On the Use of Perfectly Matched Layers to capture confined plasmonic waves

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ANR Project METAMATH

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A «sign-changing» electromagnetic scattering problem

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

negative material: \( \epsilon_1, \mu_1 \)

vacuum: \( \epsilon_0, \mu_0 > 0 \)
A «sign-changing» electromagnetic scattering problem

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

negative material : \( \varepsilon_1, \mu_1 \)

vacuum : \( \varepsilon_0, \mu_0 > 0 \)

Exemples of negative materials :
A «sign-changing» electromagnetic scattering problem

\[ u^{inc} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

Exemples of negative materials:
For a metal:

negative material : \( \varepsilon_1, \mu_1 \)
vacuum : \( \varepsilon_0, \mu_0 > 0 \)
A «sign-changing» electromagnetic scattering problem

\[ u^{inc} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

Exemples of negative materials:
For a metal: \( \epsilon_1 = \epsilon_1(\omega) = \tilde{\epsilon}_1 + i \gamma \), \( \tilde{\epsilon}_1 < 0 \)

negative material: \( \epsilon_1, \mu_1 \)

vacuum: \( \epsilon_0, \mu_0 > 0 \)
A «sign-changing» electromagnetic scattering problem

\[ u^{inc} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

negative material : \( \varepsilon_1, \mu_1 \)

vacuum : \( \varepsilon_0, \mu_0 > 0 \)

Exemples of negative materials :
For a metal : \( \varepsilon_1 = \varepsilon_1(\omega) = \varepsilon_\infty + i\gamma \) but at optical frequencies :

\[ \varepsilon_\infty < 0 \]
A «sign-changing» electromagnetic scattering problem

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

Exemples of negative materials:
For a metal: \( \epsilon_1 = \epsilon_1(\omega) = \bar{\epsilon}_1 + i \gamma \) but at optical frequencies: \( |\bar{\epsilon}_1| >> \gamma \)

vacuum: \( \epsilon_0, \mu_0 > 0 \)

negative material: \( \epsilon_1, \mu_1 \)
A «sign-changing» electromagnetic scattering problem

\[ u^{\text{inc}} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

For a metal : \( \varepsilon_1 = \varepsilon_1(\omega) = \varepsilon_1 + i \gamma \) but at optical frequencies : \( |\varepsilon_1| \gg \gamma \)

Exemples of negative materials :

\( \varepsilon_1 \sim \varepsilon_1 < 0 \)
A «sign-changing» electromagnetic scattering problem

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

Negative material: \( \epsilon_1, \mu_1 \)
\( \epsilon_1 < 0 \)

Vacuum: \( \epsilon_0, \mu_0 > 0 \)

Exemples of negative materials:
For a metal: \( \epsilon_1 = \epsilon_1(\omega) = \epsilon_1 + i\gamma \) but at optical frequencies: \( |\epsilon_1| >> \gamma \)

For a metamaterial:
\[ \epsilon_1 \sim \tilde{\epsilon}_1 < 0 \]
A «sign-changing» electromagnetic scattering problem

\[ u_{inc} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

negative material : \( \epsilon_1, \mu_1 \)
\[ \epsilon_1 < 0 \]
or
\[ \epsilon_1, \mu_1 < 0 \]

vacuum : \( \epsilon_0, \mu_0 > 0 \)

Exemples of negative materials :
For a metal : \( \epsilon_1 = \epsilon_1(\omega) = \tilde{\epsilon}_1 + i \gamma \) but at optical frequencies : \( |\tilde{\epsilon}_1| >> \gamma \)

For a metamaterial : \( \epsilon_1 < 0 \) and \( \mu_1 < 0 \)
A «sign-changing» electromagnetic scattering problem

\[ u^{inc} = e^{i \mathbf{k} \cdot \mathbf{x}} \]

\( \varepsilon, \mu > 0 \)

but at optical frequencies:

For a metal:

\( \varepsilon_1 = \varepsilon_1(\omega) = \varepsilon_1 + i\gamma \quad \text{but at optical frequencies:} \quad |\varepsilon_1| >> \gamma \)

For a metamaterial:

\( \varepsilon_1 < 0 \quad \text{and} \quad \mu_1 < 0 \)

Exemples of negative materials:

Dissipationless

negative material: \( \varepsilon_1, \mu_1 \)

\( \varepsilon_1 < 0 \quad \text{or} \quad \varepsilon_1, \mu_1 < 0 \)

vacuum: \( \varepsilon_0, \mu_0 > 0 \)
Time harmonic equations for the TM polarization

\[ u = H_z = u^{inc} + u^{sca} \]

\[ k = \frac{\omega}{\epsilon_0} \quad c_0 = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \]

* Radiation condition at finite distance

\[ \text{div} \left( \frac{1}{\epsilon} \nabla u \right) + \omega^2 \mu u = 0 \quad \text{in } B_R \]

\[ \frac{\partial u}{\partial n} - iku = \frac{\partial u^{inc}}{\partial n} - iku^{inc} = g^{inc} \quad \text{on } \Gamma_R \]
Outline

- A sign-changing scattering problem (SCSP)
- Some classical results
- What happens when $\epsilon$ changes sign?
- Taking into account dissipation?
- Zoom at the corners and modal analysis
- Well-suited model and method for SCSP
- Conclusion and perspectives
Variational formulation

Find \( u \in H^1(B_R) \) such that \( \forall v \in H^1(B_R) \)

\[
\int_{B_R} \frac{1}{\varepsilon} \nabla u \cdot \nabla v \, dB - \frac{ik}{\varepsilon_0} \int_{\Gamma_R} uv \, d\Gamma - \omega^2 \int_{B_R} \mu uv \, dB = \frac{1}{\varepsilon_0} \int_{\Gamma_R} g^{inc} \cdot v \, d\Gamma
\]

- Classical analysis for \( \varepsilon > 0 \):
  - \( a(u, v) \) is coercive
  - \( c(u, v) \) is a compact perturbation
  - \( l = 0 \)

\[
\begin{align*}
\{ a(u, v) \} & \text{ is coercive} & \text{Fredholm property} \\
\{ c(u, v) \} & \text{is a compact perturbation} & \text{Uniqueness}
\end{align*}
\]

Conclusion: for positive \( \varepsilon \), the problem is well-posed
Numerical illustrations

* P2 Finite Element simulations: \( \frac{\varepsilon_1}{\varepsilon_0} = 2 \) \( \frac{\mu_1}{\mu_0} = 1 \)

On a coarse mesh:

On a fine mesh

* Moreover the convergence of Finite Elements is guaranteed
Outline

- A sign-changing scattering problem (SCSP)
- Some classical results
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- Conclusion and perspectives
What happens for a sign-changing $\epsilon$?

- $a(u, v) = \int_{B_R} \frac{1}{\epsilon} \nabla u \cdot \nabla v \, dB - \frac{ik}{\epsilon_0} \int_{\Gamma_R} uv \, d\Gamma$ is no longer coercive.

**T-coercivity** for scalar interface problems between dielectrics and metamaterials
Anne-Sophie Bonnet-BenDhia, Lucas Chesnel, Patrick Ciarlet, MA2N, 2012

- Under some conditions on the geometry and the contrast $\frac{\epsilon_1}{\epsilon_0}$, there exists an isomorphism $\mathbb{T}$ of $H^1(B_R)$ such that $a(u, \mathbb{T}v)$ is coercive.
Different geometries

Regular inclusion:

Problem well-posed in $H^1(D_R)$ iff $\frac{\epsilon_1}{\epsilon_0} \neq -1$

Inclusion with corners:

Problem well-posed in $H^1(D_R)$ iff $\frac{\epsilon_1}{\epsilon_0} \notin I$

$$\phi \in \{\phi_1, \phi_2\} \quad I(\phi) = \begin{bmatrix} \frac{\phi - 2\pi}{\phi} ; \frac{\phi}{\phi - 2\pi} \end{bmatrix}$$
Different geometries

Regular inclusion:

Problem well-posed in $H^1(D_R)$ iff $\frac{\epsilon_1}{\epsilon_0} \neq -1$

Inclusion with corners:

Problem well-posed in $H^1(D_R)$ iff $\frac{\epsilon_1}{\epsilon_0} \notin I$

$\phi_1 = \frac{\pi}{6}, \quad \phi_2 = \frac{5\pi}{12}$

$I(\frac{\pi}{6}) = \left[-11; -\frac{1}{11}\right] \quad I(\frac{5\pi}{12}) = \left[-\frac{19}{5}; -\frac{5}{19}\right] \subset \left[-4; -\frac{1}{4}\right]$
Numerical experiments

* P2 Finite Elements simulations:

Outside the critical interval:

\[
\frac{\epsilon_1}{\epsilon_0} = -13 \quad \frac{\mu_1}{\mu_0} = 1
\]

On a coarse mesh

On a fine mesh

Convergence of Finite Elements OK
Numerical experiments

- P2 Finite Elements simulations:

On a coarse mesh

On a fine mesh

No numerical convergence
Strong singularities at the corners

Inside the critical interval:
\[
\frac{\epsilon_1}{\epsilon_0} = -1.5 \quad \frac{\mu_1}{\mu_0} = 1
\]

Is neglecting dissipation a good idea?
Outline

- A sign-changing scattering problem (SCSP)
- Some classical results
- What happens when $\epsilon$ changes sign?
- Taking into account dissipation?
- Zoom at the corners and modal analysis
- Well-suited model and method for SCSP
- Conclusion and perspectives
Taking into account dissipation

Find \( u \in H^1(B_R) \) such that \( \forall v \in H^1(B_R) \)

\[
\frac{1}{\epsilon} \int_{B_R} \nabla u \cdot \nabla v \, dB - \frac{ik}{\epsilon_0} \int_{\Gamma_R} uv \, d\Gamma - \omega^2 \int_{B_R} \mu uv \, dB = \frac{1}{\epsilon_0} \int_{\Gamma_R} g^{inc} v \, d\Gamma
\]

\[
\epsilon = \begin{cases} 
\epsilon_0 \\
\epsilon_1 = \epsilon_1 + i\gamma \\
0 < \gamma << 1
\end{cases}
\]

\( a(u,v) \) is coercive \( \rightarrow \) Fredholm property
\( c(u,v) \) is a compact perturbation \( \rightarrow \) Uniqueness
\( l = 0 \)

Conclusion : the problem is well-posed
Numerical experiments

- P2 Finite Elements simulations:
  - On a coarse mesh
  - On a fine mesh

Inside the critical interval:
Numerical experiments

- P2 Finite Elements simulations:
  - On a coarse mesh
  - On a fine mesh

Inside the critical interval:

\[
\frac{\varepsilon_1}{\varepsilon_0} = -1.5 + 0.0001i \quad \frac{\mu_1}{\mu_0} = 1
\]
Numerical experiments

- P2 Finite Elements simulations:
  - Inside the critical interval:
  - On a coarse mesh
  - On a fine mesh

\[ \frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.0001i \quad \frac{\mu_1}{\mu_0} = 1 \]
Numerical experiments

• P2 Finite Elements simulations:
  - Inside the critical interval:
    - On a coarse mesh
    - On a fine mesh

\[ \frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.0001i \quad \frac{\mu_1}{\mu_0} = 1 \]

- Convergence not ensured (corners)
+ Small dissipation
Numerical experiments

* P2 Finite Elements simulations:

On a coarse mesh

On a fine mesh

Inside the critical interval:

\[
\frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.0001i \quad \frac{\mu_1}{\mu_0} = 1
\]

- Convergence not ensured (corners)
+ Small dissipation

\[
\frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.1i \quad \frac{\mu_1}{\mu_0} = 1
\]

+ Convergence ok
- Stronger dissipation
Numerical experiments

- **P2 Finite Elements simulations:**
  - On a coarse mesh
  - On a fine mesh

Inside the critical interval:

- \( \frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.0001i \quad \frac{\mu_1}{\mu_0} = 1 \)
  - Convergence not ensured (corners)
  - Small dissipation

- \( \frac{\epsilon_1}{\epsilon_0} = -1.5 + 0.1i \quad \frac{\mu_1}{\mu_0} = 1 \)
  - Convergence ok
  - Stronger dissipation

Dissipation => problem is well-posed

Particular phenomena at the corners

What happens at the corners when \( \frac{\epsilon_1}{\epsilon_0} \) lies in the critical interval?
Outline

- A sign-changing scattering problem (SCSP)
- Some classical results
- What happens when $\epsilon$ changes sign?
- Taking into account dissipation?
- **Zoom at the corners and modal analysis**
- Well-suited model and method for SCSP
- Conclusion and perspectives
**Zoom at the corners**

\[
div\left(\frac{1}{\varepsilon} \nabla u\right) + \omega^2 \mu u = 0
\]

Cartesian \((x, y)\)

\[
\frac{1}{\varepsilon} \left( r \frac{\partial}{\partial r} \right)^2 u + \frac{\partial}{\partial \theta} \left( \frac{1}{\varepsilon} \frac{\partial u}{\partial \theta} \right) + \omega^2 \mu r^2 u = 0
\]

Polar \((r, \theta)\)

\[
z = \log(r/\rho)
\]

\[
\frac{1}{\varepsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\varepsilon} \frac{\partial u}{\partial \theta} \right) + \omega^2 \mu e^{2z} u = 0
\]

Euler \((z, \theta)\)
Modal analysis in the strip

\[
\frac{1}{\epsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) + \omega^2 \mu e^{2z} u = 0 \quad \text{in the strip}
\]

* Modes of the strip: \( u(z, \theta) = \phi(\theta) e^{\lambda z} \) solutions of
\[
\frac{1}{\epsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) = 0
\]
(periodic in \( \theta \))

Outside the critical interval

No propagative mode

Inside the critical interval

Two propagative modes appear

\[ \phi(\theta) e^{\pm ikz} \notin H^1(\text{Strip}) \]
Modal analysis in the strip

\[
\frac{1}{\epsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) + \omega^2 \mu e^{2z} u = 0 \quad \text{in the strip}
\]

* Modes of the strip: \( u(z, \theta) = \phi(\theta)e^{\lambda z} \) solutions of

\[
\frac{1}{\epsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) = 0
\]

(periodic in \( \theta \))

Back to the physical domain:

\[
\phi(\theta) r^{\pm ik}
\]

Black hole wave propagating towards the corner / emitted by the corner

Inside the critical interval

Two propagative modes appear

\[
\phi(\theta)e^{\pm ikz} \notin H^1(\text{Strip})
\]
Need for a condition radiation at infinity in the strip

- Select the «outgoing» propagative mode/singularity
- Use of the Limiting Absorption Principle

\[ \epsilon_1^\gamma = \epsilon_1 + i\gamma \quad 0 < \gamma \ll 1 \]

- Effect on the modes:
Need for a condition radiation at infinity in the strip

- Select the «outgoing» propagative mode/singularity

- Use of the Limiting Absorption Principle

\[ \epsilon_1^\gamma = \epsilon_1 + i\gamma \quad 0 < \gamma \ll 1 \]

- Effect on the modes:

![Diagram showing the effect on modes with points on the complex plane]
Need for a condition radiation at infinity in the strip

* Select the «outgoing» propagative mode / singularity

* Use of the Limiting Absorption Principle

\[ \epsilon_1^\gamma = \epsilon_1 + i\gamma \quad 0 < \gamma \ll 1 \]

* Effect on the modes:

the outgoing propagative mode becomes evanescent at infinity

the ingoing propagative mode becomes exponentially increasing at infinity
Need for a condition radiation at infinity in the strip

- Select the «outgoing» propagative mode/singularity

- Use of the Limiting Absorption Principle

\[ \epsilon_1^\gamma = \epsilon_1 + i\gamma \quad 0 < \gamma \ll 1 \]

- Effect on the modes:

the ingoing propagative mode becomes exponentially increasing at infinity
Limiting Absorption Principle

P2 Finite Element simulations on a fine mesh

Inside the critical interval:

\[ \epsilon_1^\gamma = \epsilon_1 \]

\[ \epsilon_1^\gamma = \epsilon_1 + 0.0001i \]

\[ \epsilon_1^\gamma = \epsilon_1 + 0.1i \]
Limiting Absorption Principle

P2 Finite Element simulations on a fine mesh

\[ \varepsilon'_1 = \varepsilon_1 \]

\[ \varepsilon'_1 = \varepsilon_1 + 0.0001i \]

\[ \varepsilon'_1 = \varepsilon_1 + 0.1i \]

Inside the critical interval:

Similar: small dissipation \( \Rightarrow \) oscillations \( \Rightarrow \) must refine mesh.

\( \gamma \)
Limiting Absorption Principle

P2 Finite Element simulations on a fine mesh

\[ \varepsilon_1^\gamma = \varepsilon_1 \]

\[ \varepsilon_1^\gamma = \varepsilon_1 + 0.0001i \]

\[ \varepsilon_1^\gamma = \varepsilon_1 + 0.1i \]

Inside the critical interval:

Similar: small dissipation => oscillations => must refine mesh

Different: stronger dissipation => Can we decrease \( \gamma \)?
Limiting Absorption Principle

P2 Finite Element simulations on a fine mesh

$\epsilon'_1 = \epsilon_1$

$\epsilon'_1 = \epsilon_1 + 0.0001i$

$\epsilon'_1 = \epsilon_1 + 0.1i$

Dealing with dissipation small enough and mesh fine enough

$\Rightarrow$ Expensive method

Similar: small dissipation => oscillations => must refine mesh

Different: stronger dissipation $\Rightarrow$ Can we decrease $\gamma$?
Limiting Absorption Principle

P2 Finite Element simulations on a fine mesh

\[ \epsilon_1^\gamma = \epsilon_1 \]

\[ \epsilon_1^\gamma = \epsilon_1 + 0.0001i \]

\[ \epsilon_1^\gamma = \epsilon_1 + 0.1i \]

Similar: small dissipation => oscillations => must refine mesh

Different: stronger dissipation => Can we decrease \( \gamma \)?

Dealing with dissipation small enough and mesh fine enough => Expensive method

Is there another way to capture numerically the singularities?
Outline

- A sign-changing scattering problem (SCSP)
- Some classical results
- What happens when $\epsilon$ changes sign?
- Taking into account dissipation?
- Zoom at the corners and modal analysis
- **Well-suited model and method for SCSP**
- Conclusion and perspectives
An adapted numerical method

- Use «Perfectly Matched Layers» (PML) in the strip

\[ \frac{\partial}{\partial z} \rightarrow \alpha \frac{\partial}{\partial z} \quad \alpha \in \mathbb{C}, \quad 0 < \text{arg}(\alpha) < \frac{\pi}{2} \]

- Modal analysis: the eigenvalues \( \lambda \) become \( \lambda/\alpha \)

The effect of PMLs on the propagative modes is similar to that of dissipation
Splitting in four problems

$$div\left(\frac{1}{\varepsilon} \nabla u\right) + \omega^2 \mu u = 0 \quad BR \setminus \bigcup_{i=1}^{i=3} B_{\rho,i}$$

$$\frac{\partial u}{\partial n} - iku = \frac{\partial u^{inc}}{\partial n} - iku^{inc} = g^{inc} \quad \Gamma_R$$

Matching conditions

$$\frac{1}{\varepsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left(\frac{1}{\varepsilon} \frac{\partial u}{\partial \theta}\right) + \omega^2 \mu \rho^2 e^{2z} u = 0 \quad \bigcup_{i=1}^{i=3} Strip_i$$

periodic conditions in $\theta$

Radiation conditions at infinity
New equations with PMLs

\[ \text{div}(\frac{1}{\epsilon} \nabla u) + \omega^2 \mu u = 0 \quad B_R \setminus \bigcup_{i=1}^{i=3} PML_i \]

\[ \frac{\partial u}{\partial n} - ik u = \frac{\partial u^{inc}}{\partial n} - ik u^{inc} = g^{inc} \quad \Gamma_R \]

+ \( \alpha \) Matching conditions

+ \[ \frac{\alpha^2}{\epsilon} \frac{\partial^2 u}{\partial z^2} + \frac{\partial}{\partial \theta} \left( \frac{1}{\epsilon} \frac{\partial u}{\partial \theta} \right) + \omega^2 \mu \rho^2 e^{2z/\alpha} u = 0 \quad \bigcup_{i=1}^{i=3} PML_i \]

periodic conditions in \( \theta \)

+ \[ \frac{\partial u}{\partial z} (z = -L, \cdot) = 0 \]
Numerical results

* Results with and without PMLs, for a contrast $\frac{\varepsilon_1}{\varepsilon_0} = -1.5$

* Movies of the time-harmonic solutions $e^{-i\omega t}$
Numerical results

- Results with and without PMLs, for a contrast $\frac{\varepsilon_1}{\varepsilon_0} = -1.5$

- Movies of the time-harmonic solutions $(e^{-i\omega t})$
Numerical results

* Results with and without PMLs, for a contrast $\frac{\varepsilon_1}{\varepsilon_0} = -1.5$

* Movies of the time-harmonic solutions $(e^{-i\omega t})$

Results with dissipation:

$\varepsilon_1' = \varepsilon_1 + 0.0001i$

$\varepsilon_1' = \varepsilon_1 + 0.1i$
Numerical results

- Results with and without PMLs, for a contrast $\frac{\varepsilon_1}{\varepsilon_0} = -1.5$
- Movies of the time-harmonic solutions $(e^{-i\omega t})$

Results with dissipation:

$\varepsilon_1^\gamma = \varepsilon_1 + 0.0001i$

$\varepsilon_1^\gamma = \varepsilon_1 + 0.1i$
Conclusion and perspectives

- The PML method:
  - allows us to capture efficiently propagative singularities near the corners
  - is less expensive method than dissipation + refinement mesh

- Black hole waves have been studied in other applications like elastodynamics or gravity waves, but generally require cupsidal geometries. (cf. G. Cardone, S.A. Nazarov and J. Taskinen)

- The PML error estimate is the next step (proof of the numerical convergence)

- 3D extensions (conical tip, edge) are considered

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