Limiting amplitude principle for plasmonic structures

Camille Carvalho
Collaboration with Claire Scheid (INRIA Sophia-Antipolis, University of Nice, France)

Wave seminar Fall 2020

CLOVERS
Carvalho Lab for exOtic waVes in Electromagnetics, Resonances and Scattering

The limiting amplitude principle

Example: consider the wave equation

$$\partial_{tt} u - c^2 \Delta u = 0$$

Assuming we can write $u = \underline{u} e^{-i\omega t}$ then the problem boils down to

$$\Delta \underline{u} + k^2 \underline{u} = 0 \quad \text{with} \quad k = \frac{\omega}{c}$$

When can we make this assumption ?

There is a boundary/source term that behaves like $f = \underline{f} e^{-i\omega t}$

then after a long time (or asymptotically) the solution admits the same behavior.

Why considering the time-harmonic problem ?

Only spatial dependence

Lots of efficient methods available to solve problems in frequency domains

Is the limiting amplitude principle valid for all problems ?

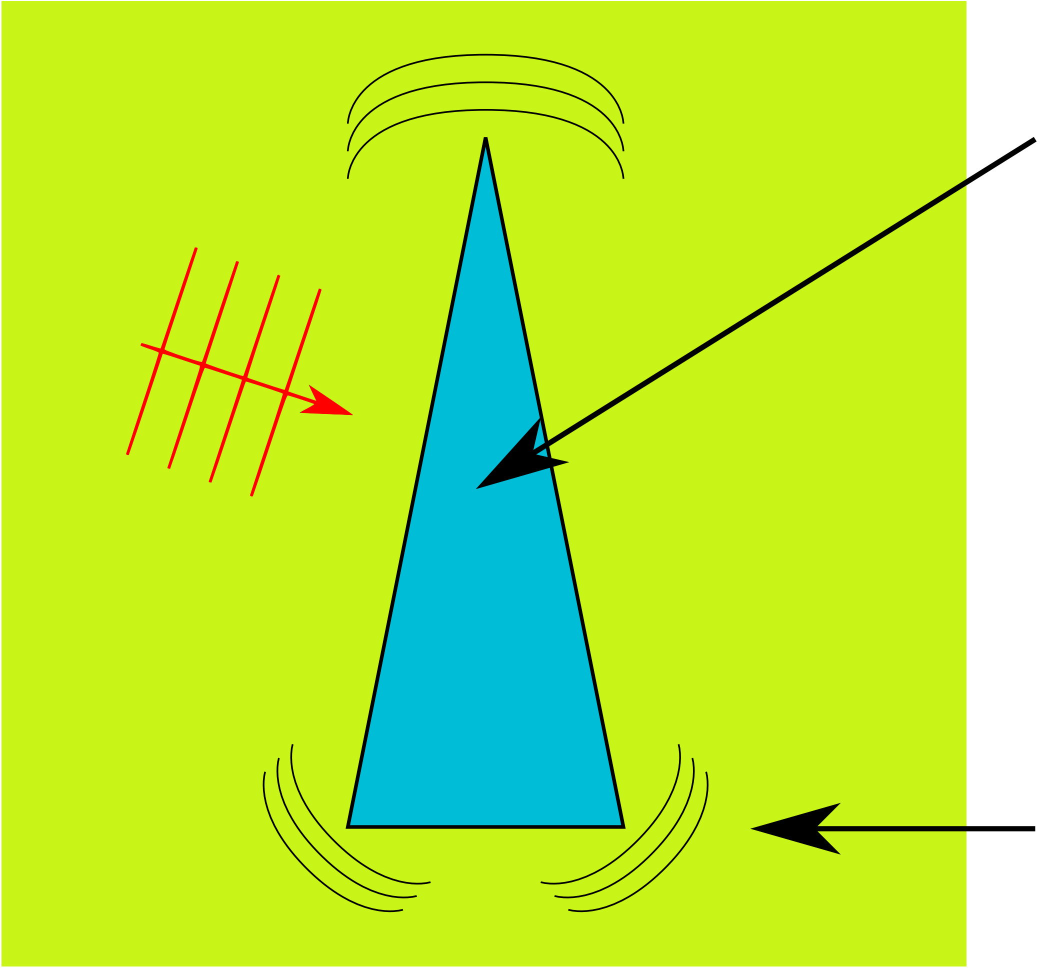
Outline

- Introduction
- Scattering in plasmonic structures
- Validating the Limiting Amplitude Principle
- Conclusion

Scattering in plasmonic structures (TD)

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

Consider the Transverse Magnetic polarization: $(E_x, E_y, H_z) = (\vec{E}_\perp, H_z)$



Maxwell equations reduce to:

$$\mu_0 \frac{\partial H_z}{\partial t} = -\nabla \times \vec{E}_\perp \ \text{ in } \mathbb{R}^2$$

$$\varepsilon_0 \varepsilon_d \frac{\partial \vec{E}_\perp}{\partial t} = \vec{\nabla} \times H_z \ \text{ in } \mathbb{R}^2 \setminus \bar{\Omega}$$

$$\varepsilon_0 \varepsilon_\infty \frac{\partial \vec{E}_\perp}{\partial t} = \vec{\nabla} \times H_z - \vec{J}_\perp \ \text{ in } \Omega$$

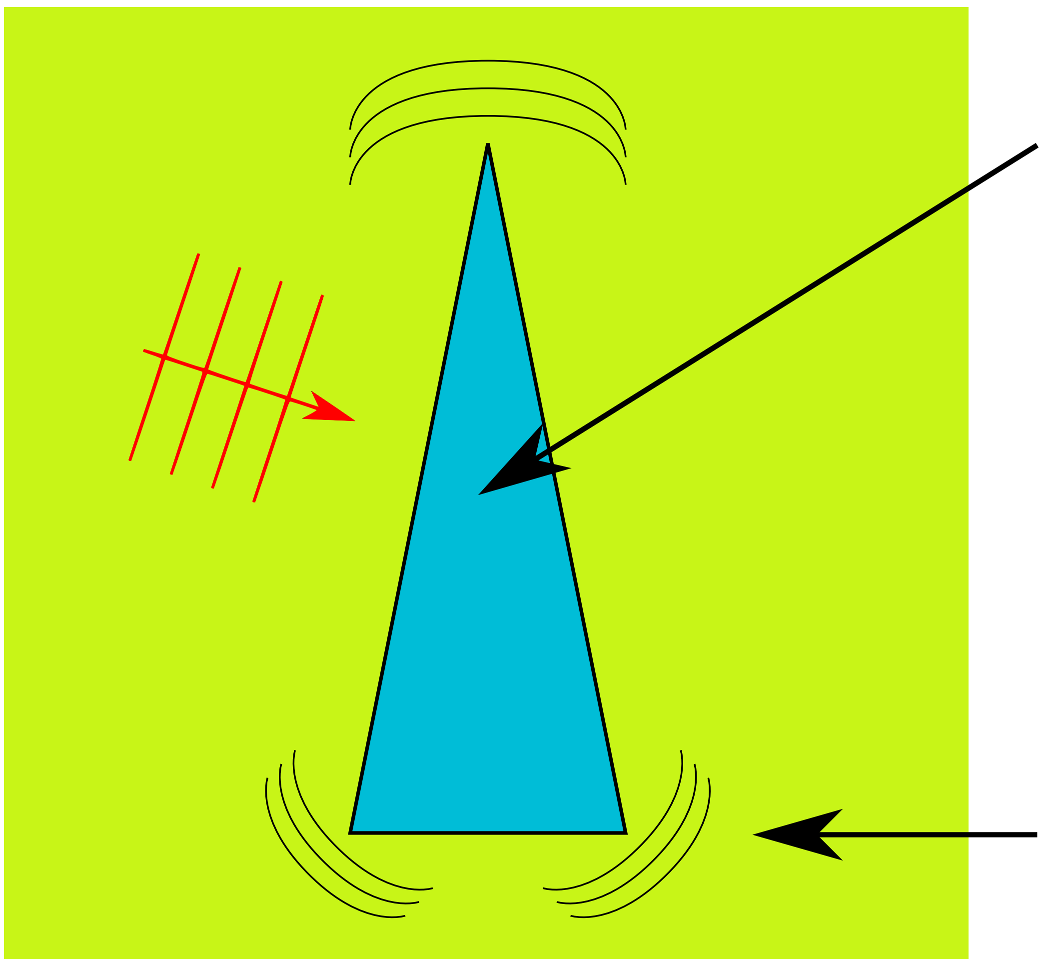
$$\frac{\partial \vec{J}_\perp}{\partial t} = \omega_p^2 \varepsilon_0 \vec{E}_\perp \ \text{ in } \Omega$$

$$\vec{J}_\perp = 0 \text{ in } \mathbb{R}^2 \setminus \Omega$$

Scattering in plasmonic structures (TD)

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

Consider the Transverse Magnetic polarization: $(E_x, E_y, H_z) = (\vec{E}_\perp, H_z)$



Maxwell equations reduce to:

$$\mu_0 \frac{\partial H_z}{\partial t} = -\nabla \times \vec{E}_\perp \text{ in } \mathbb{R}^2$$

$$\varepsilon_0 \varepsilon \frac{\partial \vec{E}_\perp}{\partial t} = \vec{\nabla} \times H_z - \vec{J}_\perp \text{ in } \mathbb{R}^2$$

$$\frac{\partial \vec{J}_\perp}{\partial t} = \omega_p^2 \varepsilon_0 \vec{E}_\perp \text{ in } \Omega$$

$$\vec{J}_\perp = 0 \text{ in } \mathbb{R}^2 \setminus \Omega$$

$$\varepsilon := \begin{cases} \varepsilon_d & \mathbb{R}^2 \setminus \bar{\Omega} \\ \varepsilon_\infty & \Omega \end{cases}$$

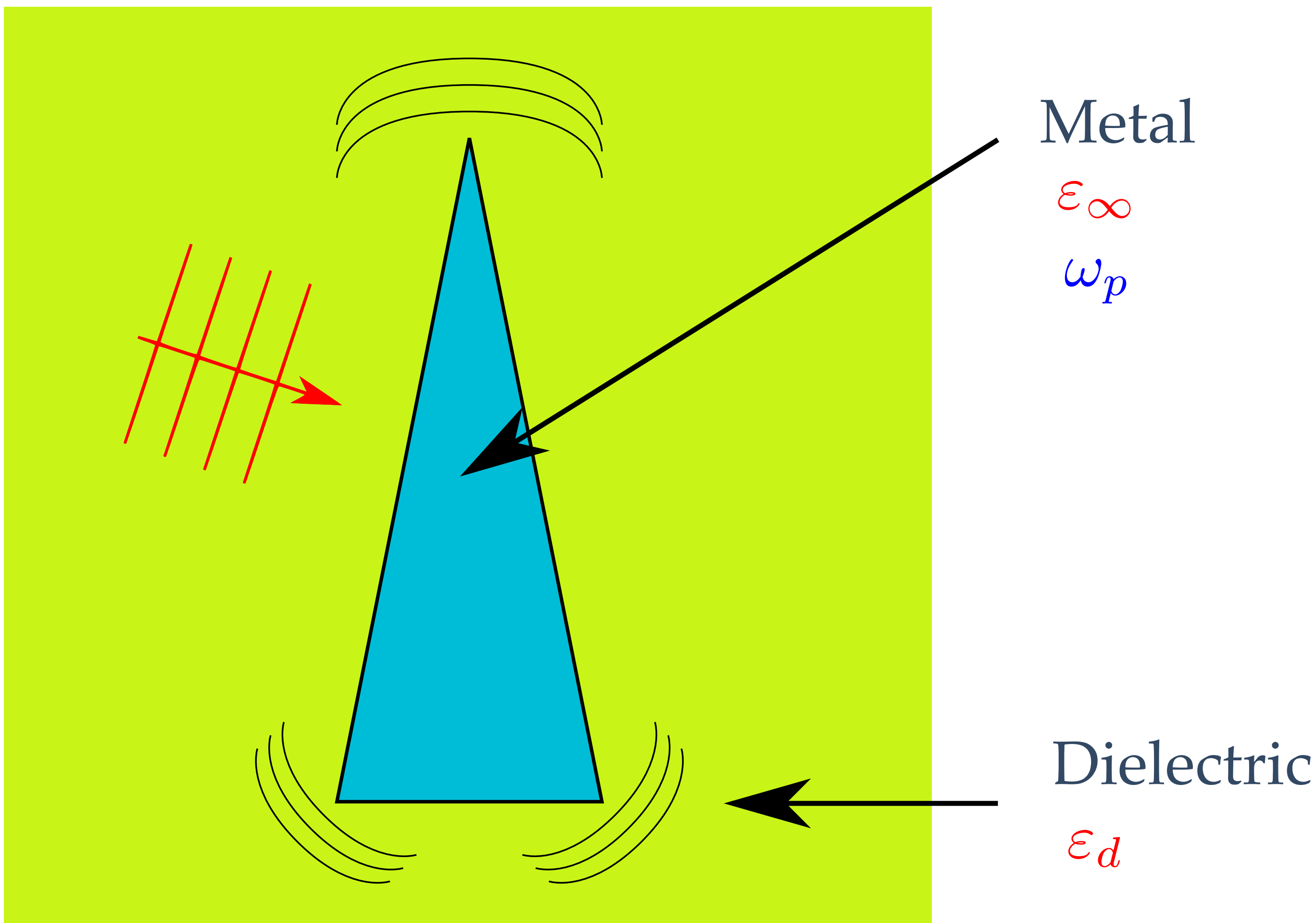
This problem is well-posed (truncate domain with Silver-Müller condition)

Nicaise (2018)

Scattering in plasmonic structures (FD)

Consider the Transverse Magnetic polarization: $(E_x, E_y, H_z) = (\vec{E}_\perp, H_z)$

Assume we can write: $(\vec{E}_\perp, H_z, \vec{J}_\perp) = (\underline{\vec{E}}_\perp, \underline{H_z}, \underline{\vec{J}}_\perp)e^{-i\omega t}$



Maxwell equations reduce to:

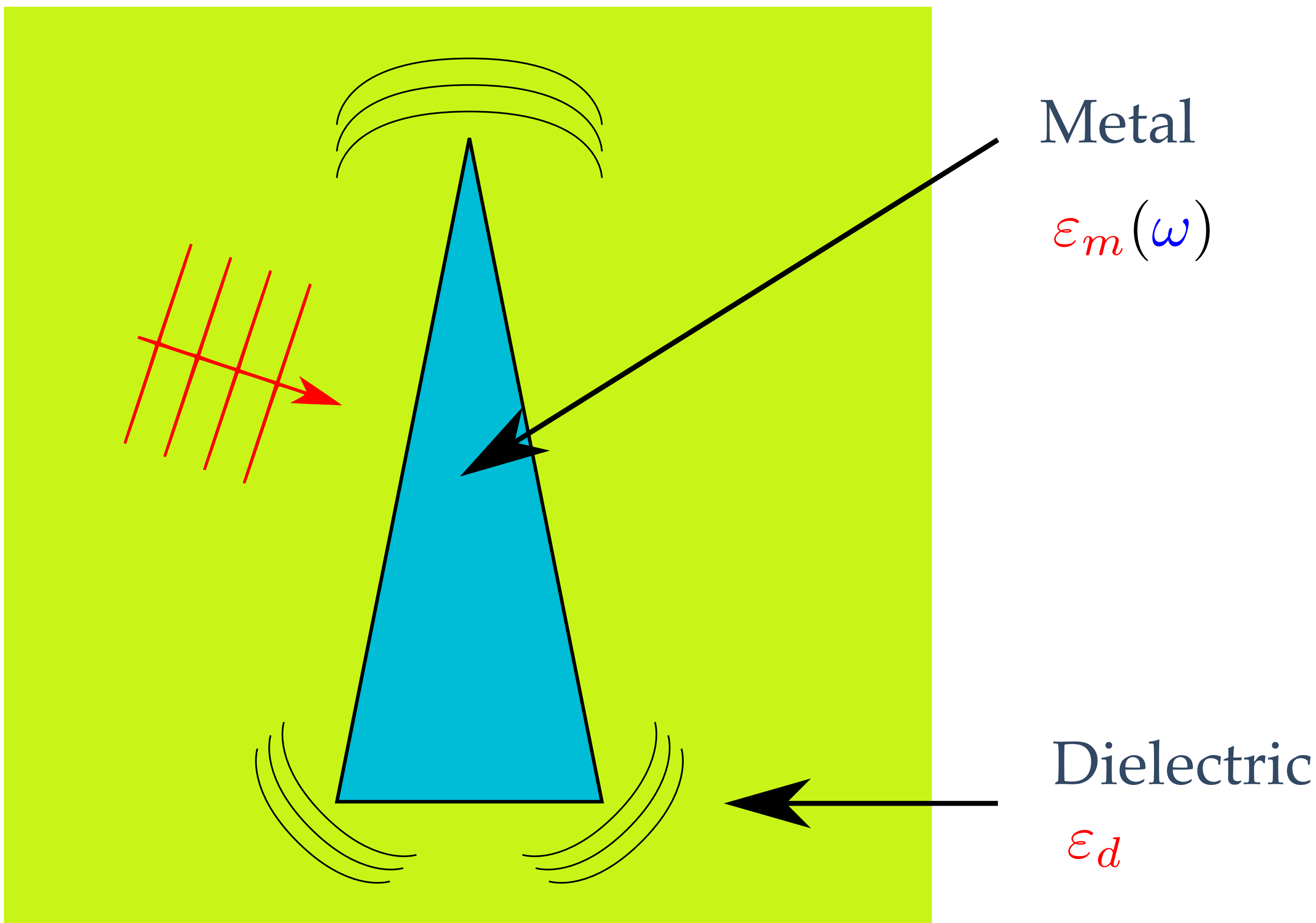
$$-i\omega\mu_0 \underline{H_z} = -\nabla \times \underline{\vec{E}}_\perp \quad \text{in } \mathbb{R}^2$$
$$-i\omega\varepsilon_0\varepsilon \underline{\vec{E}}_\perp = \vec{\nabla} \times \underline{H_z} - \underline{\vec{J}}_\perp \quad \text{in } \mathbb{R}^2$$
$$-i\omega \underline{\vec{J}}_\perp = \omega_p^2 \varepsilon_0 \underline{\vec{E}}_\perp \quad \text{in } \Omega$$
$$\underline{\vec{J}}_\perp = 0 \text{ in } \mathbb{R}^2 \setminus \Omega$$

$$\varepsilon := \begin{cases} \varepsilon_d & \mathbb{R}^2 \setminus \bar{\Omega} \\ \varepsilon_\infty & \Omega \end{cases}$$

Scattering in plasmonic structures (FD)

Consider the Transverse Magnetic polarization: $(E_x, E_y, H_z) = (\vec{E}_\perp, H_z)$

Assume we can write: $(\vec{E}_\perp, H_z, \vec{J}_\perp) = (\underline{\vec{E}}_\perp, \underline{H_z}, \underline{\vec{J}}_\perp)e^{-i\omega t}$



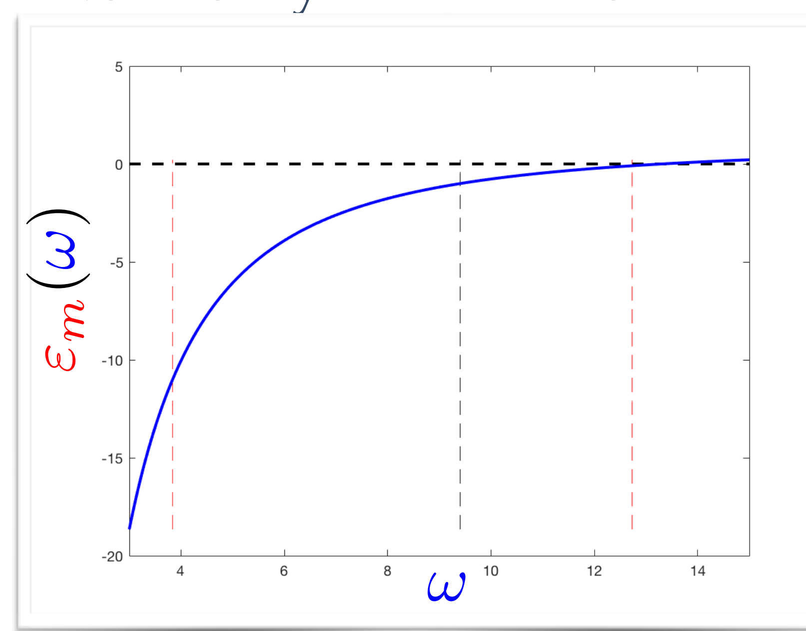
Maxwell equations reduce to:

$$-i\omega\mu_0 \underline{H_z} = -\nabla \times \underline{\vec{E}}_\perp \quad \text{in } \mathbb{R}^2$$

$$-i\omega\varepsilon_0\varepsilon(\omega)\underline{\vec{E}}_\perp = \vec{\nabla} \times \underline{H_z} \quad \text{in } \mathbb{R}^2$$

$$\varepsilon(\omega) := \begin{cases} \varepsilon_d & \mathbb{R}^2 \setminus \bar{\Omega} \\ \varepsilon_\infty - \dfrac{\omega_p^2}{\omega^2} & \Omega \end{cases}$$

Non lossy Drude model:



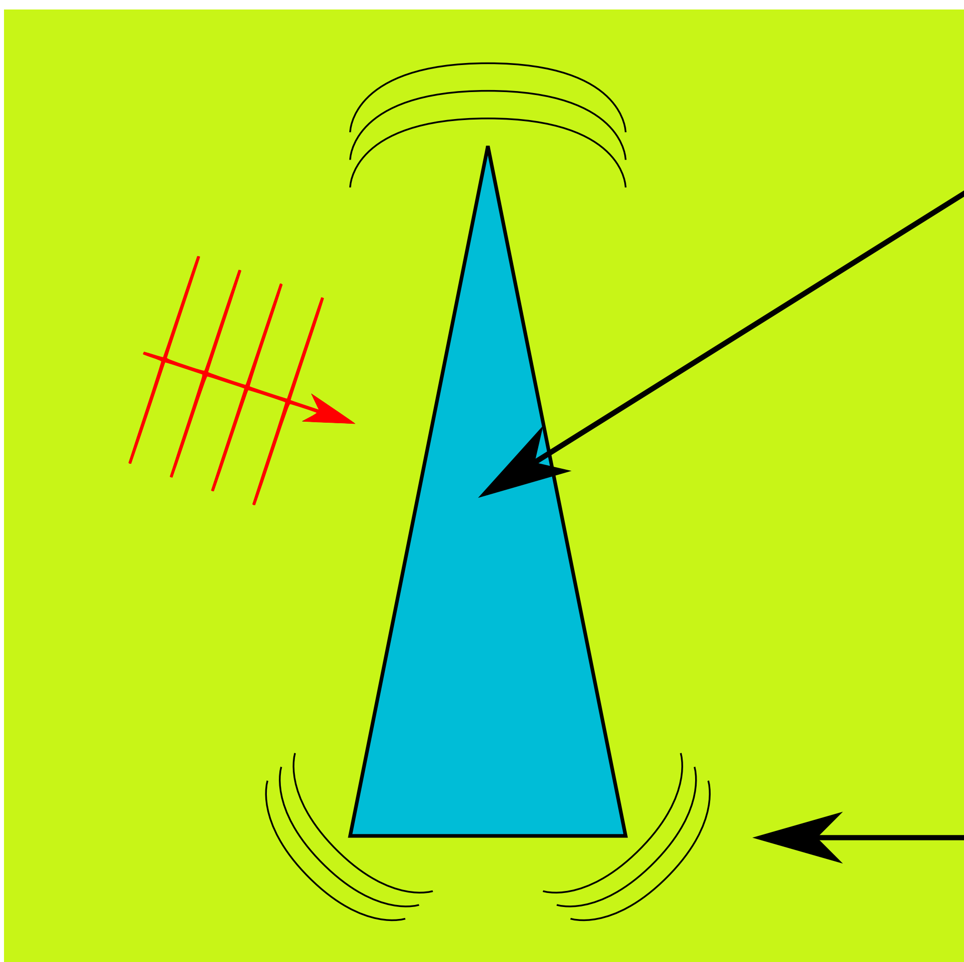
Problem with sign-changing coefficients.

Bonnet-Ben Dhia, Chesnel, Ciarlet (2012,2014)

Scattering in plasmonic structures (FD)

Consider the Transverse Magnetic polarization in time-harmonic regime:

$$(\vec{E}_\perp, H_z, \vec{J}_\perp) = (\underline{\vec{E}}_\perp, \underline{H_z}, \underline{\vec{J}}_\perp)e^{-i\omega t}$$



Metal

$\varepsilon_m(\omega)$

Dielectric

ε_d

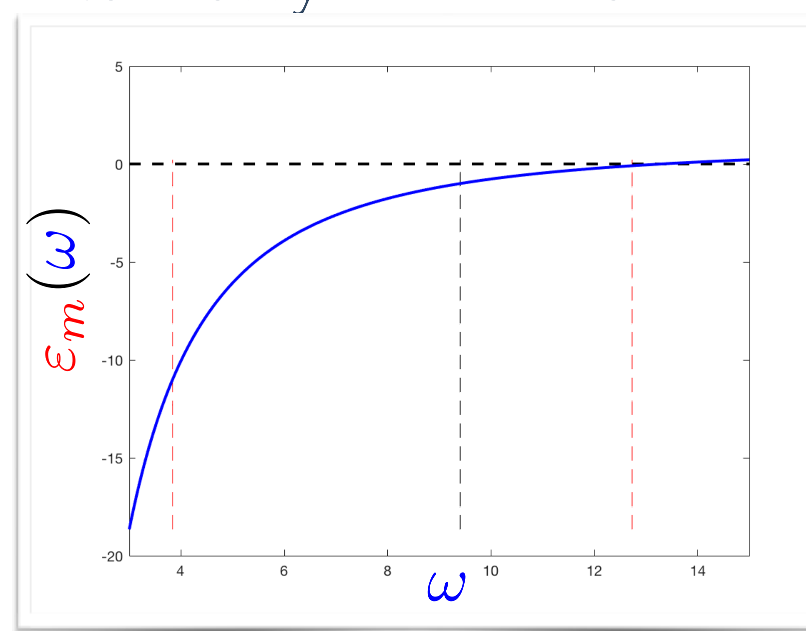
Maxwell equations reduce to:

$$\boxed{\nabla \cdot (\varepsilon(\omega)^{-1}\nabla \underline{H_z}) + k^2 \underline{H_z} = 0 \text{ in } \mathbb{R}^2}$$

$$-i\omega\varepsilon_0\varepsilon(\omega)\underline{\vec{E}}_\perp = \vec{\nabla} \times \underline{H_z} \quad \text{in } \mathbb{R}^2$$

$$\varepsilon(\omega) := \begin{cases} \varepsilon_d & \mathbb{R}^2 \setminus \bar{\Omega} \\ \varepsilon_\infty - \dfrac{\omega_p^2}{\omega^2} & \Omega \end{cases}$$

Non lossy Drude model:



This problem can be ill-posed depending on :

$$k = \omega\sqrt{\varepsilon_0\mu_0} = \frac{\omega}{c}$$

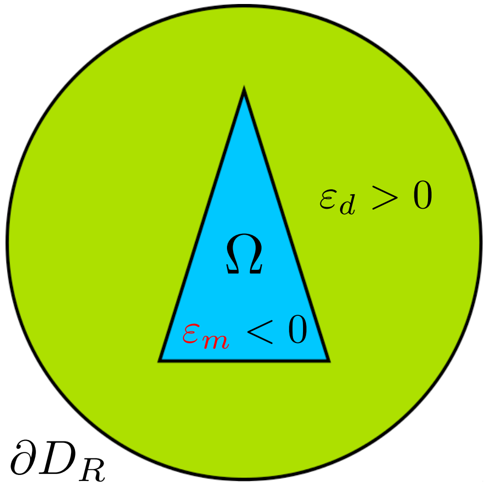
Well-posedness in frequency domain

Find $H_z \in H^1(D_R)$ such that

$\nabla \cdot (\varepsilon(\omega)^{-1} \nabla H_z) + k^2 H_z = 0$ in D_R

$\partial_n H_z - ikH_z = \partial_n u^{\mathrm{inc}} - iku^{\mathrm{inc}}$ on ∂D_R

$$H^1(D_R) := \{u | \int_{D_R} |u|^2 + |\nabla u|^2 \, d\mathbf{x} < +\infty\}$$

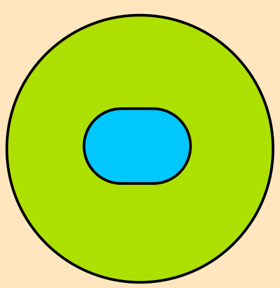


Thanks to the T-coercivity theory, one can prove well-posedness under some conditions on ε and the geometry.

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

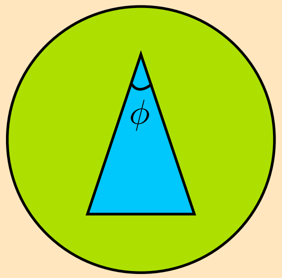
In our case: YES if and only if $\kappa_\varepsilon := \dfrac{\varepsilon_{\mathrm{m}}}{\varepsilon_{\mathrm{d}}} \notin I_c$ I_c is called critical interval.

If the interface is smooth:



$I_c = \{-1\}$

If the interface has corners:



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

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

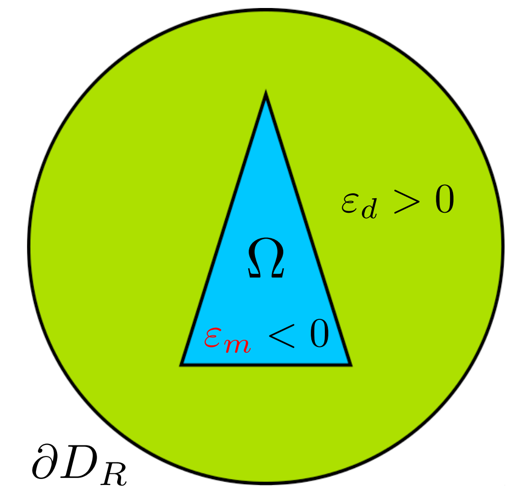
$\phi \to \pi, \ I_c \to \{-1\}$

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

Well-posedness in frequency domain

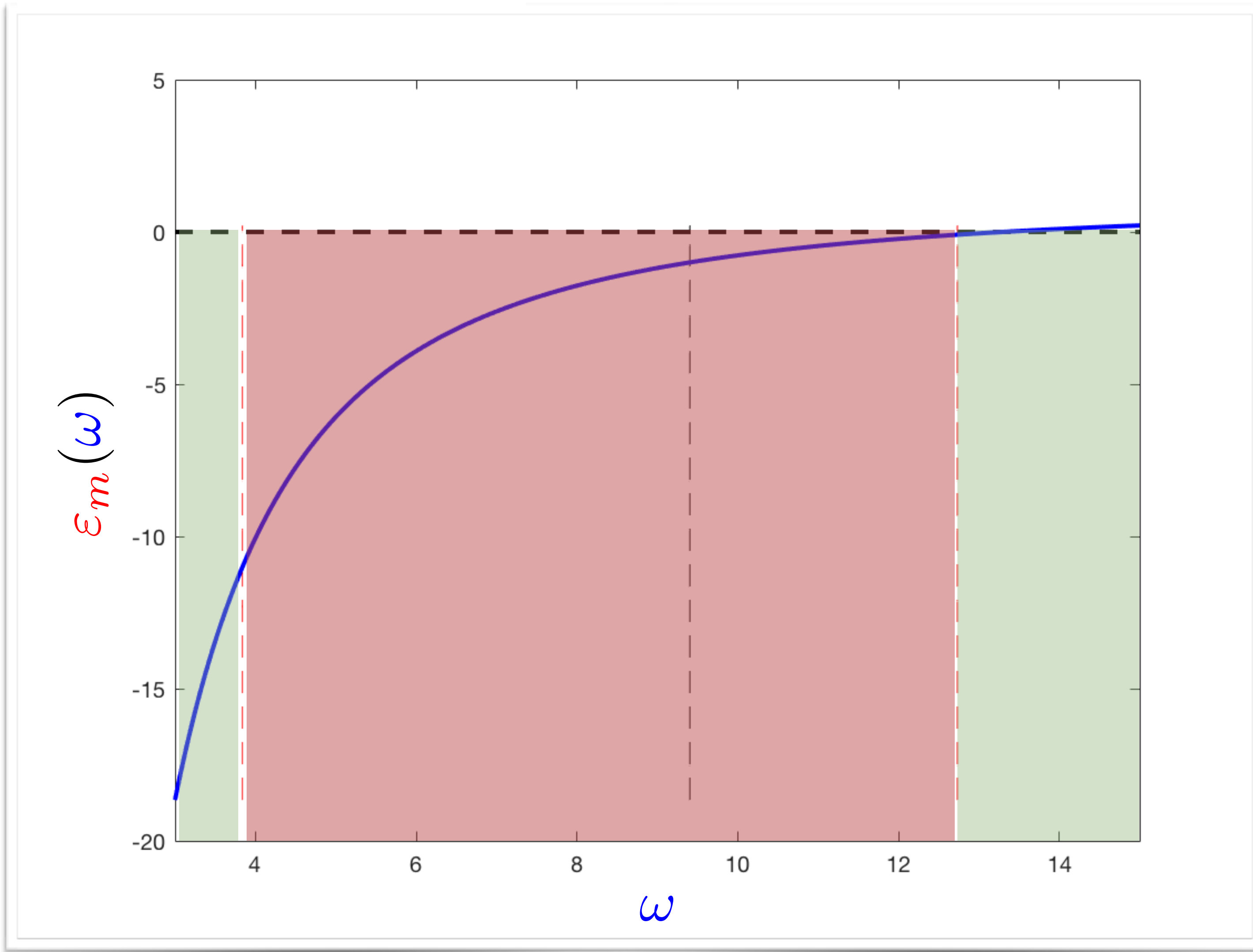
The critical interval is related to critical frequencies:

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



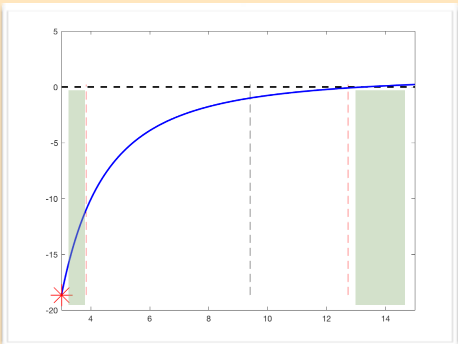
$$\kappa_\varepsilon \in \left[\frac{\phi-2\pi}{\phi}; \frac{\phi}{2\pi-\phi}\right] \iff \omega \in \left[\frac{\omega_p}{\varepsilon_\infty + \frac{\phi}{\varepsilon_d(2\pi-\phi)}}; \frac{\omega_p}{\varepsilon_\infty + \frac{\varepsilon_d \phi}{2\pi-\phi}}\right]$$

$$\kappa_\varepsilon = -1 \iff \omega = \omega_{sp} := \frac{\omega_p}{\varepsilon_\infty + \varepsilon_d}$$ Surface plasmons frequency

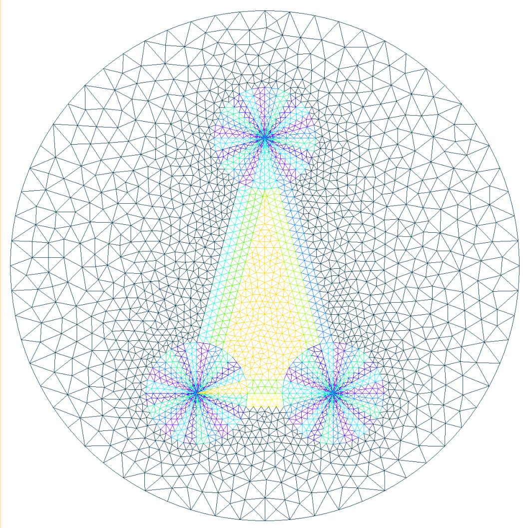


Well-posedness in frequency domain

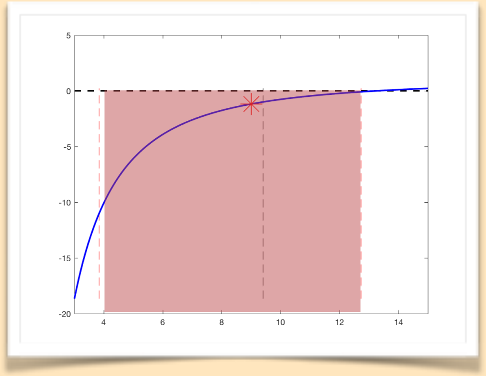
Outside I_c The scattering problem has a unique solution $H_z \in H^1(D_R)$



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

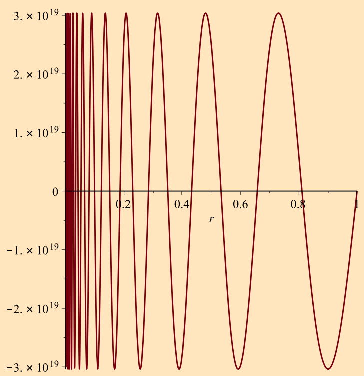


Inside $I_c \setminus \{-1\}$ The scattering problem is ill-posed in $H^1(D_R)$

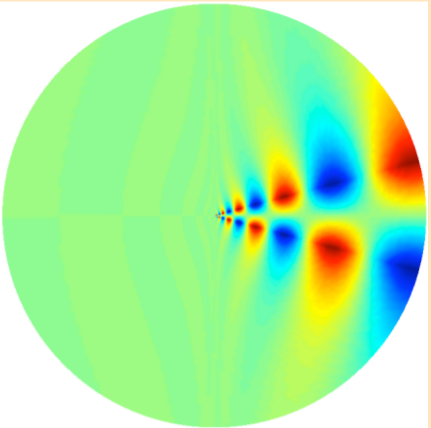


No FEM convergence
Appearance of oscillating hypersingularities at the corners

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



black-hole wave



Bonnet-Ben Dhia, Chesnel, Ciarlet (2012), Chesnel, Ciarlet (2013), Bonnet-Ben Dhia, Chesnel, Claeys (2013), Bonnet-Ben Dhia, Carvalho, Chesnel, Ciarlet (2016), Carvalho, Chesnel, Ciarlet (2017), Bonnet-Ben Dhia, Carvalho, Ciarlet (2018).

The limiting amplitude principle

Time domain

$$\mu_0 \frac{\partial H_z}{\partial t} = -\nabla \times \vec{E}_\perp \ \text{ in } \mathbb{R}^2$$

$$\varepsilon_0 \varepsilon \frac{\partial \vec{E}_\perp}{\partial t} = \vec{\nabla} \times H_z - \vec{J}_\perp \ \text{ in } \mathbb{R}^2$$

$$\frac{\partial \vec{J}_\perp}{\partial t} = \omega_p^2 \varepsilon_0 \vec{E}_\perp \ \text{ in } \Omega$$

$$\vec{J}_\perp = 0 \text{ in } \mathbb{R}^2 \setminus \Omega$$

✔ Well-posed problem
Bounded EM energy

Frequency domain

$$\nabla \cdot (\varepsilon(\omega)^{-1} \nabla \underline{H_z}) + k^2 \underline{H_z} = 0 \text{ in } \mathbb{R}^2$$

$$-i\omega\varepsilon_0\varepsilon(\omega)\underline{\vec{E}_\perp} = \vec{\nabla} \times \underline{H_z} \ \text{ in } \mathbb{R}^2$$

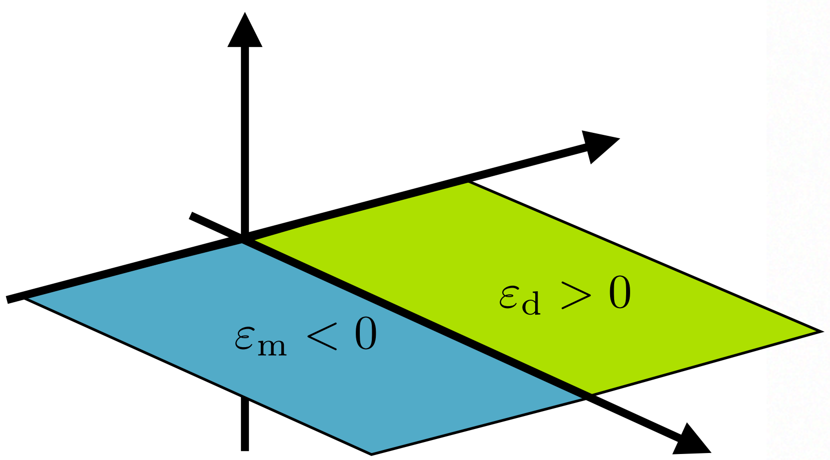
✘ Problem may be ill-posed
"Infinite" EM energy

This indicates that the limiting amplitude principle should not hold for all frequencies

Can we find underlying signatures of this break from the time domain simulations?

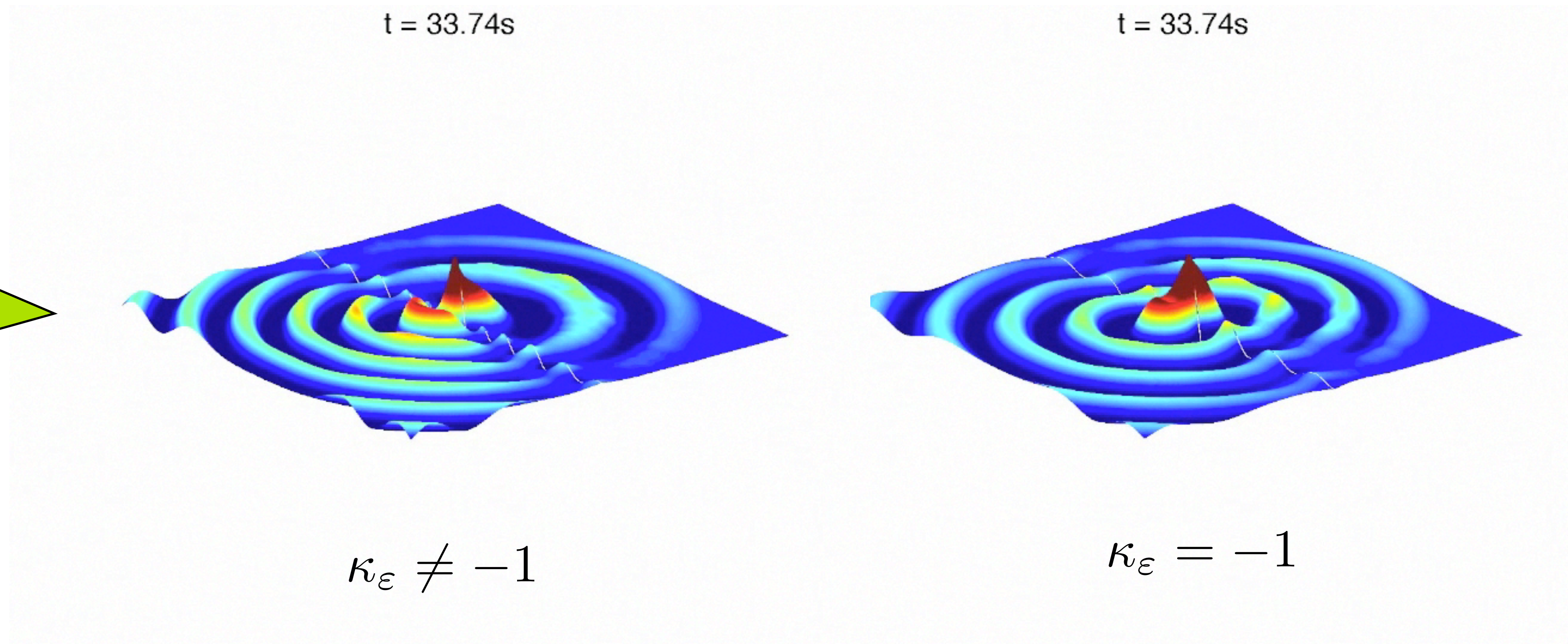
The limiting amplitude principle

The specific case of planar interface has been investigated theoretically and numerically.



$I_c = \{-1\}$

Cassier (2014), Vinoles (2016)



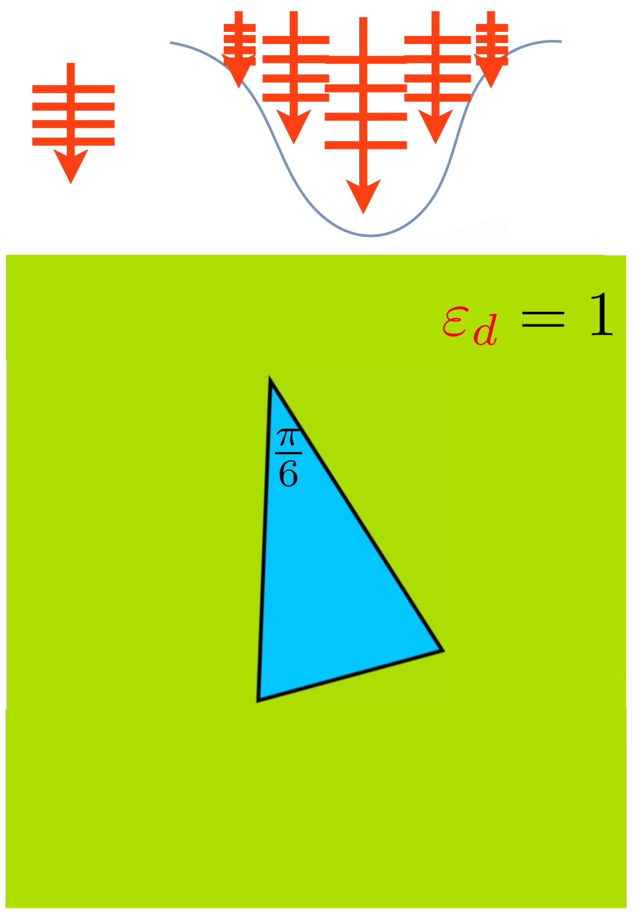
Courtesy of V. Vinoles

In presence of corners, the theory is not clear.
We propose some numerical investigations to find signature of the critical interval.

Outline

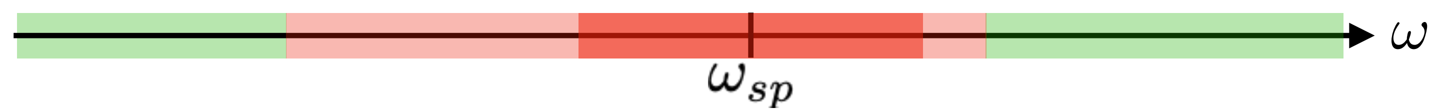
- Introduction
- Scattering in plasmonic structures
- Validating the Limiting Amplitude Principle
- Conclusion

Setting and quantities of interests

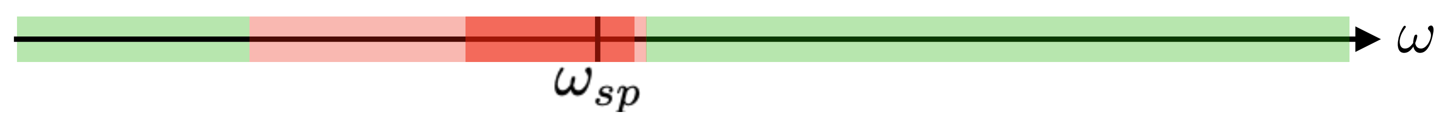


Scattering by two non lossy Drude materials in vacuum

Model 1: $\omega_p = 13.87 \times 10^{15}\mathrm{rad/s}$ $\varepsilon_\infty = 1$



Model 2: $\omega_p = 13.87 \times 10^{15}\mathrm{rad/s}$ $\varepsilon_\infty = 3.73$



We consider two incident fields:

-one plane wave (monochromatic)

-a Gaussian pulse (polychromatic)

Time-domain simulations (DGTD) Lanteri, Scheid, Viquerat (2017).

EM Energy (evolution over time, average, FFT, etc.)

$$\mathcal{E}(t) = \frac{1}{2}||\sqrt{\varepsilon_0 \varepsilon}\vec{E}_\perp(\cdot,t)||^2 + \frac{1}{2}||\sqrt{\mu_0}H_z(\cdot,t)||^2 + \frac{1}{2\varepsilon_0\omega_p^2}||\vec{J}_\perp(\cdot,t)||^2 \qquad \underline{\mathcal{E}} = \frac{1}{T}\int_0^T \mathcal{E}(t)dt$$

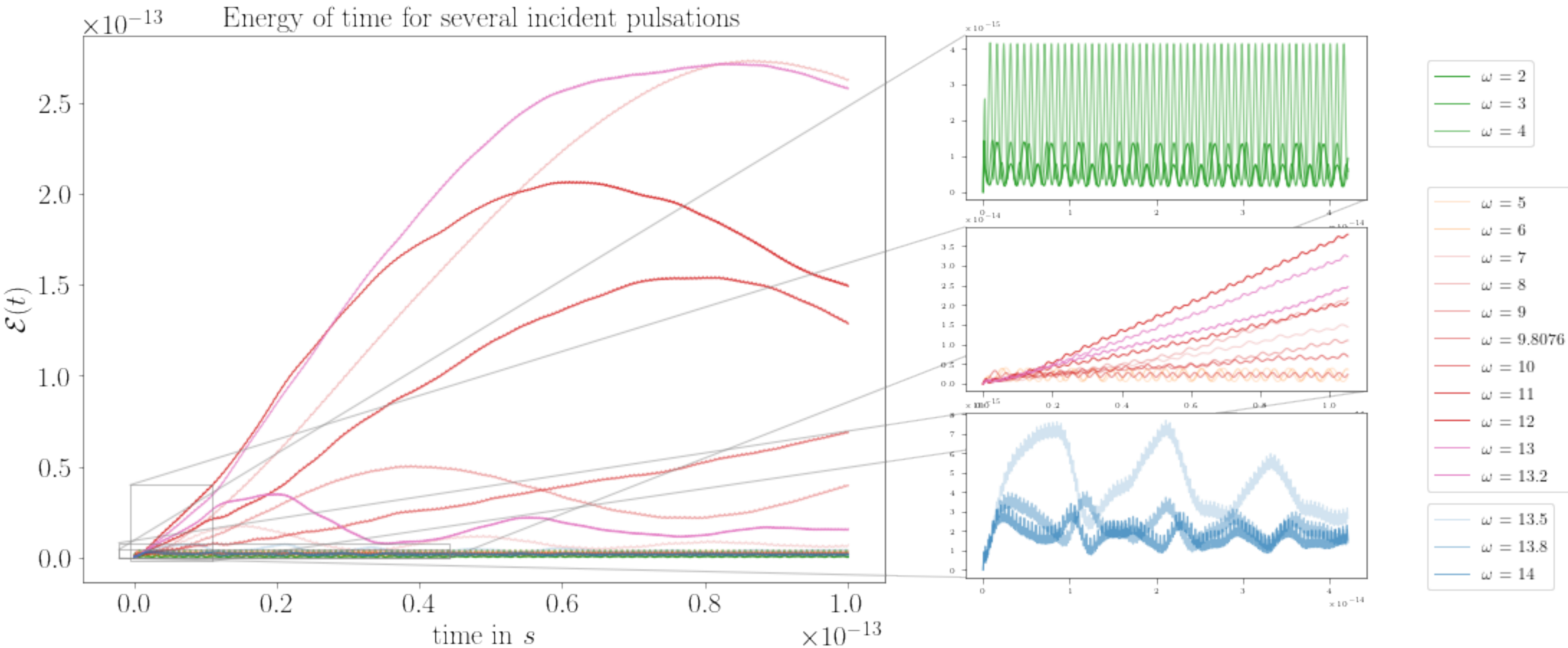
Cross sections

$$C = -\frac{1}{|\underline{\Pi}_{\mathrm{inc}}|}\int_S \underline{\Pi}\cdot d\vec{S} \qquad \underline{\Pi} = \frac{1}{T}\int_0^T \Pi(t)dt$$

FFT field at probe points

Energy $\mathcal{E}(t)$

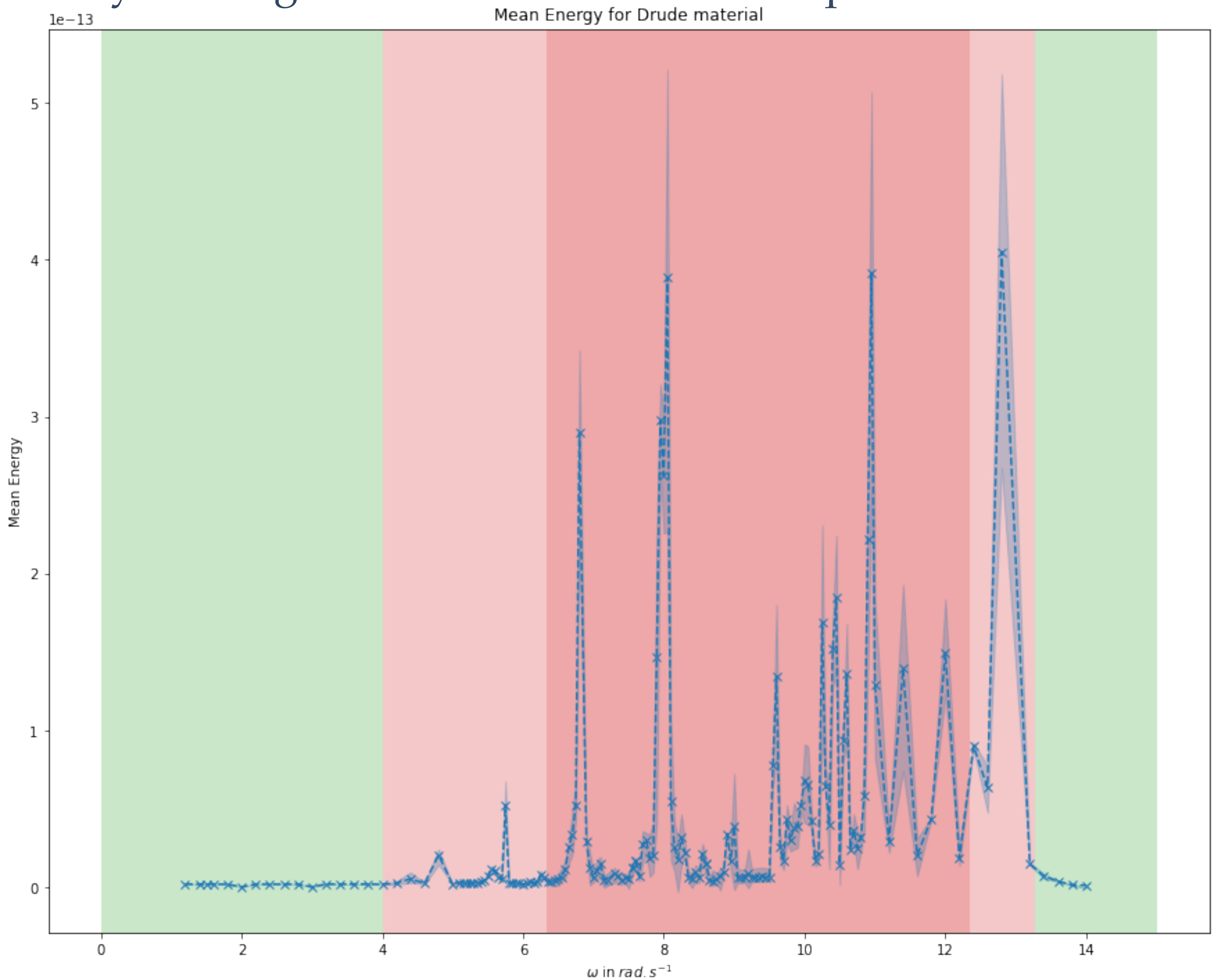
- We consider Model 1 for a monochromatic source.



Change of behavior at critical frequencies, but difficult to quantify.

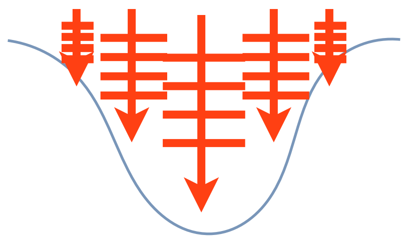
Energy $\mathscr{E}$

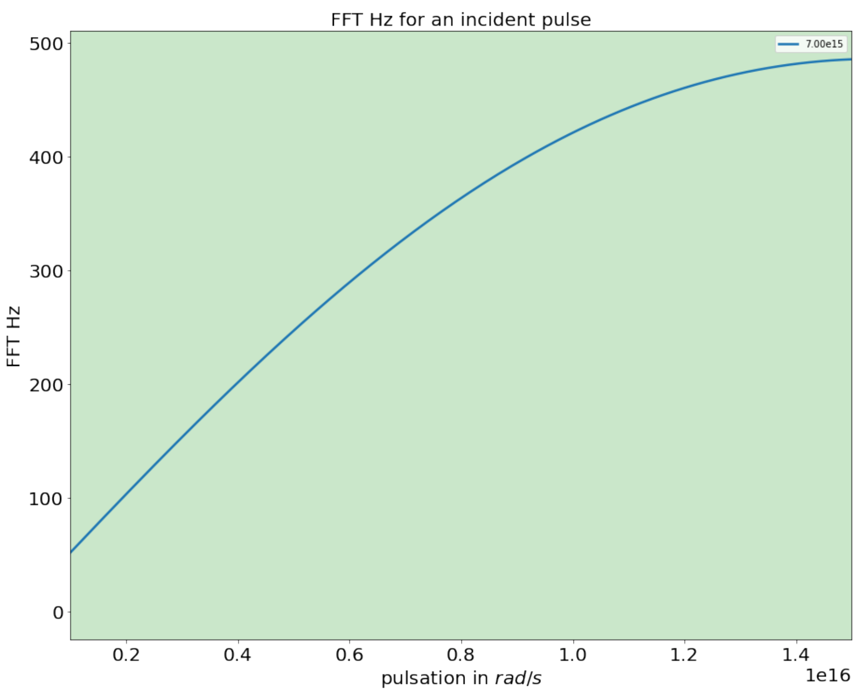
We identify a change of behavior at critical frequencies.



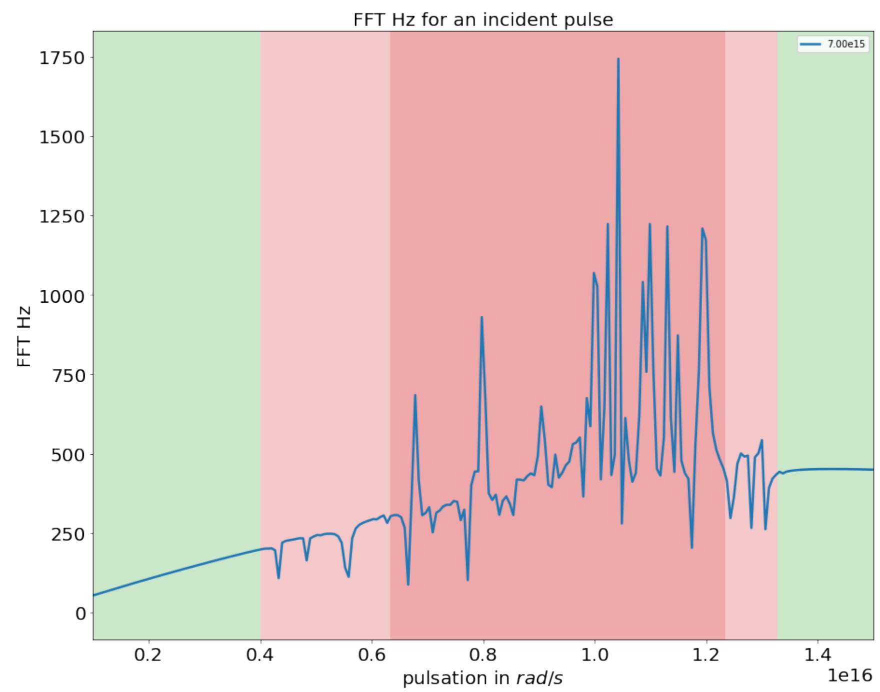
Can we provide a better signature ?

FFT fields at probe points

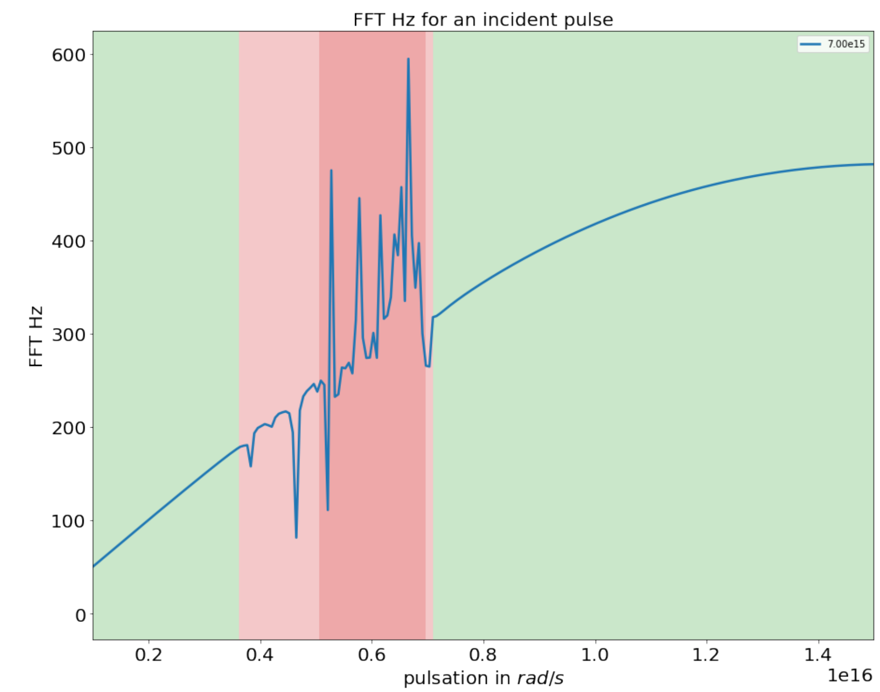




Dielectric



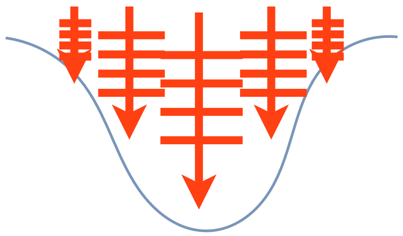
Model 1



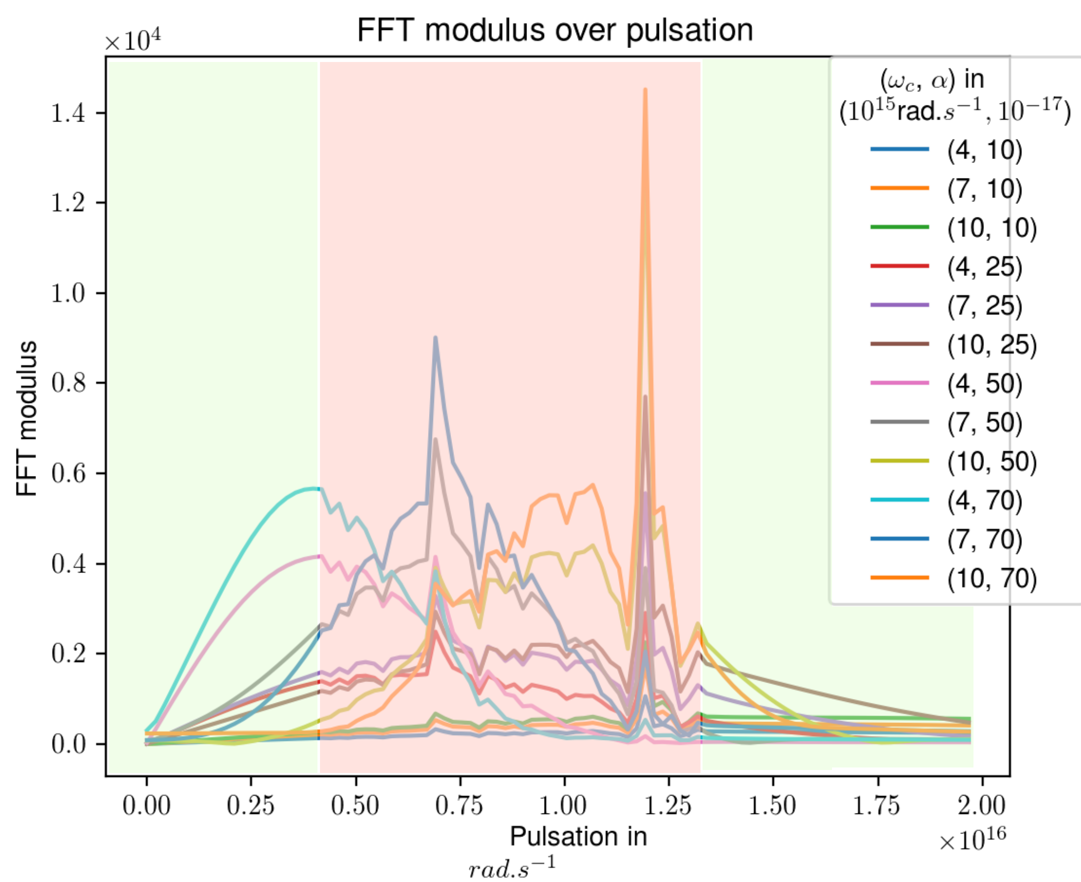
Model 2

If the limiting amplitude principle holds, the field should have the same Fourier signature as the incident field.

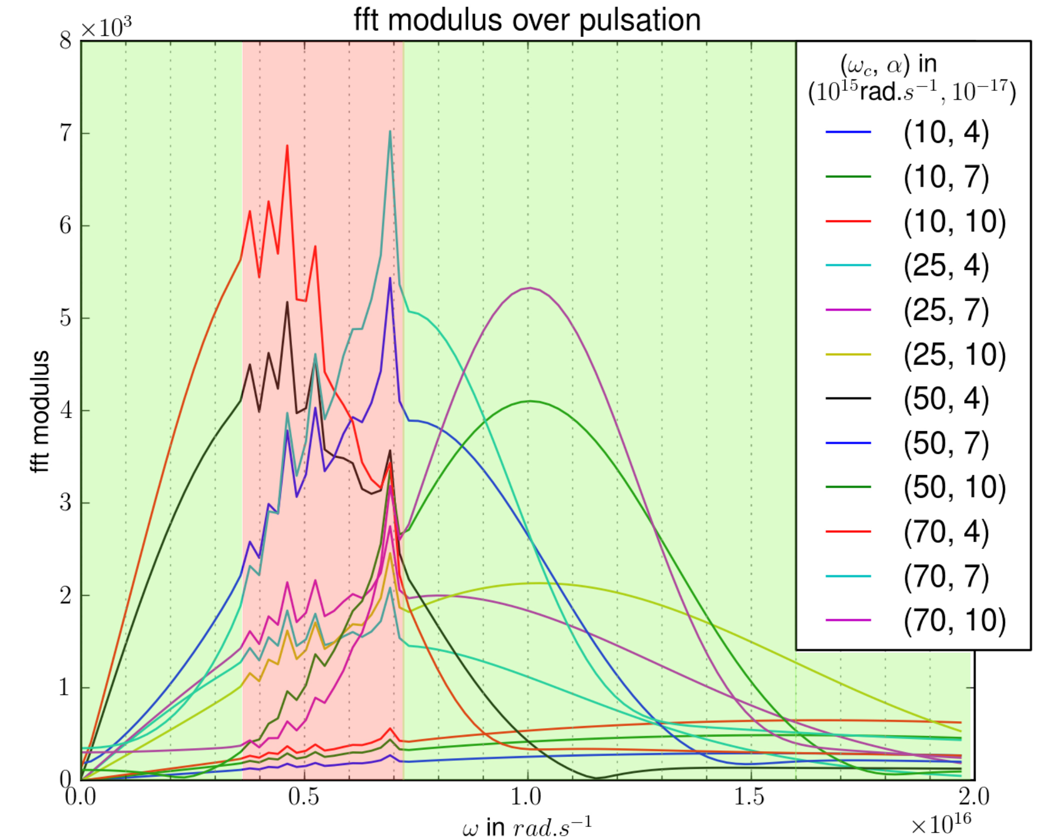
FFT fields at probe points



This phenomenon happens for any type of incident pulse.

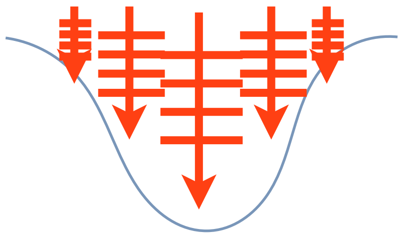


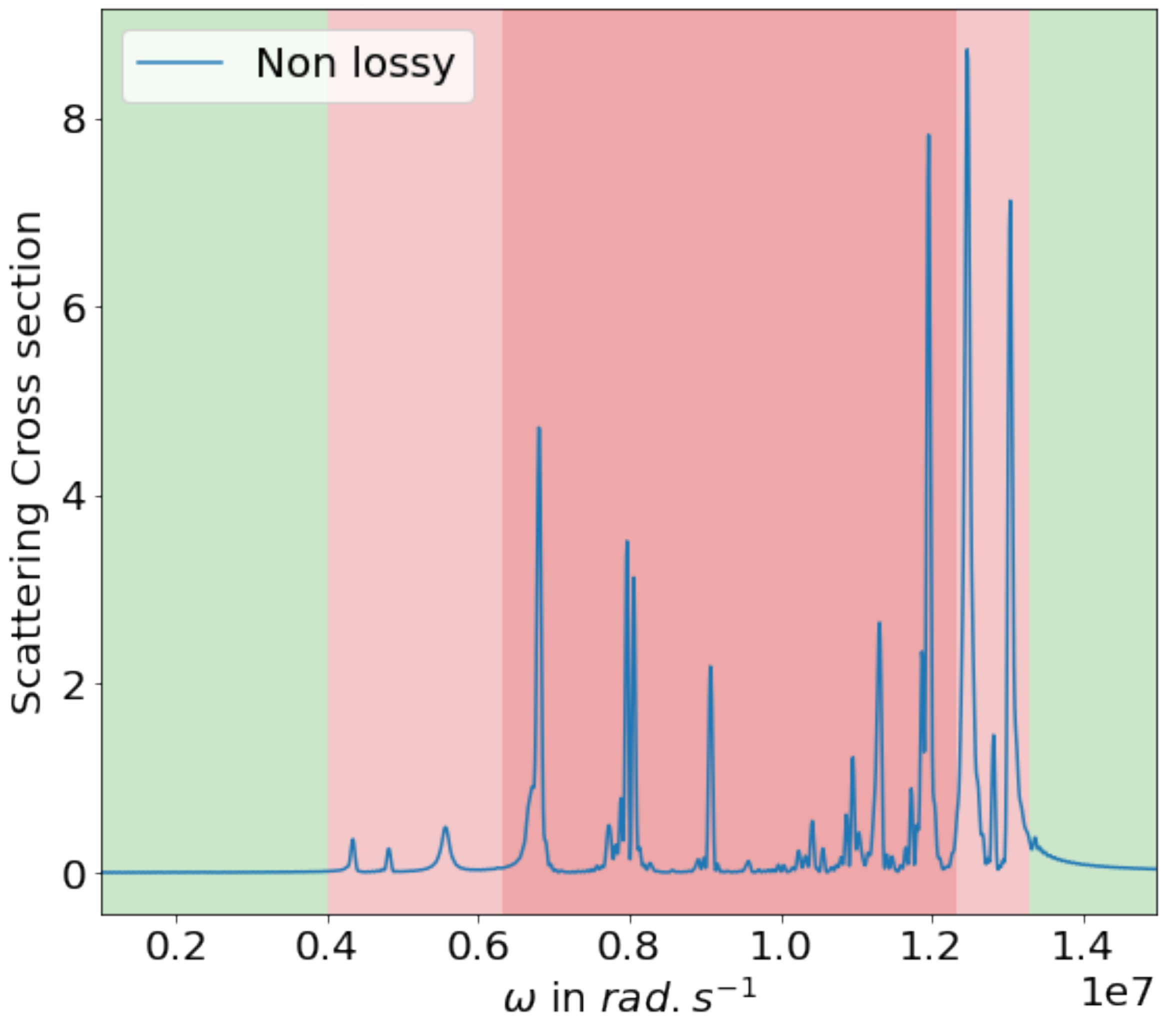
Model 1



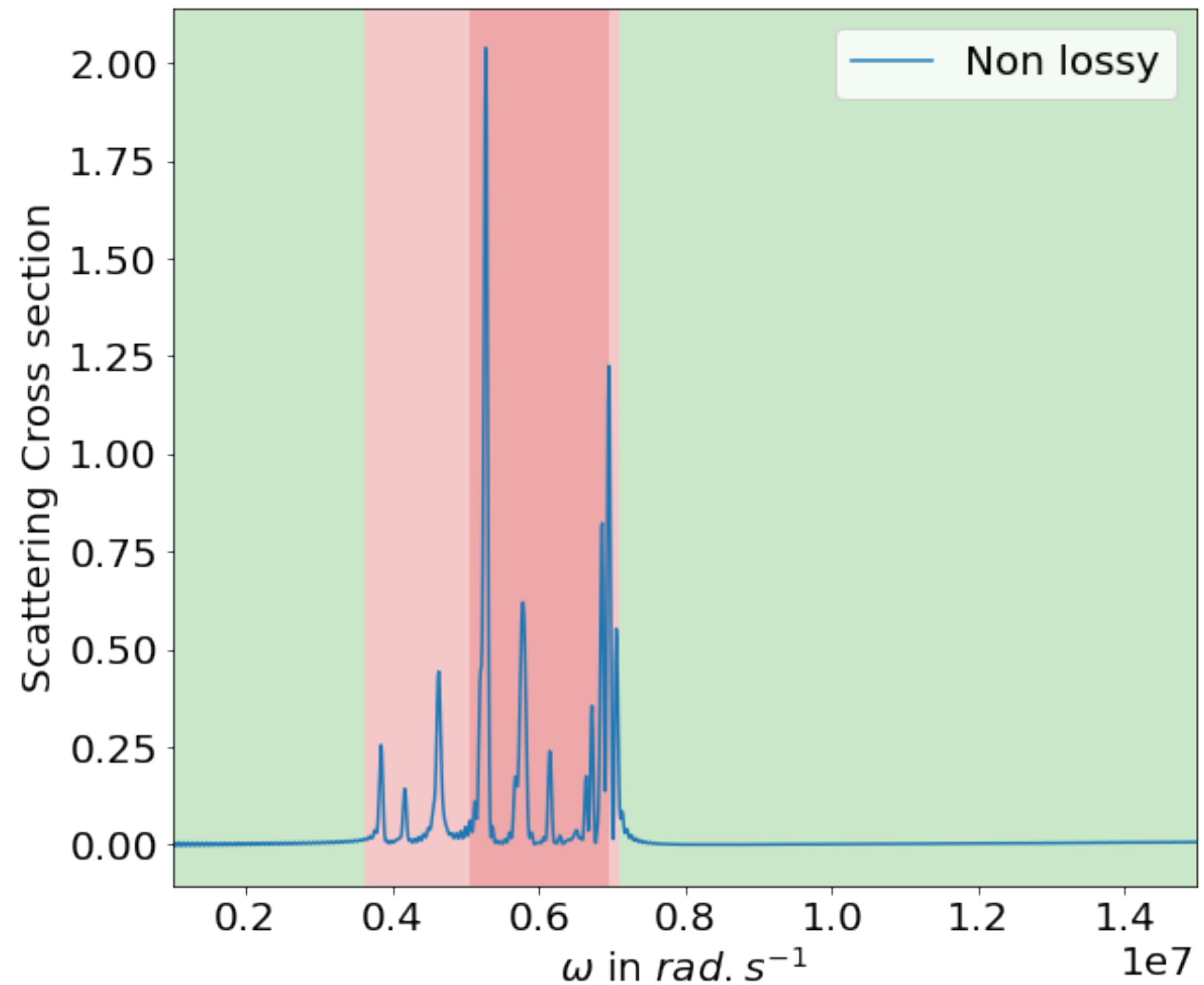
Model 2

Cross-sections





Model 1

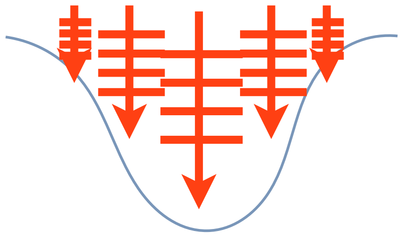


Model 2

Black-hole resonances appear at critical frequencies.

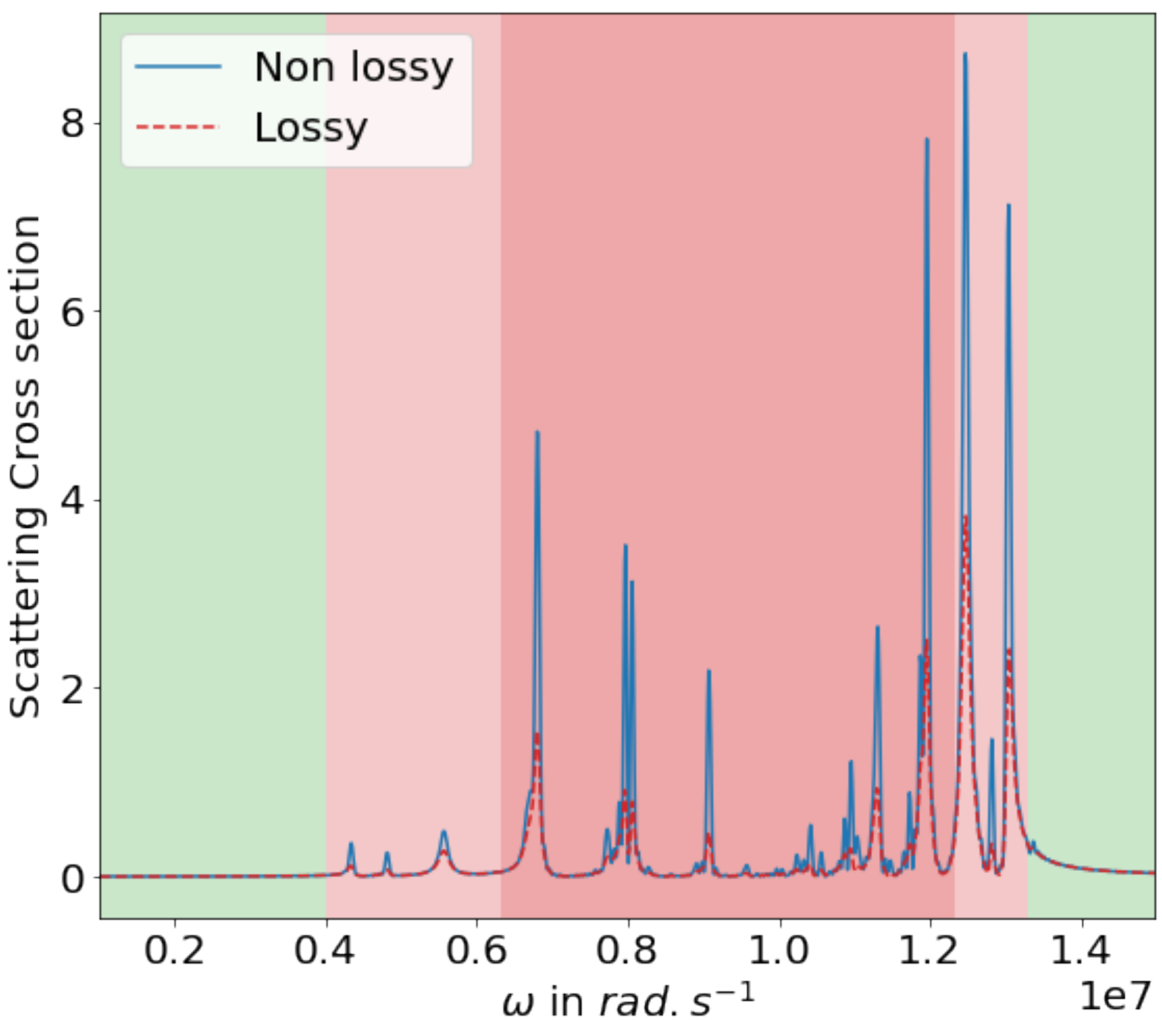
When dissipation comes into play

Metals are lossy. Adding dissipation into the problem makes the FD problem is well-posed.

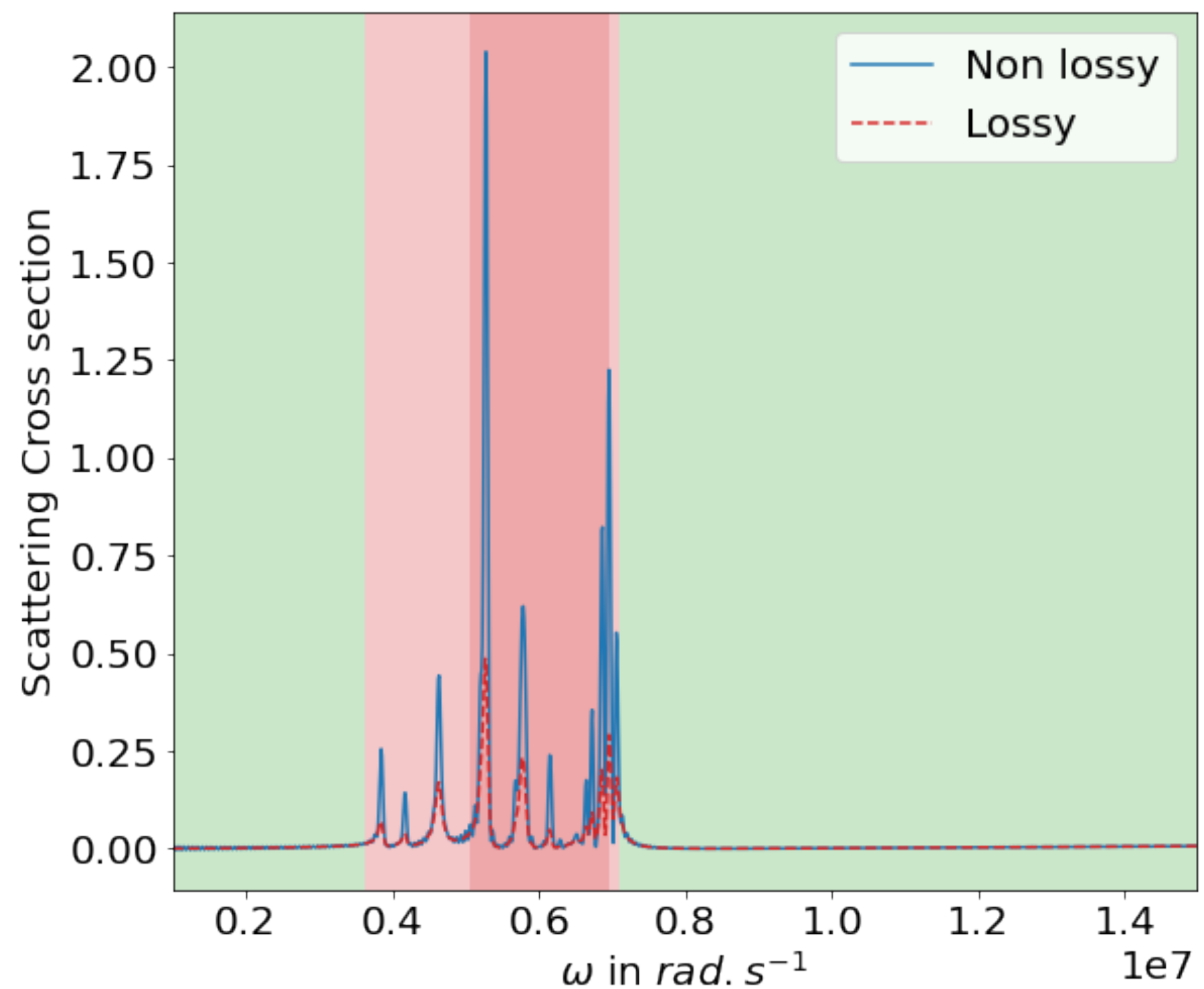


Can we still find signature of this critical interval with dissipation ?

The underlying resonances can be explained via the limit problem !



Model 1



Model 2

Outline

- Introduction
- Scattering in plasmonic structures
- Validating the Limiting Amplitude Principle
- Conclusion

Summary

It is important de (re)connect time-domain and frequency-domain problems.

In non lossy AND lossy materials, unusual phenomena arise in frequency domain, and the premises can be found in time-dependent simulations.

The limiting amplitude principle allows to validates (or not) considered models.

In lossy materials, underlying resonances can be explained by the limit (non lossy) problem.

<u>Perspectives</u>:

Consider more relevant models for the metal's permittivity.
(Drude-Lorentz model or hydrodynamic Drude's model)

Schmitt, Scheid, Lanteri, Viquerat, Moreau, (2016).

Consider Maxwell 3D

Bonnet-Ben Dhia, Chesnel, Ciarlet (2014)

Characterize the underlying black-hole waves

Carvalho, Moitier (2020)

Thank you for your attention.

Carvalho, Scheid (2020, to be submitted soon.)