Finite Elements for Electrodynamics and Modal Analysis of Dispersive Structures

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What do we want to do?

To develop

- Numerical models (using Finite Elements)
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- for Electrodynamics (to solve Maxwell's equations)
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- to provide Physical Understanding (modes, resonances, etc.)
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- Numerical models (using Finite Elements)
- for Electrodynamics (to solve Maxwell’s equations)
- to provide Physical Understanding (modes, resonances, etc.)
- of Photonic Devices (taking into account realistic materials e.g. with time dispersive permittivity)
Solving a practical problem

How to obtain a given set of IR multispectral filters like these?

Transmission enhancement through square coaxial aperture arrays in metallic film: when leaky modes filter infrared light for multispectral imaging, Benjamin Vial, Mireille Commandré, Guillaume Demésy, André Nicolet, Frédéric Zolla et al., Optics letters 39 (16), 4723-4726
Finite elements

Find $u(\mathbb{R}^2 \rightarrow \mathbb{R})$ of $\text{div}(\alpha \text{grad } v)) = f \ (\text{+B.C.})$
Numerical solution using a piecewise 1st order polynomial approximation function defined based on a triangular mesh - unknowns are nodal values en.wikipedia.org/wiki/Finite_element_method

Integration by parts lowers regularity requirement on the approximation function

$$
\int_{\Omega} (\text{div}(\alpha \text{grad } v))w \ dV = -\int_{\Omega} \alpha \text{grad } v \cdot \text{grad } w \ dV + \int_{\partial \Omega} w\alpha \text{grad } v \cdot n \ dS.
$$
Maxwell’s equations

\[
\begin{align*}
\text{curl } H &= J + \partial_t D \\
\text{curl } E &= -\partial_t B \\
\text{div } D &= \rho \\
\text{div } B &= 0
\end{align*}
\]

with Boundary Conditions (possibly \( \to \infty \) such as the Outgoing Wave Condition, Floquet–Bloch periodicity conditions...)

and (Macroscopic) Constitutive Laws for Media relating \( D, H, J \) to \( E, B \) whichever "relating" means with \( D = \varepsilon E, B = \mu H, J = \sigma E \) as simplest cases...
Edge elements

Finite elements for 3D vectors fields (E, H, A...)

- Unknown parameters are **line integrals** of the field along the **edges** of the mesh...
Edge elements

Finite elements for 3D vectors fields (E, H, A...)

- Unknown parameters are **line integrals** of the field along the **edges** of the mesh...
- ... with vector-valued interpolation functions:
  - Line integral of a "shape field" associated to an edge
    is $= 1$ along this edge and is $= 0$ along the other edges.


2D example:
Edge elements

Some references:

Edge elements

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Modes are solutions without a source (in a bounded domain)

Mode : Finite energy

\[ T = \frac{2L}{c} \quad \omega_0 = \frac{\pi c}{L} \]
Consider the following eigenvalue problem:

Find \( \lambda \in \mathbb{R} \) and \( 0 \neq u \in H(\text{curl}, \Omega) \) such that:

\[
\begin{align*}
\text{curl} \; \text{curl} \; u &= \lambda u \quad \text{in} \; \Omega \quad (\ast) \\
\text{div} \; u &= 0 \quad \text{in} \; \Omega \\
u \times n|_{\partial \Omega} &= 0
\end{align*}
\]

The condition on the divergence is nearly redundant since taking the divergence of (\ast) gives \( \lambda \; \text{div} \; u = 0 \).

For the non-zero eigenvalues this is equivalent to the null divergence condition but not for the zero eigenvalue. In this case, \( \lambda = 0 \) would be associated with the infinite dimensional eigenspace made of gradients:

\( \{ \text{grad} \; \phi, \; \phi \in H^1(\Omega) \} \).

The null divergence condition eliminates such eigenvectors.
Vector Eigenvalue Problem with Edge Elements

The weak discrete formulation can be expressed as:

Find $\lambda_h \in \mathbb{R}$ and $0 \neq u \in V_h \subset H_0^0(\text{curl}, \Omega)$ such that:

$$\int_{\Omega} \text{curl } u_h \cdot \text{curl } v \, dx = \lambda_h \int_{\Omega} u_h \cdot v \, dx \quad , \forall v \in V_h \subset H_0^0(\text{curl}, \Omega) \quad (1)$$

If old-fashioned nodal elements are used, the result is plagued with spurious modes and **ALL** the eigenvalue are possibly wrong!
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\[
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\]

\[
\int_{\Omega} \text{curl } u_h \cdot \text{curl } v \ dx = \lambda_h \int_{\Omega} u_h \cdot v \ dx, \forall v \in V_h \subset H_0(\text{curl}, \Omega)
\]  \( (1) \)

- If old-fashioned nodal elements are used, the result is plagued with spurious modes and ALL the eigenvalues are possibly wrong!
- If \( V_h \) is taken to be the space of edge elements and the zero divergence condition is not included in the formulation, in practice, the zero divergence modes appear to be well associated with eigenvalues equal to zero within numerical round-off and the other numerical eigenvalues provide good approximations of the true ones.
Vector Eigenvalue Problem with Edge Elements

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- see Bossavit (1990), Arnold (2002)
Vector Eigenvalue Problem with Edge Elements

- \( \text{grad} \, P_h \subset V_h \) with \( P_h = P_1(\mathcal{T}_h) \), the Lagrange elements, and \( V_h = \mathcal{N}_0(\mathcal{T}_h) \), the edge elements.

- This property is fundamental and can be encoded in a **commutative diagram** (interpolation and differential operator (grad) commute).

- Choose \( v = \text{grad} \, \varphi \) with \( \varphi \) in \( P_h \). In this case
  \[
  \int_{\Omega} \text{curl} \, u_h \cdot \text{curl} \, \text{grad} \, \varphi \, dx = \lambda_h \int_{\Omega} u_h \cdot \text{grad} \, \varphi \, dx = 0, \quad \forall \varphi \in P_h
  \]
  and for non-zero eigenvalues: \( \int_{\Omega} u_h \cdot \text{grad} \, \varphi \, dx = 0, \quad \forall \varphi \in P_h \), the divergence of \( u_h \) is weakly equal to zero.
Commutative Diagram: de Rham Complex and Discrete Fields

\[ C^\infty(\mathbb{R}^3) \xrightarrow{\text{grad}} [C^\infty(\mathbb{R}^3)]^3 \xrightarrow{\text{curl}} [C^\infty(\mathbb{R}^3)]^3 \xrightarrow{\text{div}} C^\infty(\mathbb{R}^3) \]

\[ \Pi^0_h \downarrow \quad \Pi^1_h \downarrow \quad \Pi^2_h \downarrow \quad \Pi^3_h \downarrow \]

\[ w^0_h \quad \xrightarrow{\text{G}} \quad w^1_h \quad \xrightarrow{\text{C}} \quad w^2_h \quad \xrightarrow{\text{D}} \quad w^3_h \]

**Figure** – Commutative diagram for the discrete topological operators and the projection operators on discrete fields. \( w^0_h \) are sets of nodal values, \( w^1_h \) are sets of line integrals along edges, \( w^2_h \) are sets of fluxes through facets, \( w^3_h \) are sets of volume integrals on tetrahedra, \( G \) is the node-edge incidence matrix, \( C \) is the edgefacet incidence matrix, \( D \) is the facet-tetrahedron incidence matrix, an incidence matrix has coefficients \( \in \{1, -1, 0\} \).
Commutative Diagram : de Rham Complex and Edge Elements

\[
\begin{array}{cccccc}
C^\infty(\mathbb{R}^3) & \xrightarrow{\text{grad}} & [C^\infty(\mathbb{R}^3)]^3 & \xrightarrow{\text{curl}} & [C^\infty(\mathbb{R}^3)]^3 & \xrightarrow{\text{div}} & C^\infty(\mathbb{R}^3) \\
\Pi^0_h & \downarrow & \Pi^1_h & \downarrow & \Pi^2_h & \downarrow & \Pi^3_h \\
W^0_h & \xrightarrow{\text{grad}} & W^1_h & \xrightarrow{\text{curl}} & W^2_h & \xrightarrow{\text{div}} & W^3_h \\
\end{array}
\]

**Figure** – Commutative diagram for the discrete topological operators and the projection operators on interpolated finite dimensional function spaces. \(W^0_h\) nodal elements, \(W^1_h\) edge elements, \(W^2_h\) facet elements, \(W^3_h\) volume elements.

\[ d\varphi = d \left( g \, dx^{i_1} \wedge \cdots \wedge dx^{i_k} \right) \\
= dg \wedge (dx^{i_1} \wedge \cdots \wedge dx^{i_k}) + g \, d (dx^{i_1} \wedge \cdots \wedge dx^{i_k}) \\
= dg \wedge dx^{i_1} \wedge \cdots \wedge dx^{i_k} + g \sum_{p=1}^{k} (-1)^{p-1} dx^{i_1} \wedge \cdots \wedge dx^{i_{p-1}} \wedge d^2 x^{i_p} \wedge dx^{i_{p+1}} \wedge \cdots \wedge dx^{i_k} \\
= dg \wedge dx^{i_1} \wedge \cdots \wedge dx^{i_k} \\
= \frac{\partial g}{\partial x^i} dx^i \wedge dx^{i_1} \wedge \cdots \wedge dx^{i_k} \]
Exterior Calculus and Maxwell’s Equations

- Natural framework for Maxwell equations
  - $E$, $H$ are 1-forms (intensities).
  - $D$, $B$, $J$ are 2-forms (flux densities).
  - $\rho$ is a 3-form (volume density).
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- **Edge elements** (and facet elements...) are discrete differential forms (Whitney elements) (that make imposing boundary conditions easy!).
- Clear explanation of the general structure of Maxwell equations and their topological properties such as the existence of potentials and cuts (PR Kotiuga, "An algorithm to make cuts for magnetic scalar potentials in tetrahedral meshes based on the finite element method" IEEE Transactions on Magnetics 25 (5), 4129-413, 1989) with de Rham complex and cohomology.
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- Does not introduce spurious use of metric and is the natural framework for **transformation optics**.

$F = E + B \wedge dt$.

Invariant global quantities are integrals of differential forms.

$d \circ d = 0 \iff$ Stokes formula

$\int_{\Omega} d\alpha = \int_{\partial\Omega} \alpha \Rightarrow \partial \circ \partial = \emptyset$.

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- Ready for higher dimensions (Einstein’s relativity) : \( F = E + B \wedge dt \).

- Invariant global quantities are integrals of differential forms.

\[
d \circ d = 0 \iff \text{Stokes formula} \quad \int_{\Omega} d\alpha = \int_{\partial \Omega} \alpha \quad \Rightarrow \quad \partial \circ \partial = 0
\]
Electrodynamics

- **Maxwell’s equations (exterior calculus)**

\[
\begin{align*}
dH &= J + \partial_t D \\
d\mathbf{E} &= -\partial_t \mathbf{B} \\
dD &= \rho \\
dB &= 0
\end{align*}
\]

- **Poynting identity**

\[
d(\mathbf{E} \wedge \mathbf{H}) = J \wedge \mathbf{E} + \mathbf{E} \wedge \partial_t D + \mathbf{H} \wedge \partial_t B
\]

- **These relations are metric free!**
Metric

- **Distance, angle...**
- Hodge star operator $\ast$ maps $p$-forms on $(3 - p)$-forms.
- It is a linear algebraic operator that expresses the metric action on $p$-forms.
- Example of Euclidean metric in Cartesian coordinates:

\[
\begin{align*}
\ast dx &= dy \wedge dz \\
\ast dy &= dz \wedge dx \\
\ast dz &= dx \wedge dy
\end{align*}
\]

- This simplicity hides metric aspects in Cartesian coordinates but the relations are more complicated with a general coordinate system...
... and electromagnetic constitutive laws!

For example in free space:

\[ D = \varepsilon_0 \times E \]

\[ B = \mu_0 \times H \]

The Hodge star operator is necessary to transform fields (1-forms) into flux densities (2-forms)!
Commutative Diagram : de Rham Complex and Whitney Forms

\[ C^\infty(\mathbb{R}^3) \xrightarrow{d} [C^\infty(\mathbb{R}^3)]^3 \xrightarrow{d} [C^\infty(\mathbb{R}^3)]^3 \xrightarrow{d} C^\infty(\mathbb{R}^3) \]

\[ \Pi^0_h \downarrow \quad \Pi^1_h \downarrow \quad \Pi^2_h \downarrow \quad \Pi^3_h \downarrow \]

\[ W^0_h \xrightarrow{d} W^1_h \xrightarrow{d} W^2_h \xrightarrow{d} W^3_h \]

**Figure** – Commutative diagram for the discrete topological operators and the projection operators on interpolated finite dimensional function spaces. \( W^0_h \) nodal elements, \( W^1_h \) edge elements, \( W^2_h \) facet elements, \( W^3_h \) volume elements.

The role of the finite element interpolation together with the weak formulation (involving the scalar product) is to provide a numerical approximation to the Hodge star operator!

Remark : FDTD rather uses two dual rectangular and orthogonal meshes.
Interlude: Transformation Optics

- Geometrical transformation: change of coordinates:
  \[(x, y, z) \mapsto (x_s, y_s, z_s)\] and \(J_s\) is the Jacobian matrix and \(J_s^{-1} = (J_s^{-1})^T\).
Geometrical transformation: change of coordinates: 
\[(x, y, z) \mapsto (x_s, y_s, z_s)\] and \(J_s\) is the Jacobian matrix and 
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Rule: from initial material "tensor" properties \(\varepsilon, \mu\), the transformation is encapsulated in equivalent material properties \(\varepsilon_s\) and \(\mu_s\):

\[\varepsilon_s = J_s^{-1} \varepsilon J_s^{-T} \det(J_s)\]

\[\mu_s = J_s^{-1} \mu J_s^{-T} \det(J_s)\]
Geometrical transformation: change of coordinates: 
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\[
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\]

Global quantities (measurements) are integral of differential forms and are therefore invariant with respect to the transformation!
Interlude: Transformation Optics

- Geometrical transformation: change of coordinates: 
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  is encapsulated in **equivalent** material properties \(\varepsilon_s\) and \(\mu_s\):

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- **Nicolet, A., Zolla, F., Guenneau, S.,** A finite element modelling for 
From modes to quasimodes (also called quasinormal modes (QNM) or leaky modes)

Quasimodes are solutions without a source in unbounded domains corresponding to resonances...

Mode : Finite energy

\[ \omega_0 = \frac{\pi c}{L} \]
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Mode: Finite energy

\[ \omega_0 = \frac{\pi c}{L} \]

Quasimode: Infinite energy

\[ \omega = \tilde{\omega}_0 - i\gamma \quad \gamma > 0 \]
Leaky modes have an infinite power

Heuristics:
- Far enough, homogeneous medium: \( \Delta u + k_\infty^2 u = 0 \)
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- Far enough, homogeneous medium: \( \Delta u + k_\infty^2 u = 0 \)
- Far field, outgoing wave:
  \[
  e^{-i(\omega t - k_\infty r)} \frac{1}{4\pi r} \text{(or higher order multipole...)}
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- \( \Rightarrow \text{Im}(k_\infty) < 0 \) (exponential divergence of \( e^{ik_\infty r} \) w.r.t. \( r \))!
Naive spectral theory

\( \mathcal{L} \) is a linear operator acting on a Hilbert space \( \mathcal{H} \) (with a scalar product noted \((\cdot, \cdot)\)).

"Eigenvalue problem" : Is there \( \mathcal{L}u = \lambda u \) with \( \lambda \in \mathbb{C} \) and \( u \in \mathcal{H} \) (typically corresponding to "finite power")?

- Yes \( \Rightarrow \lambda \) corresponds to an eigenvalue (real for Hermitian/self-adjointed operators i.e. lossless media...).
  The set of these \( \lambda \) is the discrete spectrum (modes).

Scalar products \((u, u)\) and Rayleigh quotients \( R_\mathcal{L}(u) = \frac{(\mathcal{L}u, u)}{(u, u)} \) are well defined.

No but almost... There is an "eigenfield" of "infinite power" (not in the suitable space) e.g. plane waves... this can be formalized via Weyl criterion (Weyl sequence).

The set of these \( \lambda \) is the continuous spectrum (radiating modes).

Some trick is needed to see the resonances/leaky modes in the case of unbounded domains corresponding to complex \( \lambda \) (even with lossless media) : non-Hermitian extension of the operator (analytic dilation/Perfectly Matched Layers : complex valued coordinates).
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Naive spectral theory

$L$ is a linear operator acting on a Hilbert space $\mathcal{H}$ (with a scalar product noted $(\cdot, \cdot)$).

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Leaky modes and PMLs (Perfectly Matched Layers)

An extension of the (self-adjoined) operator, formally the same operator but acting on a larger domain (function space including "infinite power leaky modes"), is required i.e. an non-Hermitian extension with complex eigenvalues...


In the harmonic, they can be viewed as a complex-valued change of coordinates: W. C. Chew and W. H. Weedon, A 3D perfectly matched medium from modified Maxwell’s equations with stretched coordinates, Microwave Optical Tech. Letters, vol. 7, no 13, 1994, p. 599-604.

In this case, they are a useful tool to perform spectral analysis: Discretization of Continuous Spectra Based on Perfectly Matched Layers, F. Olyslager, SIAM Journal on Applied Mathematics, Vol. 64, No. 4 (Apr. – Jun., 2004), pp. 1408–1433.
Geometrical transformation: complex valued change of coordinates:

\((x, y, z) \mapsto (x_s, y_s, z_s)\)

e.g. Cartesian PML \(x = x_s e^{-i\phi}\)
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\[(x, y, z) \mapsto (x_s, y_s, z_s)\]
e.g. Cartesian PML \(x = x_s e^{-i\phi}\)

Let \(k_\infty = |k| e^{-i\kappa}\) with \(\kappa > 0\),
we have \(k_\infty x_s = |k| e^{-i\kappa} xe^{i\phi} = k x e^{-i(\kappa - \phi)}\)
\[\implies \text{Im}(k_\infty x_s) = |k| x \sin(\phi - \kappa)\]
Taking \(\phi > \kappa\) to have \(\text{Im}(k_\infty x_s)\) kills the exponential divergence of \(e^{ik_\infty x_s}\) w.r.t. \(x_s\).
Geometrical transformation: complex valued change of coordinates: \((x, y, z) \mapsto (x_s, y_s, z_s)\)

\[ e.g. \text{ Cartesian PML } x = x_s e^{-i\phi} \]

Let \( k_\infty = |k|e^{-i\kappa} \) with \( \kappa > 0 \), we have

\[ k_\infty x_s = |k|e^{-i\kappa}xe^{i\phi} = |k|x e^{-i(\kappa - \phi)} \]

\[ \Rightarrow \text{Im}(k_\infty x_s) = |k|x \sin(\phi - \kappa) \]

Taking \( \phi > \kappa \) to have \( \text{Im}(k_\infty x_s) \) kills the exponential divergence of \( e^{ik_\infty x_s} \) w.r.t. \( x_s \).

New scalar product \((u, v)_\phi\) and a non-Hermitian extension \( L_\phi \) of the operator can be defined...
Geometrical transformation: complex valued change of coordinates: 
\((x, y, z) \mapsto (x_s, y_s, z_s)\) is turned into equivalent permittivity and permeability \(\varepsilon_s\) and \(\mu_s\) in the PML.

- Point spectrum: Rayleigh quotients 
  \(R_L(u) = \frac{(Lu, u)}{(u, u)}\) are invariant under the change of coordinates and modes are not modified!

- Quasinormal Modes: Rayleigh quotients 
  \(R_L(\phi(u)) = \frac{(Lu, u)}{(\phi u, \phi u)}\) becomes well defined for \(\phi\) large enough and do not change for larger \(\phi\): Quasimodes are unveiled!

- Continuous spectrum: Weyl sequences still correspond to \(k_s \in \mathbb{R}\) and therefore the \(k\) are multiplied by \(e^{-i\phi}\): the continuous spectrum is rotated!
Geometrical transformation: complex valued change of coordinates: 
\((x, y, z) \mapsto (x_s, y_s, z_s)\) is turned into equivalent permittivity and permeability \(\varepsilon_s\) and \(\mu_s\) in the PML.

- **Point spectrum**: Rayleigh quotients 
  \[ R_L(u) = \frac{(Lu, u)}{(u, u)} \]
  are invariant under the change of coordinates and modes are not modified!

- **Quasinormal Modes**: Rayleigh quotients 
  \[ R_{L\phi}(u) = \frac{(Lu, u)_\phi}{(u, u)_\phi} \]
  becomes well defined for \(\phi\) large enough and do not change for larger \(\phi\): Quasimodes are unveiled!
PML and Transformation Optics

Geometrical transformation: complex valued change of coordinates: 
\[(x, y, z) \mapsto (x_s, y_s, z_s)\] is turned into equivalent permittivity and permeability \(\varepsilon_s\) and \(\mu_s\) in the PML.

- **Point spectrum**: Rayleigh quotients 
  \[R_L(u) = \frac{(\mathcal{L}u, u)}{(u, u)}\] are invariant under the change of coordinates and modes are not modified!

- **Quasinormal Modes**: Rayleigh quotients 
  \[R_{\mathcal{L}_\phi}(u) = \frac{(\mathcal{L}u, u)_\phi}{(u, u)_\phi}\] becomes well defined for \(\phi\) large enough and do not change for larger \(\phi\): Quasimodes are unveiled!

- **Continuous spectrum**: Weyl sequences still correspond to \(kx_s \in \mathbb{R}\) and therefore the \(k\) are multiplied by \(e^{-i\phi}\): the continuous spectrum is rotated!
Rotation of continuous spectrum with PML unveils leaky modes

An old technique in Quantum Mechanics: Balslev, E.; Combes, J. M. Spectral properties of many-body Schrödinger operators with dilatation-analytic interactions. Communications in Mathematical Physics 22 (1971), no. 4, 280–294. This is an EXACT modification of the initial problem, not an approximation! \( \phi \) is the phase of the PML complex parameter \( s \) used for the complex stretch of the initial coordinates.
Bounded scatterer: (from Benjamin Vial Ph.D.)

triangular rod $\varepsilon^d = 13 + 0.2i$
Bounded scatterer:

triangular rod $\varepsilon^d = 13 + 0.2i$
Two leaky modes and one from the continuous spectrum (Bérenger mode)...

\[ \omega_1 = 1.77 \cdot 10^{14} - 6.36 \cdot 10^{12} i \, \text{rad.s}^{-1} \]

\[ \omega_2 = 1.90 \cdot 10^{14} - 1.01 \cdot 10^{13} i \, \text{rad.s}^{-1} \]

\[ \omega_3 = 1.57 \cdot 10^{14} - 1.29 \cdot 10^{14} i \, \text{rad.s}^{-1} \]
InfraRed Multispectral Filter Conception using QNM

How to obtain a given set of IR multispectral filters like these?

Transmission enhancement through square coaxial aperture arrays in metallic film: when leaky modes filter infrared light for multispectral imaging, Benjamin Vial, Mireille Commandré, Guillaume Demésy, André Nicolet, Frédéric Zolla et al., Optics letters 39 (16), 4723-4726
Filters conception

Modelling: parametric study
Spectral parameters of the resonance as a function of the period $d$ obtained from calculated transmission spectra (blue line) and extracted from the degenerated eigenfrequencies (red crosses). (a): resonant wavelength, (b): spectral width. Electric (c) and magnetic (d) field maps of the leaky mode in the Oyz plane for $d = 2.4 \mu m$. 

\[ \log |E|^2 \]

\[ \log |H|^2 \]
Filters conception

$\lambda^r$ targets: gives the conception parameter $d$

$d$ (µm) $\lambda^r$ (µm) M1 M2 M3 M4
2 2.5 3 7 8 9 10 11 12 13

Finite Elements for Electrodynamics and Modal Analysis of Dispersive Structures
Fabrication

Centre Interdisciplinaire des NAnosciences de Marseille (CINAM), UMR CNRS 7325, plateforme de lithographie électronique Planète (CT-PACA, FEDER funding)
Multispectral chip

Focused beam, not polarized

Simulations

Measurements
Modes in presence highly dispersive permittivities

- Handling frequency dispersion is naturally built-in when dealing with direct time-harmonic problems: setting $\omega$ sets the value of $\epsilon_r(\omega)$ explicitly.

- What should be done in spectral problems, where $\omega$ is the eigenvalue? This is of particular interest in the optical range:
  - dispersion relations for waveguides, fibers, photonic crystals, ...
  - study of resonant cavities
  - quasi-modal analyses

...where metals (Au, Ag, Al...) and semi-conductors (Si, GaAs, Ge...) exhibit resonant permittivities!
Why do we want the modes of dispersive structures? 
example: frequency selective reflective surface with Au/Ag nano-particles

Structure:

Design - « optimization »:

Fabrication:

Characterisation:

Causal permittivity models in very short... 

- Causal frequency dispersive materials ⇔ permittivity $\varepsilon_r(\omega)$ fulfills Kramers–Kronig relations.
- Causal materials can be modeled as a continuous sum of Lorentz resonances.
- Materials can be modeled as an infinite discrete sum of Lorentz resonances (still causal).
- On a limited spectral range, this sum can be truncated (still causal).
- In the visible range, 1 Lorentz + 1 Drude fits (and is still causal) for most metals and SC.
Permittivity models

Typically, $\varepsilon_r$ writes as a rational function of $\omega$:

- Drude model: 
  \[ \varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_d^2}{\omega(\omega + i\gamma_d)} \]

- Lorentz model: 
  \[ \varepsilon_r(\omega) = \varepsilon_\infty - \frac{\Delta\varepsilon \omega_l^2}{\omega^2 + i\gamma_l \omega - \omega_l^2} \]

- Drude-Lorentz model:
  \[ \varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_d^2}{\omega(\omega + i\gamma_d)} - \frac{\Delta\varepsilon \omega_l^2}{\omega^2 + i\gamma_l \omega - \omega_l^2} \]

In general: 
\[ \varepsilon_r(\omega) = \frac{N(\omega)}{D(\omega)} \]

arxiv.org/abs/1612.01876 "Extracting an accurate model for permittivity from experimental data: Hunting complex poles from the real line" Mauricio Garcia-Vergara, Guillaume Demésy, Frédéric Zolla
The eigenvalue problem in a simple 2D case

We are looking for non trivial solutions of the source-free equation:

\[ \mathcal{L}^{2D}(u) := -\varepsilon_r(x, \omega)^{-1} \text{div}(\mu_r^{-1} \text{grad} u) = \left( \frac{\omega}{c} \right)^2 u \]

- i.e. the eigenvalues \( \omega_n \) and associated eigenvectors \( u_n \) of the operator \( \mathcal{L}^{2D} \)
- \( \mathcal{L}^{2D}(u) \) depends on \( \omega \) we are looking for!

Let us compare two possible solutions:

- Physical linearization construction of an augmented system where auxiliary fields are added to \((E, H)\)
- **Numerical linearization**

---

The polynomial eigenvalue problem (PEP)

With a Drude material $\varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_d^2}{\omega(\omega + i\gamma_d)}$, $L^{2D}(u) = \left(\frac{\omega}{c}\right)^2 u$

becomes:

$$L_3^{2D}(u) \omega^3 + L_2^{2D}(u) \omega^2 + L_1^{2D}(u) \omega^1 + L_0^{2D}(u) = 0,$$

where:

$$L_3^{2D}(u) := \varepsilon_\infty u,$$

$$L_2^{2D}(u) := i \gamma_d \varepsilon_\infty u,$$

$$L_1^{2D}(u) := -\omega_d^2 u + c^2 \text{div} \left[ \mu_r^{-1} \text{grad} u \right],$$

$$L_0^{2D}(u) := i \gamma_d c^2 \text{div} \left[ \mu_r^{-1} \text{grad} u \right].$$

This is a third order polynomial (nonlinear) EVP.
Implementation

Solved as-is in GetDP (http://getdp.info, C. Geuzaine, Université de Liège) with two-level orthogonal Arnoldi eigensolver from SLEPc (http://slepc.upv.es, J. E. Roman, Universitat Politècnica de València)

Formulation {
   { Name modal_o3; Type FemEquation;
      Quantity {
         { Name u; Type Local; NameOfSpace H1;}
      }
      Equation {
         Galerkin{ [ r0[] * Dof{Grad u}, {Grad u} ]; ... }
         Galerkin{ DtDof[ -I[] * c1[] * Dof{u}, {u} ]; ... }
         Galerkin{ DtDof[ -I[] * r1[] * Dof{Grad u}, {Grad u} ]; ... }
         Galerkin{ DtDtDof[ - c2[] * Dof{u}, {u} ]; ... }
         Galerkin{ DtDtDtDof[ I[] * c3[] * Dof{u}, {u} ]; ... }
      }
   }
}
Drude model: \( \varepsilon_r(\omega) = 3 - \frac{(0.6\eta)^2}{\omega(\omega + i0.2\eta)} \)

Rectangular box – \( u|_{\partial\Omega} = 0 \)

\[ \eta = \frac{2\pi c}{a} \]

\( \mathcal{L}_3^{2D}(u) := \varepsilon_\infty u, \)
\( \mathcal{L}_2^{2D}(u) := i\gamma_d \varepsilon_\infty u, \)
\( \mathcal{L}_1^{2D}(u) := -\omega_d^2 u + c^2 \text{div} \left[ \mu_r^{-1} \text{grad} u \right], \)
\( \mathcal{L}_0^{2D}(u) := i\gamma_d c^2 \text{div} \left[ \mu_r^{-1} \text{grad} u \right], \)
\( \mathcal{L}_3^{2D}(u) \omega^3 + \mathcal{L}_2^{2D}(u) \omega^2 + \mathcal{L}_1^{2D}(u) \omega + \mathcal{L}_0^{2D}(u) = 0. \)
Lorentz model: \( \varepsilon_r(\omega) = 3 - \frac{4 (0.6\eta)^2}{\omega^2 + i 0.2\eta \omega - (0.6\eta)^2} \)

Rectangular box – \( u |_{\partial \Omega} = 0 \)

\[ \eta = \frac{2\pi c}{a} \]

PEP writes as:

\[ \sum_{k=0}^{4} L_k^{2D}(u) \omega^k = 0. \]
Drude-Lorentz model: 

\[ \varepsilon_r(\omega) = 2 - \frac{(0.5\eta)^2}{\omega(\omega + i0.3\eta)} - \frac{2(0.6\eta)^2}{\omega^2 + i0.1\eta \omega - (0.6\eta)^2} \]

Rectangular box – \( u|_{\partial \Omega} = 0 \)

\[ \eta = \frac{2\pi c}{a} \]

PEP writes as:

\[ \sum_{k=0}^{5} L^{2D}_k(u) \omega^k = 0. \]
And now with two boxes!

\[ \partial \Omega = \Omega_l \cup \Omega_r \]

- \( \varepsilon_r(x, \omega) \) piecewise constant on \( \Omega \)
- \( \varepsilon_{r,1} = \frac{\sum_{k=0}^{N} n_{1,k} \omega^k}{\sum_{k=0}^{N} d_{1,k} \omega^k} \) and \( \varepsilon_{r,2} = \frac{\sum_{k=0}^{N} n_{2,k} \omega^k}{\sum_{k=0}^{N} d_{2,k} \omega^k} \)
- \( \int_{\Omega} \left( f(x) \, \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) u' \, d\Omega \) with \( f(x) \) piecewise constant
Boundary term

\[ \int_{\Omega} \left( f(x) \, \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) \, u' \, d\Omega = \int_{\Omega} \left( \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) \, (f(x) \, u') \, d\Omega \]
Boundary term

\[
\int_{\Omega} \left( f(x) \, \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) u' \, d\Omega = \int_{\Omega} \left( \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) \left( f(x) \, u' \right) \, d\Omega
\]

\[
= -\int_{\Omega} \left[ \mu_r^{-1} \, \text{grad} \, u \right] \cdot \left[ f(x) \, \text{grad} \, u' + u' \, \text{grad} \, f(x) \right] \, d\Omega
\]

\[
+ \int_{\partial \Omega} \left( \mu_r^{-1} \, \text{grad} \, u \cdot n_{|\partial \Omega} \right) f(x) \, u' \, dl
\]
Boundary term

$$\int_{\Omega} \left( f(x) \, \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) \, u' \, d\Omega = \int_{\Omega} \left( \text{div} \, \mu_r^{-1} \, \text{grad} \, u \right) \, (f(x) \, u') \, d\Omega$$

$$= -\int_{\Omega} \left[ \mu_r^{-1} \, \text{grad} \, u \right] \cdot \left[ f(x) \, \text{grad} \, u' + u' \, \text{grad} \, f(x) \right] \, d\Omega$$

$$+ \int_{\partial \Omega} \left( \mu_r^{-1} \, \text{grad} \, u \cdot n_{|\partial \Omega} \right) \, f(x) \, u' \, dl$$

$$= -\int_{\Omega} \left[ \mu_r^{-1} \, \text{grad} \, u \right] \cdot \left[ f(x) \, \text{grad} \, u' \right] \, d\Omega$$

$$- \int_{\Omega} \left[ \mu_r^{-1} \, \text{grad} \, u \right] \cdot \left[ u' \, \text{grad} \, f(x) \right] \, d\Omega$$

$$+ \int_{\partial \Omega} \left( \mu_r^{-1} \, \text{grad} \, u \cdot n_{|\partial \Omega} \right) \, f(x) \, u' \, dl$$
Boundary term

\[
\int_{\Omega} \left( f(x) \text{ div } \underline{\mu_r}^{-1} \text{ grad } u \right) u' \, d\Omega = \int_{\Omega} \left( \text{ div } \underline{\mu_r}^{-1} \text{ grad } u \right) (f(x) u') \, d\Omega
\]

\[
= -\int_{\Omega} \left[ \underline{\mu_r}^{-1} \text{ grad } u \right] \cdot [f(x) \text{ grad } u' + u' \text{ grad } f(x)] \, d\Omega
\]

\[
+ \int_{\partial \Omega} \left( \underline{\mu_r}^{-1} \text{ grad } u \cdot n_{\partial \Omega} \right) f(x) u' \, dl
\]

\[
= -\int_{\Omega} \left[ \underline{\mu_r}^{-1} \text{ grad } u \right] \cdot [f(x) \text{ grad } u'] \, d\Omega
\]

\[
- \int_{\Omega} \left[ \underline{\mu_r}^{-1} \text{ grad } u \right] \cdot [u' \text{ grad } f(x)] \, d\Omega
\]

\[
+ \int_{\partial \Omega} \left( \underline{\mu_r}^{-1} \text{ grad } u \cdot n_{\partial \Omega} \right) f(x) u' \, dl
\]

\[
= -\int_{\Omega} \left[ \underline{\mu_r}^{-1} \text{ grad } u \right] \cdot [f(x) \text{ grad } u'] \, d\Omega
\]

\[
- \int_{\Omega} \left[ \underline{\mu_r}^{-1} \text{ grad } u \right] \cdot [u' \text{ jump}_{\Gamma} \delta_{\Gamma} n_{\Gamma}] \, d\Omega
\]

\[
+ \int_{\partial \Omega} \left( \underline{\mu_r}^{-1} \text{ grad } u \cdot n_{\partial \Omega} \right) f(x) u' \, dl
\]
Boundary term

\[
\int_{\Omega} \left( f(x) \, \text{div} \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \right) \, u' \, d\Omega = \int_{\Omega} \left( \text{div} \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \right) \, (f(x) \, u') \, d\Omega
\]

\[
= -\int_{\Omega} \left[ \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \right] \cdot \left[ f(x) \, \text{grad} \, u' \right] \, d\Omega
\]

\[
- \int_{\Gamma} f_{jump} \, \left[ \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \right] \cdot n_{\mid \Gamma} \, u' \, dl
\]

\[
+ \int_{\partial \Omega} \left( \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \cdot n_{\mid \partial \Omega} \right) \, f(x) \, u' \, dl
\]

- We need to impose jumps to \( f \left[ \frac{\mu_r^{-1}}{\mu_r} \, \text{grad} \, u \right] \cdot n_{\mid \Gamma} \), i.e. jumps on the tangential trace of \( f \, \mathbf{H} \) on \( \Gamma \)

- Yet we do not have access to this quantity directly...
Lagrange multipliers – Split one equation into three equations:

\[ u_1 = 0 \text{ on } \partial \Omega_1 \]
\[ u_2 = 0 \text{ on } \partial \Omega_2 \]

\[
\sum_{k=0}^{N} \omega^k \left[ \int_{\Omega_1} d_{1,k} \, \text{grad} \, u_1 \cdot \text{grad} \, u_1' + \omega^2 \, n_{1,k} \, u_1 \, u_1' \, d\Omega_1 \right]
\]
\[
\sum_{k=0}^{N} \omega^k \left[ \int_{\Omega_2} d_{2,k} \, \text{grad} \, u_2 \cdot \text{grad} \, u_2' + \omega^2 \, n_{2,k} \, u_2 \, u_2' \, d\Omega_2 \right]
\]
\[
+ \sum_{k=0}^{N} \omega^j \left[ \int_{\Gamma} d_{j,1} \lambda \, u_1' \, d\Gamma \right] - \sum_{k=0}^{N} \omega^j \left[ \int_{\Gamma} d_{j,2} \lambda \, u_2' \, d\Gamma \right]
\]
\[
= 0 = 0
\]

and \[ \int_{\Gamma} (u_1 - u_2) \lambda' \, d\Gamma = 0 \]
Results for the two-box

Semi-analytical vs. FEM-augmented vs. FEM-polynomial

\[ \varepsilon_{r,1}(\omega) = 3 - \frac{4(0.6\eta)^2}{\omega^2 + i0.2\eta\omega - (0.6\eta)^2} \quad \text{with} \quad \eta = \frac{2\pi c}{a} \]

\[ \varepsilon_{r,2}(\omega) = 2 \]
Other polarization case

\[ E = [E_x(x, y), E_y(x, y), 0] \]

with edge elements

\[ \varepsilon_{r,1}(\omega) = 3 - \frac{4 (0.6\eta)^2}{\omega^2 + i 0.2\eta \omega - (0.6\eta)^2} \]

\[ \varepsilon_{r,2} = 2 \]
Other polarization case

\( \mathbf{E} = [E_x(x, y), E_y(x, y), 0] \) with edge elements

- **pole**
  \[ \varepsilon_{r,1}(\omega) \to \infty \]
  accumulation point

- \( \varepsilon_{r,1}(\omega) = -\varepsilon_{r,2} \)
  surface plasmon
  +accumulation point

- \( \varepsilon_{r,1}(\omega) = 0 \)
  (many) spurious modes
  divergence condition failure

\[ \varepsilon_{r,1}(\omega) = 3 - \frac{4 (0.6\eta)^2}{\omega^2 + i 0.2\eta \omega - (0.6\eta)^2} \]

\[ \varepsilon_{r,2} = 2 \]
Other polarization case

\[ \mathbf{E} = [E_x(x,y), E_y(x,y), 0] \] with edge elements
Drude photonic crystal

- Single Drude resonance $\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$

- With: $\frac{\omega_p a}{2\pi c} = 1.1, \quad \frac{\gamma a}{2\pi c} = 0.05$

- Material filling fraction = 0.65 for both $\bigcirc$ and $\Box$

- $r = 0.455a$ for $\bigcirc$

- $(w = 0.806a)$ for $\Box$
Drude photonic crystal

\[ \mathbf{E} = [E_x(x, y), E_y(x, y), 0] \] with edge elements
Drude photonic crystal

\( \mathbf{E} = [E_x(x, y), E_y(x, y), 0] \) with edge elements

\( \Gamma X - XM - MT \) (zoom)
Conclusion and perspectives

- Edge elements (and higher order generalizations) are a good tool for the direct discretization of PDE operators of classical electrodynamics...

- Spectral problems for dispersive media – 2 linearization strategies:
  - Augmented formalism – Auxiliary fields
  - Direct calculation of plasmonic resonances through solution of polynomial eigenvalue problem with GetDP+SLEPc

- Lagrange multipliers to deal with boundary terms in order to limit the degree of the PEP in the case of several dispersive media.

- To do:
  - Spectral transformations to explore specific regions of the spectrum.
  - Fix divergence condition failure ($\varepsilon(\omega) = 0$).
  - Merge with PMLs for QNM of dispersive structures.
  - QNM expansion.
  - 3D …
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- and many others...
- THANK YOU FOR YOUR ATTENTION!
Tonti Diagram for Electrodynamics (in vector analysis)
two formulations for $E_z$
(direct and Lagrange mult.)

\[ \epsilon_{\infty_1} = 3.00 \quad \omega_1 = 0.60 \quad \gamma_1 = 0.20 \quad \omega_l = 0.00 \quad \gamma_l = 0.00 \quad \epsilon_1 = 0.00 \]

\[ \epsilon_{\infty_2} = 2.00 \quad \omega_2 = 0.00 \quad \gamma_2 = 0.00 \quad \omega_l = 0.00 \quad \gamma_l = 0.00 \quad \epsilon_2 = 0.00 \]
two formulations for $H_z$
($H_z$ direct and $E_x, E_y$ Lagrange mult.)