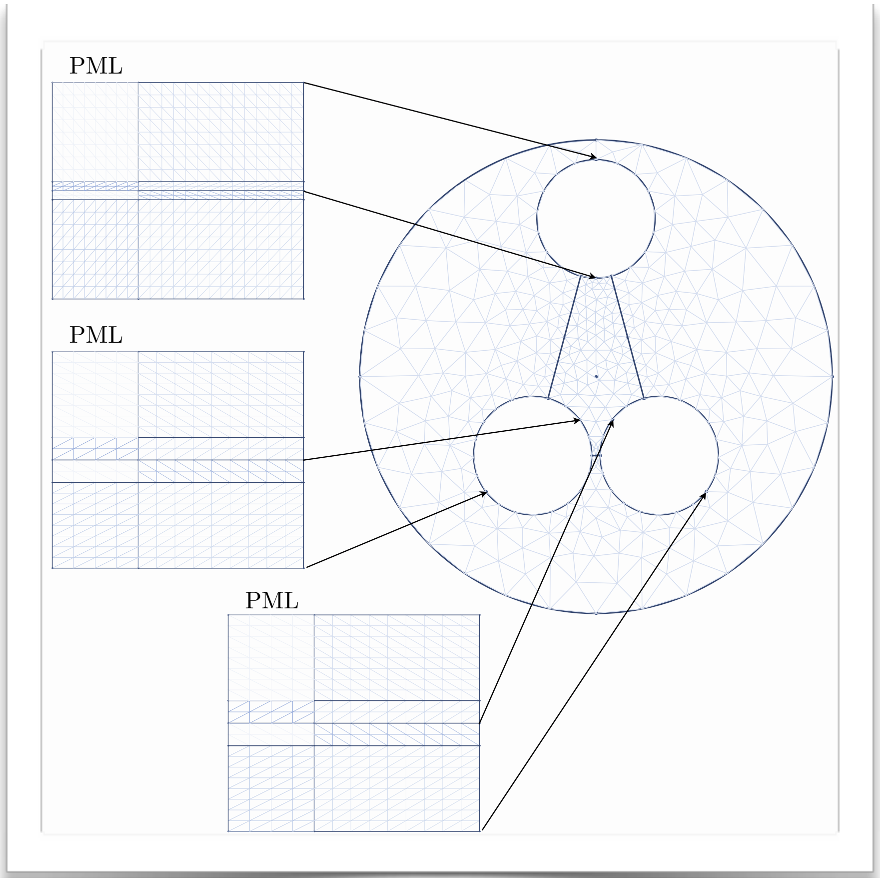

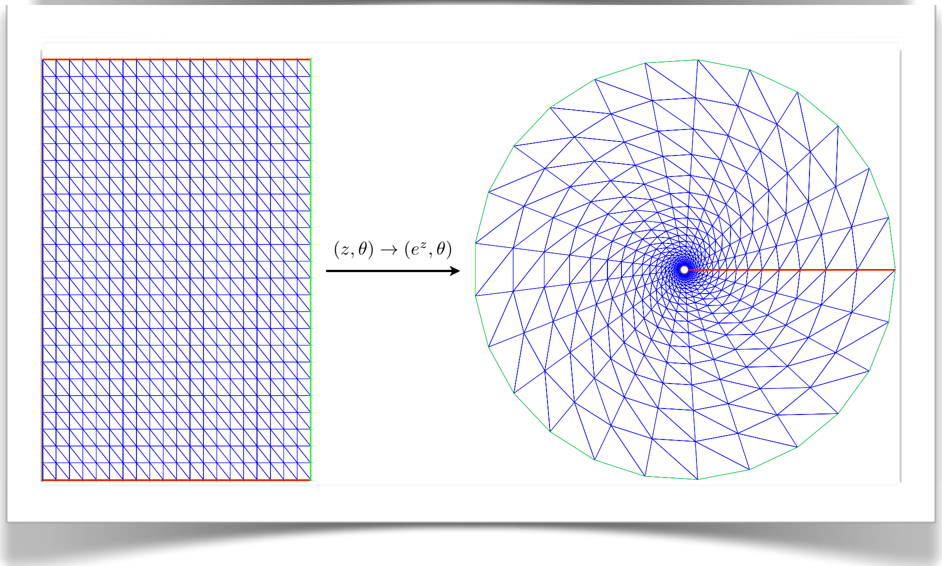

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Computation with Lagrange FE of order 2 with a Matlab code

Numerical results

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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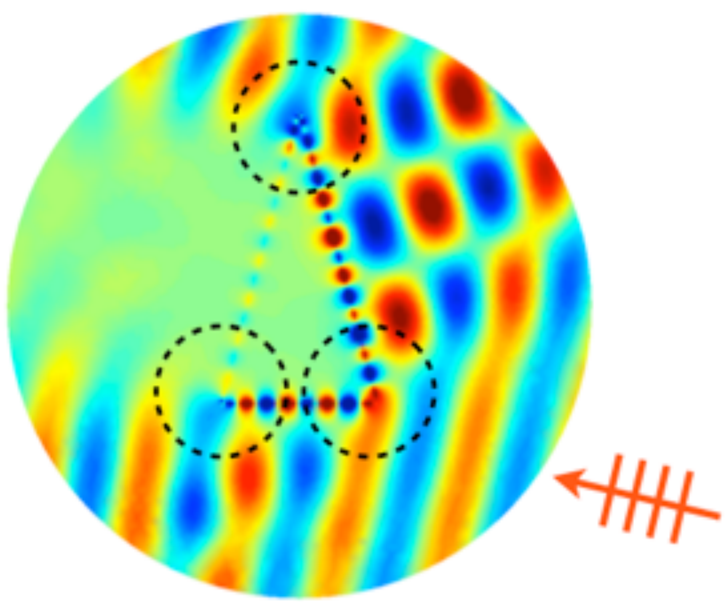
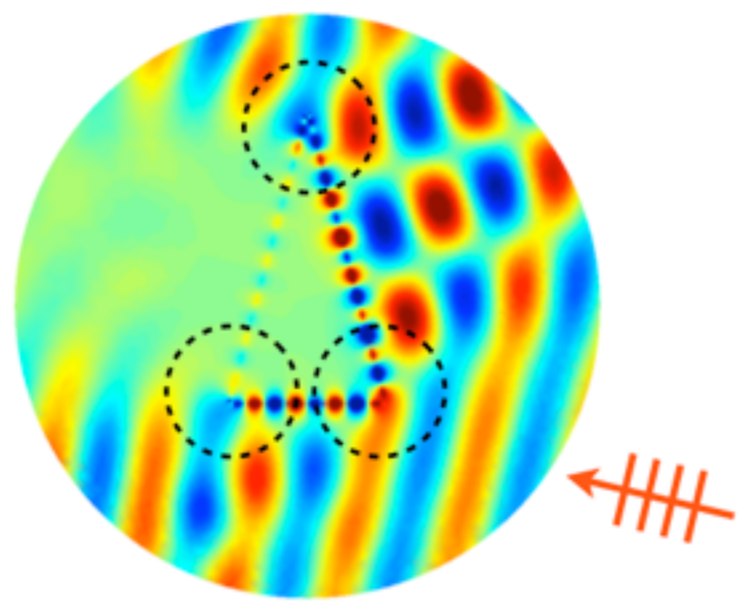
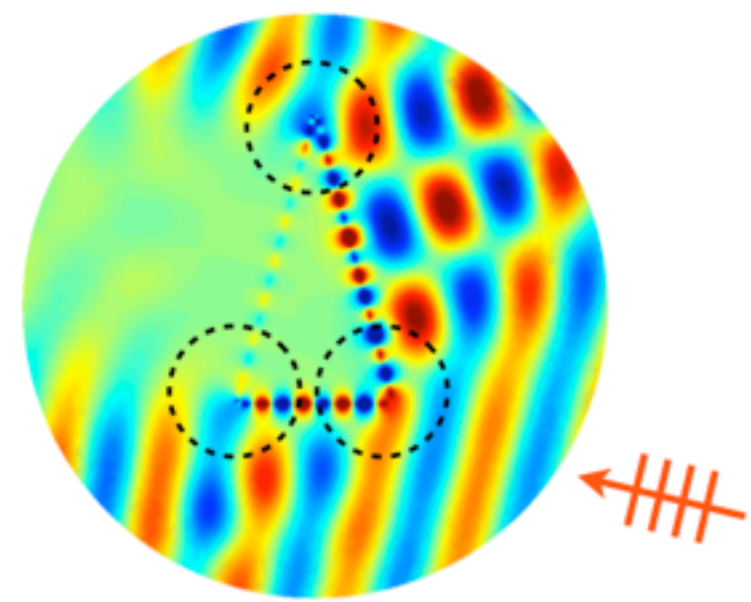


coarse mesh



intermediate mesh



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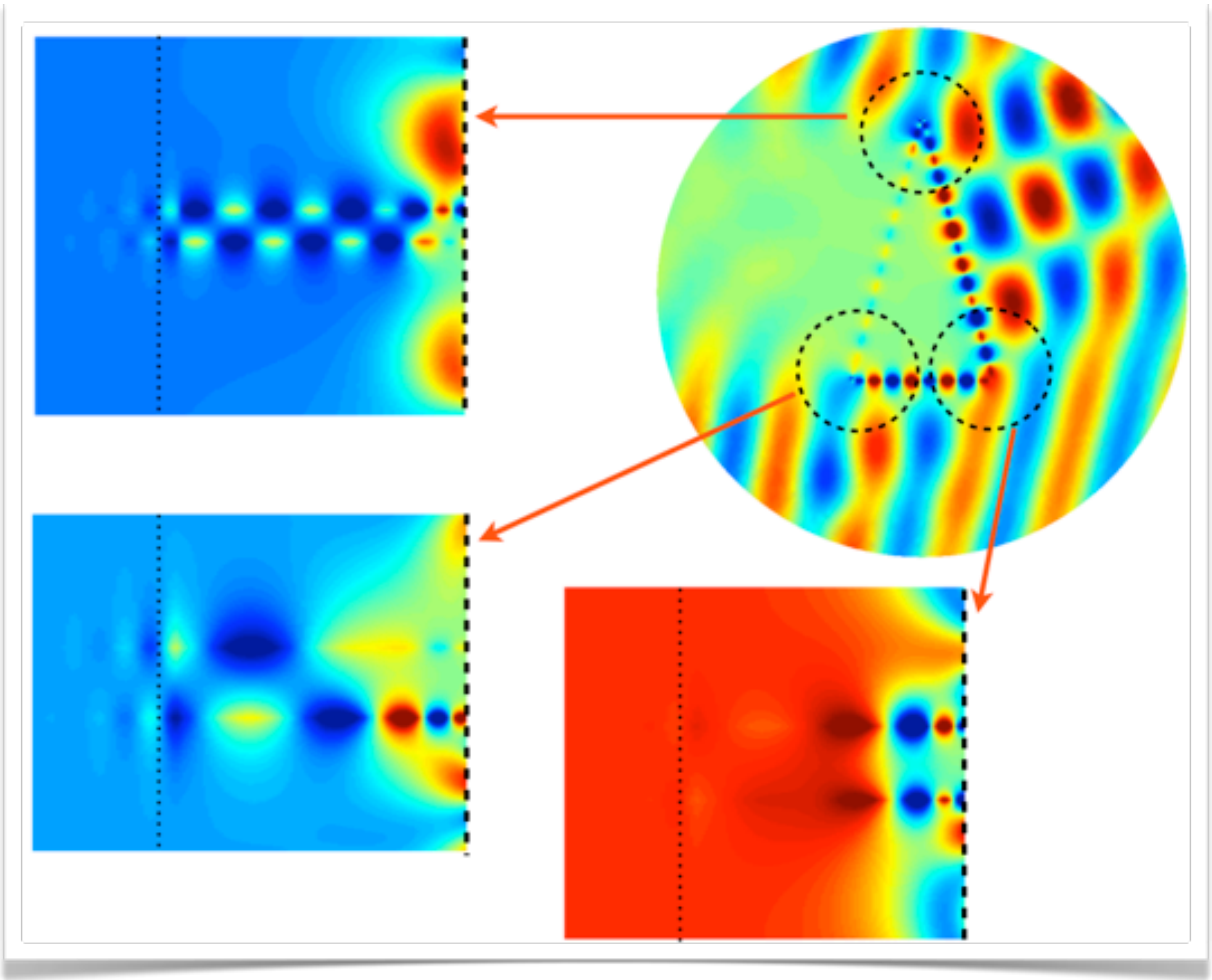

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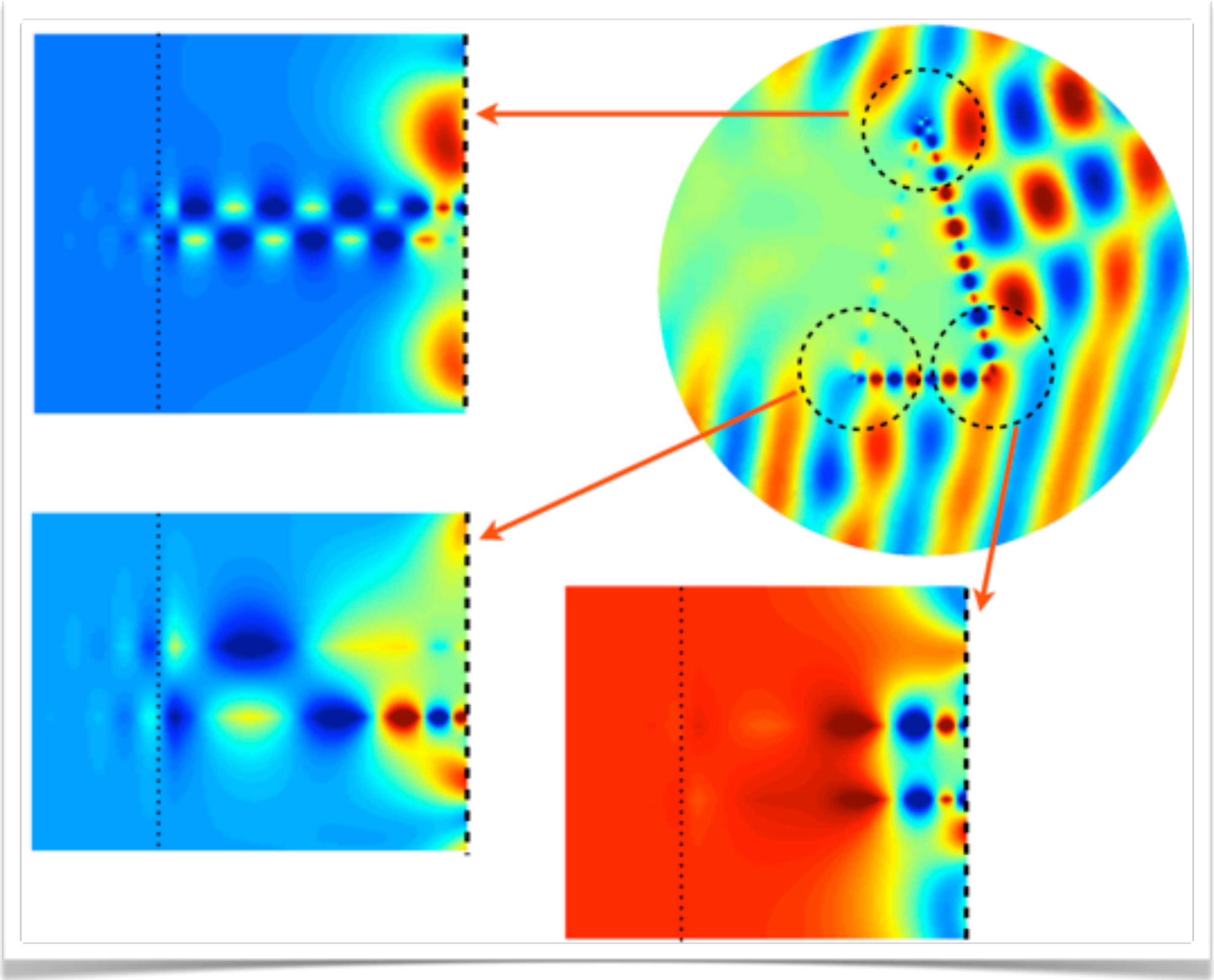

The numerical method with PMLs is stable. Let us go back to the dissipative problem.

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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Without PMLs

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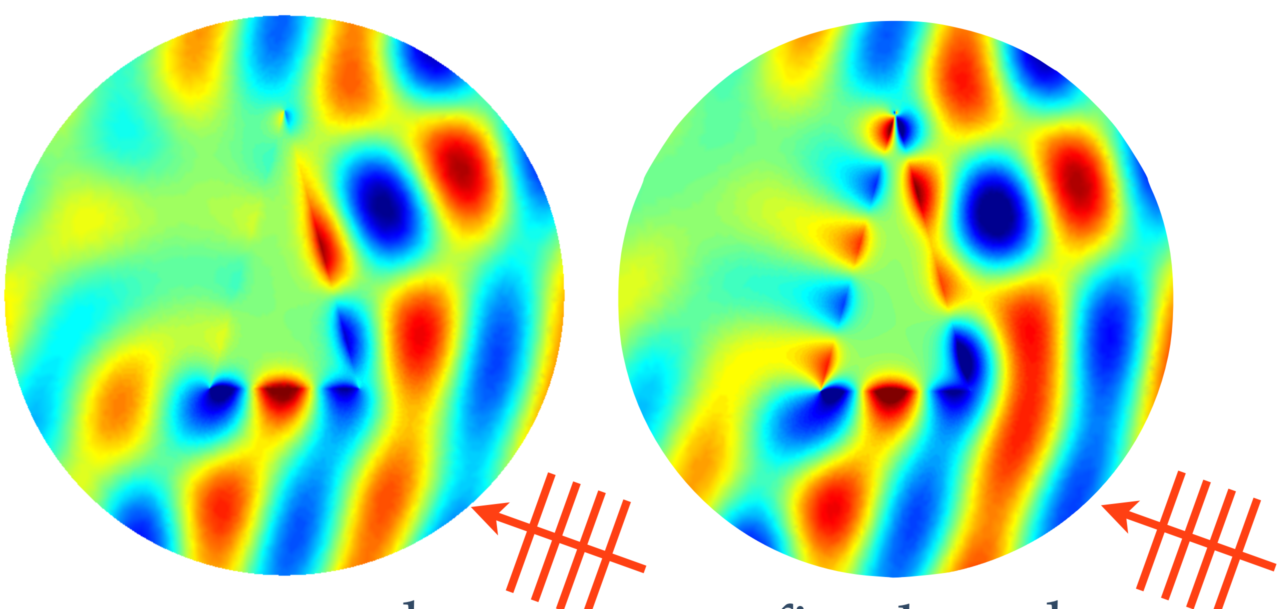

coarse mesh refined mesh

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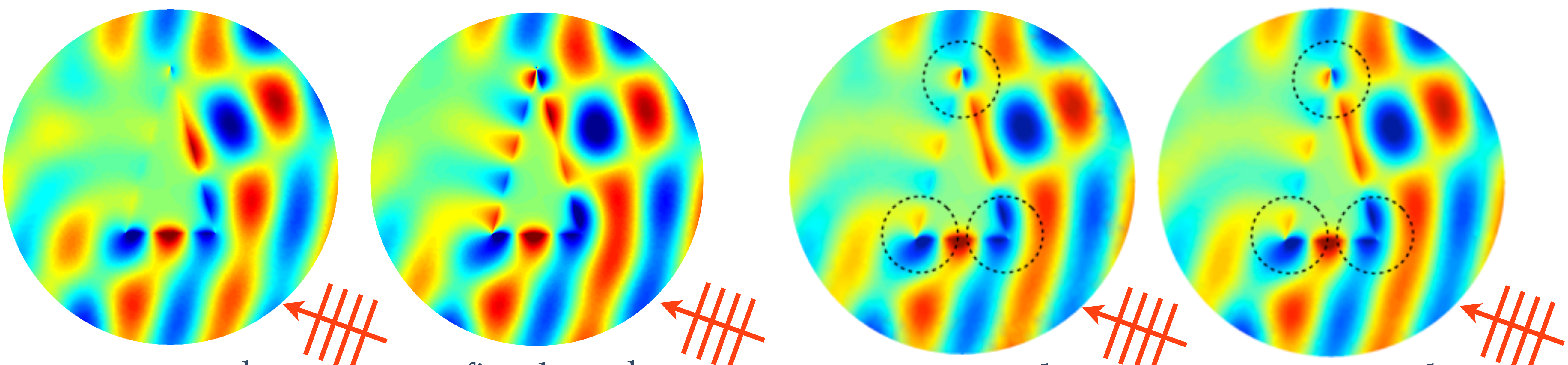
Without PMLs | With PMLs



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Without PMLs

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

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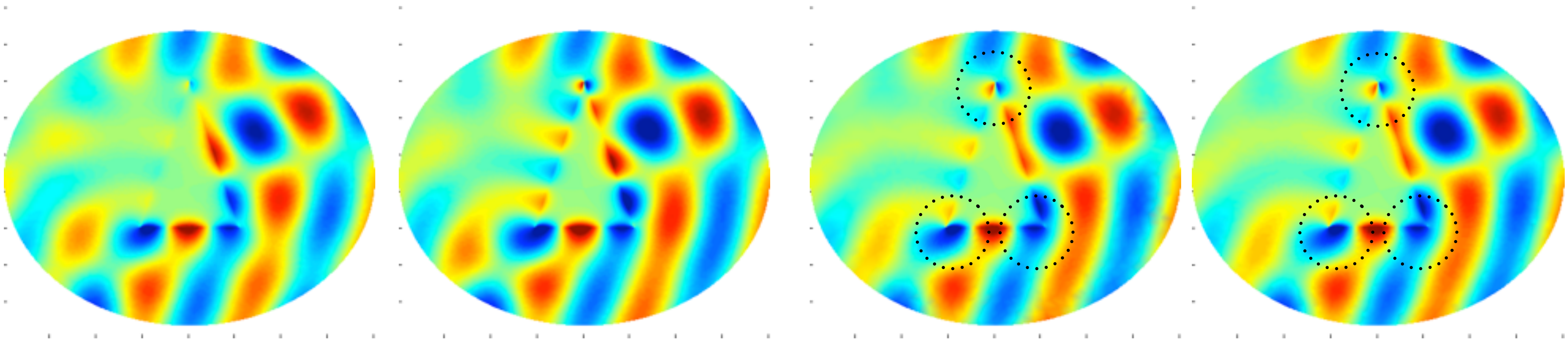
Without PMLs

With PMLs



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

Outline

- Part I: meshing rules for the corners case for $\kappa_\varepsilon \notin I_c$
- Part II: scattering problem with sign-changing coefficients
- **Perspectives**

Perspectives and ongoing work

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- Limit amplitude principle: validate the existence of a time-harmonic regime according to the critical interval. These questions are investigated in the ANR project METAMATH, and with C. Scheid in team NACHOS (Nice, France).

Thank you for your attention.