Discontinuities in open photonic waveguides: Rigorous 3D modeling with the finite element method

Guillaume Demésy∗and Gilles Renversez

Aix Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille, France.

July 29, 2019

Abstract

In this paper, we present a general framework to study rigorously discontinuities in open waveguides using a full vector description given by Maxwell’s equations and using the finite element method. The discontinuities are not necessarily a small perturbation of the initial waveguide and can be very general, such as plasmonic inclusions of arbitrary shape. The leaky modes of the invariant structure are computed first ; then serve as incident fields on the full structure with obstacles using a scattered field approach ; the resulting scattered field is finally projected on the modes of the invariant structure making use of their bi-orthogonality. A complete energy balance is performed. Finally, the modes open waveguides periodically structured along the propagation direction are computed we compare the relevant complex propagation constants to the transmission obtained for a finite number of identical cells. The relevance and complementarity of the two approaches are highlighted on a numerical example encountered in infrared sensing. Finally, open source models allowing to retrieve most of the results of this paper are provided.

1 Introduction

The study of discontinuities is an old research topic in waveguide studies due to its importance for practical applications in many areas of physics. One must cite the seminal contribution of Schwinger for the development of variational methods in the forties [1] and the results obtained by Lewin [2].

These methods, often complex and specific, do not generally consider the exact solutions of Maxwell’s equation and rely on specific configurations, hypotheses, initial guesses for the solution forms. During the last two decades, the versatile Finite-Difference Time-Domain (FDTD) method allowed the study of waveguide discontinuities, including 3D ones, taking into account the full set of Maxwell’s equations [3, 4]. Nevertheless, the computational resources both in terms of memory and time requirements are huge when realistic 3D photonic devices are considered with a uniform square grid, especially nanophotonic ones with high quality factors. As for harmonic methods, Fourier modal methods [5, 6] also allow to tackle discontinuities in waveguides but they are restricted to geometries with straight walls. In acoustics and optics,

∗Corresponding author: guillaume.demesy@fresnel.fr
coupled modal-finite element techniques have been successfully used in varying cross-section waveguides [7, 8].

In the present work, we demonstrate that such studies of 3D waveguide discontinuities can be carried out efficiently with adapted formulations of the finite element method (FEM) which already proved its power and versatility in many field of computational electrodynamics [9].

We can state four main advantages of the FEM-based method: i) curved geometries are naturally treated using high order mesh elements and corresponding shape functions, ii) conforming non-uniform meshing is now a standard for mesh generators which is particularly relevant when rapid and strong permittivity changes must be tackled, iii) the domain decomposition method is now available in several FEM solvers allows the treatment of large scale 3D problem, iv) and the possibility to reuse the inverse matrix for several incident modes propagating in the invariant structure – a subtlety detailed later which is a key advantage for the optimization multi-mode guides. This is especially worthy when the simulations are performed within a topology optimization frame [10].

The practical context motivating this theoretical and numerical study is the design of efficient plasmonic waveguides for infrared sensing [11] since the mid-IR spectral domain is known to be the molecular fingerprint region, due to the fact that most molecule including pollutants have intense fundamental vibrational bands in this spectral range. The device configuration is fully integrated and based on a ridge waveguide upon which metallic scattering nano-objects will ensure the coupling between the guided modes and superstrate of the device. Chalcogenide glasses are chosen for the main layers due to their high transparencies for infrared wavelengths. Ultimately, the metallic scatterers are planned to be functionalized in order to react to the targeted chemical species. The sensing property relies on the subsequent modification of the guidance of the full structure.

In this paper, we present a general framework to study rigorously discontinuous waveguides using a full vector description given by Maxwell’s equations in the framework of the finite element method. The discontinuity can be very general and is not necessarily a small perturbation of the initial waveguide. The full structure under investigation is made of 3 segments: The input one is a uniform waveguide invariant along its main propagation axis, the intermediate one contains the opto-geometrical modifications of the waveguide (see Fig. 1), the output one is again an invariant waveguide. In order to model the response of the resulting 3D guiding structure, we adopt a scattered field formulation consisting of three sequential steps, the output of first step being the input of the second one, the output of the first and second being the input of the third one.

First, we determine the leaky guided modes for a fixed frequency, corresponding to the wavelength of interest, of the unperturbed 2D waveguide. This is a ridge waveguide made of chalcogenide layers on a silicon substrate, assumed to be invariant along its propagation axis. We use our usual vector FEM method with the Galerkin approach to solve the associated eigenvalue problem [9, 12, 13]. This first step provides both the propagation constants (eigenvalues) and the associated modes profiles (eigenvectors).

Second, these guided modes are used as incident fields for the full 3D problem in the modified segment. The electromagnetic problem to solve for this second step is then a scattering problem [14]. It is possible to define a proper energy balance (transmission and reflection into the ridge guide, absorption taking place into the plasmonic rods, radiation losses) allowing to fully evaluate the impact of the modified segment on the energy propagation.

Third, outside of the modified region, the total field is projected on a fixed number of leaky modes of the output segment of the full structure, eventually only the main one. Our method
allows to compute all the required energy-related quantities to investigate quantitatively the behavior of the full structure, notably the impact of the modified segment, and to take into account the way it is excited by the selected propagating mode.

Note that our approach differs from the one exposed in Ref. [9] where total field formulations making use of port boundary conditions are applied to closed discontinuous waveguides, whereas it is proposed here to use a general scattered field formulation to deal with in open discontinuous waveguides.

Finally, we also compute the modes of infinitely periodically structured waveguides and compare the relevant complex propagation constants to the transmission obtained with a finite number of identical cells. After deriving the formulation, the relevance and complementarity of the two approaches are highlighted on a numerical example.

2 Direct problem

In this section, a direct – as opposed to modal – scattering approach is demonstrated. A typical and realistic structure addressed in this paper is sketched in Fig. 1: A z-invariant dielectric rectangular waveguide (of width $w$ and thickness $h_g$ in blue) is deposited on a low index spacer (of thickness $h_l$, in green) lying on a semi-infinite substrate (in purple). The z-invariance of this guiding structure is locally broken, by adjunction of a finite number of obstacles. These obstacle can be in practice any bounded modification of permittivity: Ellipsoidal patches above the guiding layer labelled $\bullet$ in Fig. 1, holes $\circ$ in the guiding layer, obstacles or resonators next to the waveguide $\circ$ or even a combination of all $\bullet$, $\circ$. . . . Note that the method applies irrespectively of the number of layers of the z-invariant structure and that the obstacles can be arbitrarily shaped and located in (or above) the structure. It is shown how the obstacles (more generally the modified waveguide segment) perturb a mode propagating in the z-invariant structure. A first step consists in the numerical computation of the modes of the invariant structure, which are used in a second step as incident fields for the full 3D structure.

2.1 Obtaining the incident fields

The classical guiding z-invariant structure is characterized by its permittivity function defined by parts as:

$$
\varepsilon_{r,2D}(x, y) = \begin{cases} 
\varepsilon_{r,g} & \text{in the guide,} \\
\varepsilon_{r,l} & \text{in the low index region,} \\
\varepsilon_{r,s} & \text{in the substrate,} \\
\varepsilon_{r,t} & \text{in the superstrate.}
\end{cases}
$$

(1)

Between $z_{\text{min}}$ and $z_{\text{max}}$, one can now break the z-invariance by a local modification of the permittivity function which leads to a 3D scattering problem, which in turn can be characterized by its permittivity function defined by parts:

$$
\varepsilon_{r,3D}(x, y, z) = \begin{cases} 
\varepsilon_{r,g} & \text{in the guide,} \\
\varepsilon_{r,l} & \text{in the low index region,} \\
\varepsilon_{r,s} & \text{in the substrate,} \\
\varepsilon_{r,t} & \text{in the superstrate,} \\
\varepsilon_{r,d}(x, y, z) & \text{in the obstacles}
\end{cases}
$$

(2)
Figure 1: Scheme of the \(z\)-invariant structure (substrate in purple, low index layer in green and a rectangular waveguide in blue) with various discontinuities (or obstacles) breaking the \(z\)-invariance locally in region called modified. Discontinuities can be ellipsoidal patches above the guiding layer labelled \(\odot\), holes \(\odot\) in the guiding layer, obstacles or resonators next to the waveguide \(\odot\) or even a combination of all \(\odot\)...

The starting point consists in computing the modes of an annex problem formed by the \(z\)-invariant structure solely. This is a very classical problem [13, 15] where one introduces the ansatz \(E(x) = e(x)e^{-i(\omega_0 t - \beta z)}\) in the source-free Helmholtz equation:

\[
\text{curl} \left( \mu^{-1}_{r,2D} \text{curl} E \right) = \varepsilon_{r,2D} \left( \frac{\omega_0}{c} \right)^2 E
\]

(3)

for a given \(\omega_0 \in \mathbb{R}^+\), e.g. the pulsation of the wave. Note that the permittivity and permeability are now tensors fields, corresponding to their scalar counterparts defined above. Indeed, cartesian PMLs adapted to each infinite (along the transverse directions) domain are used to damp the radially blowing leaky modes of this open structure [13]. It results in a quadratic non-Hermitian eigenvalue problem amounting to find non trivial pairs \((\beta_k, e_k) \in \mathbb{C} \times H^1(\Omega_{2D}, \text{curl})\) such that :

\[
\text{curl} \left( \mu^{-1}_{r,2D} \text{curl} e_k \right) - k_0^2 \varepsilon_{r,2D} e_k + i \beta_k \left( \hat{z} \times \left( \mu^{-1}_{r,2D} \text{curl} e_k \right) + \text{curl} \left( \mu^{-1}_{r,2D} \hat{z} \times e_k \right) \right) + \left( i \beta_k \right)^2 \hat{z} \times \left( \mu^{-1}_{r,2D} \hat{z} \times e_k \right) = 0.
\]

(4)

This equation can be solved using a mixed finite element formulation involving edge elements for the discretization of the transverse component \((e_x, e_y)\) coupled to a nodal basis for the (continuous) longitudinal component \(e_z\) [13, 16].

Throughout the paper, the following numerical values are considered for the \(z\)-invariant waveguide [17]: The operating freespace wavelength \(\lambda_0 = 7.7 \mu\text{m}, \varepsilon_{r,g} = 7.1824 \quad (\text{Se}_4), \varepsilon_{r,l} = 6.2001 \quad (\text{Se}_2), \varepsilon_{r,s} = 11.69024481 \quad (\text{silicon}) \quad [18], \varepsilon_{r,t} = 1 \quad (\text{air}), w_g = 14 \mu\text{m}, h_g = 2.2 \mu\text{m} \quad \text{and} \quad h_l = 5.3 \mu\text{m}. \) All the materials are assumed to be non-magnetic: \(\mu_{r,2D} = 1\) \((\text{except in the PMLs where } \mu_{r,2D} \text{ takes the appropriate value). The six best guided modes supported by the}$$
(a) Mode 1: −2.7 dB/cm
(b) Mode 2: −4.3 dB/cm
(c) Mode 3: −12.9 dB/cm
(d) Mode 4: −18.8 dB/cm
(e) Mode 5: −18.8 dB/cm
(f) Mode 6: −48.4 dB/cm

Figure 2: Six best guided modes supported by the z-invariant structure (edges in colors matching the domains shown in Fig. 1) at $\lambda_0 = 7.7 \mu m$. The black and white maps indicate the norm of the modes (white is high) and the orange arrows indicate the real part of the mode that belong to the waveguide cross-section.

z-invariant structure are depicted in Fig. 2(a-f), sorted in ascending losses (i.e. $\text{Im}\{\beta_1\}$ is the smallest).

Finally, all geometries and conformal meshes have been obtained using the Gmsh software [19] and all the finite element formulations in this paper are implemented thanks to the flexibility of the finite element software GetDP [20]. Open source models allowing to retrieve most of the results of this paper are provided.

2.2 Computation of the scattered field

One can now use any of these 2D modes $E_{k,2D} := e_k e^{i(\beta_k z - \omega_0 t)}$ as an incident field $E^\text{inc}$ on the obstacles and look for $E^\text{tot}$, the total field solution of the source-free Helmholtz equation:

$$-\text{curl} \left[ \mu_{r,3D}^{-1} \text{curl} E^\text{tot} \right] + k_0^2 \varepsilon_{r,3D} E^\text{tot} = 0. \quad (5)$$

with $k_0 \equiv \omega_0/c$. Let us define the scattered field as $E^d \equiv E^\text{tot} - E^\text{inc}$ and from the linearity of Eqs. (3,5), we obtain the following scattering problem:

$$-\text{curl} \left[ \mu_{r,3D}^{-1} \text{curl} E^d \right] + k_0^2 \varepsilon_{r,3D} E^d = k_0^2 (\varepsilon_{r,3D} - \varepsilon_{r,2D}) E^\text{inc}. \quad (6)$$
Note that the support of the effective sources \((\epsilon_{r,3D} - \epsilon_{r,2D})\) in this scattering problem has to be bounded to ensure a proper outgoing wave condition \cite{21} to the scattered field \(E_d\), which is the case in our examples. Finally, 3D cartesian PMLs are bound the computational domain. Compared to a total field approach with a port condition, it is stressed that the electromagnetic sources of our equivalent radiation problem are located within the discontinuities. The PMLs of elongated structures are naturally build in to damp fields radiating from the center of the computation box more efficiently than the total field radiating from a port located at one extremity of the elongated box, the resulting total field being more grazing than the scattered field when entering the PMLs.

### 2.3 Energy balance

The Poynting vectors associated with the incident, diffracted and total fields are classically defined by respectively \(S_{\text{inc}} = \text{Re}\{E_{\text{inc}} \times H_{\text{inc}}\}/2\), \(S_d = \text{Re}\{E_d \times H_d\}/2\) and \(S_{\text{tot}} = \text{Re}\{E_{\text{tot}} \times H_{\text{tot}}\}/2\). Then, the incoming, transmitted, reflected and absorbed powers can be defined as respectively

\[
\begin{align*}
P_{\text{in}} &= \int_{\Gamma_{\text{in}}} S_{\text{inc}} \cdot n_{\Gamma} \, dS, \\
P_{\text{tr}} &= \int_{\Gamma_{\text{out}}} S_{\text{tot}} \cdot n_{\Gamma} \, dS, \\
P_{\text{ref}} &= \int_{\Gamma_{\text{in}}} S_d \cdot n_{\Gamma} \, dS, \\
P_{\text{abs}} &= \frac{\varepsilon_0 \omega_0}{2} \text{Im}\{\epsilon_{r,d}\} \int_{\Omega_d} |E_{\text{tot}}|^2 \, d\Omega,
\end{align*}
\]

where \(\Gamma_{\text{in}}\) and \(\Gamma_{\text{out}}\) are transverse plane surfaces before and after the obstacles (as depicted in blue color in Fig. 3) with \(n_{\Gamma}\) the unit vector normal to \(\Gamma_{\text{in}}\) and \(\Gamma_{\text{out}}\) as shown in Fig. 3. \(\Omega_d\) is the support of the diffractive obstacles or of the localized region where the waveguide opto-geometrical parameters are modified. Finally one can define transmission, reflection and absorption coefficients as :

\[
T = \frac{P_{\text{tr}}}{P_{\text{in}}}, \quad R = \frac{P_{\text{ref}}}{P_{\text{in}}} \quad \text{and} \quad A = \frac{P_{\text{abs}}}{P_{\text{in}}}.
\]

Note that the energy balance defined as \(T + R + A\) is expected to be less than unity since the flux contributions from four surfaces \((xOx\) and \(xOy\) planes are missing in the box chosen to apply the Poynting theorem. This translates the fact that the guide is leaky. For clarity, Fig. 3 illustrates the quantities at stake in the energy balance. This numerical set up is obtained for an incident field set to \(E_{1,2D}\) (cf Fig. 2(a)) with four ellipsoidal lossy patches placed above the same waveguide as in Section 2.1. This example will be discussed in detail in Section 4. The hot colormap represents the square norm of the total electric field \(|E_{\text{tot}}|^2\) (white is high, dark is low) involved in the computation of the Joule losses. The pink/yellow map (yellow is high, pink is low) represents the total Poynting vector \(S_{\text{tot}}\) on three planes. The first plane (see left side of the figure) corresponds to \(\Gamma_{\text{in}}\), another one (right side of the figure) to \(\Gamma_{\text{out}}\) and the last one to the symmetry plane of the structure. Along this last plane, the perturbation induced by the objects is clearly visible. The transmission \(T\) reaches 70.6%, the reflection \(R\) 0.7% and the absorption \(A\) 22.5\% \((T + R + A = 93.8\%)\) in this example. The 6.2\% remaining correspond
Figure 3: Cuts of the total Poynting vector $S_{\text{tot}}$ and square norm of the total field $E_{\text{tot}}$ inside the four lossy obstacles (ellipsoidal patches) above the waveguide. Half of the structure is computed and represented due to the symmetry properties of the structure.

to radiation leakage. This repartition of the energy can be even more precisely characterized by expansion of the diffracted and total fields on the modes of the 2D invariant structure, once away from the obstacles, as shown in the next paragraph.

### 2.4 Modal expansion of the scattered field

The modes of the 2D invariant structure satisfy the following bi-orthogonality condition equivalent to the one given in ref. [15], it also defines the normalization of each leaky modes:

$$\int_{S} \mathbf{e}_j \times \mathbf{h}_k \cdot \hat{z} \, dS = \int_{S} \mathbf{e}_k \times \mathbf{h}_j \cdot \hat{z} \, dS = A_k \delta_{kj} \quad \text{with} \quad (9)$$

In the case of leaky modes, it is suggested in [15] to perform a complex change of space variable as one moves far away from the waveguide to damp the exponential growth of the leaky mode. In our finite element approach that includes the PML which are an analytical continuation of , this integration corresponds simply to integrate over a full cross-section of computational domain including the PML regions. Hence, away from the obstacles, it is possible to expand the scattered field as $E^d = \sum_k r_k E_{k,2D}$ and the total field as $E_{\text{tot}} = \sum_k t_k E_{k,2D}$ where the reflection and transmission coefficients are simply given as:

$$\begin{align*}
t_k &= \int_{S_{\text{out}}} E_{\text{tot}} \times \mathbf{h}_k \cdot \hat{z} \, dS / A_k \\
r_k &= \int_{S_{\text{in}}} E^d \times \mathbf{h}_k \cdot \hat{z} \, dS / A_k
\end{align*} \quad (10)$$
where $S_{in}$ can be any transverse section before the obstacles ($z < z_{\text{min}}$) and $S_{out}$ can be any transverse section after the obstacles ($z > z_{\text{out}}$). Note that this can be extended to the computation of the full scattering matrix of the waveguide. Finally, $\sum_{k=1}^{6} |t_k|^2 \rightarrow T$ and $\sum_{k=1}^{6} |r_k|^2 \rightarrow R$. In this example, the values $\sum_{k=1}^{6} |t_k|^2 = 0.665$ (with $|t_1|^2 = 0.632$) and $\sum_{k=1}^{6} |r_k|^2 = 0.0002$ are obtained.

3 Modes of the infinitely periodic 3D structure

3.1 Variational formulation of the spectral problem

In this section, we are now interested in a 3D spectral problem with one direction of periodicity defined by

\[
\text{curl} \left[ \mu_{r,\#}(x)^{-1} \text{curl} E \right] = \epsilon_{r,\#}(x,\omega_0) \left( \frac{\omega_0}{c} \right)^2 E. \tag{11}
\]

where $\epsilon_{r,\#}(x,\omega_0)$ and $\mu_{r,\#}(x)$ are respectively the permittivity and permeability tensor fields at a fixed frequency $\omega_0$ exhibiting a 1D periodicity $d$ along $Oz$. Bloch’s theorem states that one can now, without loss of generality, look for solutions for the electric field $E$ of the form:

\[
E = E_{\#}(x,y,z) e^{-i(\omega_0 t - \gamma z)}, \tag{12}
\]

where $E_{\#}$ is a $d$-periodic function in $z$ and $\gamma$ is the Bloch variable lying in the first (reduced) Brillouin zone $[0, \pi/d]$ [13, 22].

One can choose to set $\gamma$ to a real value lying in the first Brillouin zone and to look for $(\omega_{\gamma,i}, E_{\gamma,i})$ eigenvalues and eigenvectors, by imposing Bloch conditions on the $z$-transverse surfaces of the cell and making the use of Eq. (11). An alternative option amounts to set $\omega_0$ to a real value, inject the form of Eq. (12) into Eq. (11) and look for eigenvectors under the form of periodic part $E_{\#}$ of the Bloch wave along with corresponding eigenvalue $\gamma$. Two equations are to be fulfilled:

\[
\begin{align*}
-\text{curl} \left[ \mu_{r,\#}^{-1} \text{curl} \left[ E_{\#} e^{i\gamma z} \right] \right] + k_0^2 \epsilon_{r,\#}(x) E_{\#} e^{i\gamma z} &= 0 \tag{13a} \\
\text{div} \left[ \epsilon_{r,\#}(x) E_{\#} e^{i\gamma z} \right] &= 0. \tag{13b}
\end{align*}
\]

Not surprisingly, expanding the curl term in Eq. (13a) in order to get rid of the $e^{i\gamma z}$ dependency, leads to an expression similar to the $z$-invariant counterpart of the problem (see Eq. (4)):

\[
-\text{curl} \left[ \mu_{r,\#}^{-1} \text{curl} E_{\#} \right] + k_0^2 \epsilon_{r,\#}(x) E_{\#} \\
- i\gamma \hat{z} \times \left[ \mu_{r,\#}^{-1} \text{curl} E_{\#} \right] \\
- i\gamma \text{curl} \left( \mu_{r,\#}^{-1} \hat{z} \times E_{\#} \right) \\
- (i\gamma)^2 \hat{z} \times \left( \mu_{r,\#}^{-1} \hat{z} \times E_{\#} \right) = 0. \tag{14}
\]

In a variational way, after classically integrating by part two curl operators, it holds that
for any $W \in H^1_\#(\Omega, \text{curl})$:

$$\begin{align*}
& - \int_{\Omega} \left[ \mu_{r, \#}^{-1} \text{curl} E_{\#} \right] \cdot \text{curl} W \, d\Omega \\
& + \int_{\Omega} k_0^2 \varepsilon_{r, \#}(x) E_{\#} \cdot \bar{W} \, d\Omega \\
& - i\gamma \int_{\Omega} \hat{z} \times \left[ \mu_{r, \#}^{-1} \text{curl} E \right] \cdot \bar{W} \, d\Omega \\
& - i\gamma \int_{\Omega} \left( \mu_{r, \#}^{-1} \hat{z} \times E_{\#} \right) \cdot \text{curl} W \, d\Omega \\
& +(i\gamma)^2 \int_{\Omega} \left( \mu_{r, \#}^{-1} \hat{z} \times E_{\#} \right) \cdot (\hat{z} \times \bar{W}) \, d\Omega \\
& - \int_{\partial\Omega} \left[ n_{\partial\Omega} \times \left( \mu_{r, \#}^{-1} \text{curl} E_{\#} \right) \right] \cdot \bar{W} \, dS \\
& - i\gamma \int_{\partial\Omega} \left[ n_{\partial\Omega} \times \left( \mu_{r, \#}^{-1} \hat{z} \times E_{\#} \right) \right] \cdot \bar{W} \, dS \\
& = 0
\end{align*}$$

(15)

Note that the two boundary terms recombine into $- \int_{\partial\Omega} [n_{\partial\Omega} \times (\mu_{r, \#}^{-1} (\text{curl} E_{\#} + i\gamma \hat{z} \times E_{\#})] \cdot \bar{W} \, dS \propto \int_{\partial\Omega} [n_{\partial\Omega} \times H] \cdot \bar{W} \, dS$ so that setting a Dirichlet or Neumann natural condition for $E_{\#}$ on non-periodic faces of the domain ($i.e.$ the PML bounds) actually corresponds to a Dirichlet or Neumann natural condition for $H$.

The divergence condition in Eq. (13b) has to be handled carefully. Indeed, we are looking for divergence free solutions such that $\text{div} (\varepsilon_{r, \#} E) = 0$, that is:

$$\text{div} \left( \varepsilon_{r, \#} E_{\#} e^{i\gamma z} \right) = 0 = \text{div} (\varepsilon_{r, \#} E_{\#}) + i\gamma \hat{z} \cdot (\varepsilon_{r, \#} E_{\#})$$

(16)

Consequently, $\varepsilon_{r, \#} E_{\#}$ is not divergence-free and, from the variational point of view, the following holds for any $\varphi \in H^1_\#(\Omega)$:

$$\begin{align*}
& \int_{\Omega} \left[ \text{div} (\varepsilon_{r, \#} E_{\#}) + i\gamma \hat{z} \cdot (\varepsilon_{r, \#} E_{\#}) \right] \varphi \, d\Omega = 0 \\
& = - \int_{\Omega} \varepsilon_{r, \#} E_{\#} \cdot \text{grad} \varphi \, d\Omega + i\gamma \int_{\Omega} \hat{z} \cdot (\varepsilon_{r, \#} E_{\#}) \varphi \, d\Omega .
\end{align*}$$

(17)

Finally, the proper way to ensure the divergence condition [23] in a weak sense is to use $\varphi$ as a Lagrange multiplier. We are now in position to reformulate the eigenvalue problem at stake in this section. We are looking for non trivial pairs $\gamma_k, (E_{\#, k}, \varphi_k) \in \mathbb{C} \times (H^1_\#(\Omega, \text{curl}) \times H^1_\#(\Omega))$. 

9
such that:

\[
\begin{aligned}
&-\int_{\Omega} \mu_{r,\#}^{-1} \text{curl} E_{\#,k} \cdot \text{curl} W \, d\Omega \\
&+ \int_{\Omega} k_0^2 \varepsilon_{r,\#}(x) E_{\#k} \cdot \overline{W} \, d\Omega \\
&-i\gamma \int_{\Omega} \hat{z} \times (\mu_{r,\#}^{-1} \text{curl} E) \cdot \overline{W} \, d\Omega \\
&-i\gamma \int_{\Omega} (\mu_{r,\#}^{-1} \hat{z} \times E_{\#k}) \cdot \text{curl} \overline{W} \, d\Omega \\
&+(i\gamma)^2 \int_{\Omega} (\mu_{r,\#}^{-1} \hat{z} \times E_{\#k}) \cdot (\hat{z} \times \overline{W}) \, d\Omega \\
&+ \int_{\Omega} \varepsilon_{r,\#} \text{grad} \varphi_k \cdot \overline{W} \, d\Omega \\
&+i\gamma \int_{\Omega} \varepsilon_{r,\#} \varphi_k \hat{z} \cdot \overline{W} \, d\Omega = 0 \\
&\int_{\Omega} \varepsilon_{r,\#} E_{\#k} \cdot \overline{\text{grad} \varphi_k} \, d\Omega \\
&-i\gamma \int_{\Omega} \hat{z} \cdot (\varepsilon_{r,\#} E_{\#k}) \overline{\varphi_k} \, d\Omega = 0
\end{aligned}
\]  

(18a)

3.2 Numerical validation

It is apropos to validate this 3D model numerically using an extruded 2D domain. The eigenvalue resulting from three finite element problems are shown in Fig. 4. Two of them (orange circles and blue crosses) are variants of the 2D problem in Eq. (4). The problem is indeed quadratic and can be solved as such using SLEPc scientific library (orange circles) which uses its internal numerical linearization. But as detailed in [13], it is possible to linearize the 2D problem by simply using for unknown \((e_x, e_y, i\gamma e_z)\) instead of \((e_x, e_y, e_z)\). The resulting sparse systems resulting from the two methods are different and it is worth noting that the 30 eigenvalues are identical up to numerical precision. Now the third eigenproblem (red pluses in Fig. 4) corresponds to Eqs. (18) applied to the 3D problem obtained by the extrusion of the previous 2D problem by a period \(d = 1 \mu m\) along the \(z\) direction. Up to the \(\pi/d\) folding of the dispersion curves expected from the application to the Bloch theorem, these 2D and 3D problems are spectrally equivalent and the eigenvalues are indeed retrieved with excellent accuracy. The discrepancies obtained for \(\text{Im}\{\gamma_k/k_0\} > 0.2\) can be simply explained by the fact that the 3D mesh used in the simulation is comparatively coarser than the 2D mesh. For the best guided modes labelled (a), (b) and (c), the relative error between the 2D and 3D eigenvalues is lower that \(10^{-4}\) in modulus. Note that convergence tests have been performed and this discrepancy decreases with a rate expected from the element type when the mesh size decreases. The real part of \(E_{\#k}\) are shown in the insets (a-c) of Fig. 4 (note that they cannot be directly compared to the yellow arrows of Fig. 2(a-c) since an eigenvector is defined up to an arbitrary phase). A small value of the period along \(z\) corresponds to a large first Brillouin zone so that the eigenvalues computed do not belong to a folded dispersion branch and the periodic part of the Bloch variable are constant along \(z\).

Now we are in position to compare the results derived from the modes of the infinitely
structured waveguide (3D modal problem defined in Sec. 3) to the transmission properties of scattering problems with a finite number of periods (3D direct problems defined in Sec. 2).

4 Discussion

The two 3D approaches are now compared on a structure made of a finite array of periodically arranged lossy ellipsoidal patches defined by their relative permittivity $\varepsilon_{r,d} = 9 + 2i$, height $h = 1\,\mu m$, transverse and longitudinal radii $r_t = 5\,\mu m$ and $r_l = 1.5\,\mu m$, and period $d = 4\,\mu m$ as shown in Fig. 1. Number of patches is $N$ and the incident field is the fundamental mode labelled 1 in Fig. 2(a).

Figure 5 shows the transmission $T_N$ (blue curve, cf. Eq. 8) as a function of the number $N$ periods (scatterers). The yellow curve represents the coefficient $|t_1|^2$ (cf. Eq. (10)), the fraction of incident energy carried into mode 1 and remaining in this channel after crossing the modified waveguide segment containing the scatterers. This last curve lies below the green curve that represents the sum of the amplitudes transmitted into all 6 channels (or modes) shown in Fig. 2 of Sec. 3. Note that this numerical set up corresponds to Fig. 3 with $N = 4$.

Finally, one can correlate these results to the infinitely periodic structure and superimpose the last red curves that represents $T_1 e^{-2i\gamma''(N-1)d}$, the spatial damping of the mode with smallest propagation losses found using the modal approach detailed in Sec. 3 (the $T_1$ factor accounts
for the fact that this quantity is clearly physically undefined in absence of any obstacle for $N = 0$). The consistency between all these quantities is remarkable.

5 Conclusion

In conclusion, we present in this paper a general finite element frame for the study of discontinuous waveguides, from isolated discontinuities to fully periodic ones. A first method, adapted to a finite set of discontinuities allows to compute, given the modes of the invariant structure, the field scattered by the local discontinuity, all relevant energy related quantities, and the projection of the scattered field on the modes of the invariant structure (that is the elements of the transition scattering matrix).

When the modified region extends to infinity with periodic discontinuities, the relevant quantity is known the dispersion relation of the so formed structured waveguide. We showed that an adequate weak treatment of divergence condition allows to determine these modes with accuracy.

The two numerical models presented in this paper show great interest for the design of structured waveguides. Note that the methodology adopted for the direct problem is very general and can readily be applied to a large variety of guiding structure and geometry of objects located in the modified waveguide segment. Finally, open source models allowing to retrieve most of the results of this paper are provided.

This work will later be extended to the case where the input and output invariant structures mismatch using a couple mode-FE approach [8] to compute the relevant incident fields.
Acknowledgement

This research was supported by ANR Louise project, grant ANR-15-CE04-000164 of the French Agence Nationale de la Recherche. The authors would like to thank the developers of MUMPS [24], PETSc [25], SLEPc [26], Gmsh [19] and GetDP [20] for maintaining and making their respective libraries freely available. Finally, the authors acknowledge Sonia Fliss (INRIA POEMS) for fruitful discussions.

References

[1] J. Schwinger and D. S. Saxon, *Discontinuities in waveguides*. Gordon and Breach, 1968.

[2] L. Lewin, *Theory of waveguides*. Newnes-Butter-worths, 1975.

[3] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*. Artech House, Boston, 3 ed., 2005.

[4] A. Taflove, A. Oskooi, and S. G. Johnson, eds., *Advances in FDTD Computational Electrodynamics*. Photonics and Nanotechnology, Artech House, Boston, 2013.

[5] P. Lalanne and E. Silberstein, “Fourier-modal methods applied to waveguide computational problems,” *Optics Letters*, vol. 25, no. 15, pp. 1092–1094, 2000.

[6] G. Lecamp, J.-P. Hugonin, and P. Lalanne, “Theoretical and computational concepts for periodic optical waveguides,” *Optics express*, vol. 15, no. 18, pp. 11042–11060, 2007.

[7] V. Pagneux, N. Amir, and J. Kergomard, “A study of wave propagation in varying cross-section waveguides by modal decomposition. part i. theory and validation,” *The Journal of the Acoustical Society of America*, vol. 100, no. 4, pp. 2034–2048, 1996.

[8] A. Pelat, S. Felix, and V. Pagneux, “A coupled modal-finite element method for the wave propagation modeling in irregular open waveguides,” *The Journal of the Acoustical Society of America*, vol. 129, no. 3, pp. 1240–1249, 2011.

[9] J. Jin, *The Finite Element Method in Electromagnetics*. John Wiley & Sons Inc., 3rd ed., 2014.

[10] M. P. Bendsoe and O. Sigmund, *Topology Optimization*. Springer-Verlag, 2nd ed., 2004.

[11] A. Gutierrez-Arroyo, E. Baudet, L. Bodiou, J. Lemaitre, I. Hardy, F. Faijan, B. Bureau, V. Nazabal, and J. Charrier, “Optical characterization at 7.7 µm of an integrated platform based on chalcogenide waveguides for sensing applications in the mid-infrared,” *Opt. Express*, vol. 24, p. 23109, 2016.

[12] T. Nédélec, *Notions sur les techniques d’éléments finis, mathématiques et applications, n° 7*. Mathématiques & Applications, Ellipses, 2nd ed., 1991.

[13] F. Zolla, G. Renversez, A. Nicolet, B. Kuhlme, D. Felbacq, A. Argyros, and S. Leon-Saval, *Foundations of Photonic Crystal Fibres*. Imperial College Press, 2nd ed., 2012.
[14] G. Demésy, F. Zolla, A. Nicolet, and M. Commandré, “All-purpose finite element formulation for arbitrarily shaped crossed-gratings embedded in a multilayered stack,” JOSA A, vol. 27, no. 4, pp. 878–889, 2010.

[15] A. Snyder and J. Love, Optical Waveguide Theory Chapman and Hall, p. 500. New York, first ed., 1983.

[16] A. Nicolet, S. Guenneau, C. Geuzaine, and F. Zolla, “Modelling of electromagnetic waves in periodic media with finite elements,” Journal of Computational and Applied Mathematics, vol. 168, no. 1-2, pp. 321–329, 2004.

[17] T. Kuriakose, E. Baudet, T. Halenkovíc, M. M. Elsawy, P. Němec, V. Nazabal, G. Renversez, and M. Chauvet, “Measurement of ultrafast optical kerr effect of ge-sb-se chalcogenide slab waveguides by the beam self-trapping technique,” Opt. Comm., vol. 403, pp. 352 – 357, 2017.

[18] D. Chandler-Horowitz and P. M. Amirtharaj, “High-accuracy, midinfrared (450 cm$^{-1}$ $\leqslant \omega \leqslant 4000$ cm$^{-1}$) refractive index values of silicon,” Journal of Applied Physics, vol. 97, no. 12, p. 123526, 2005.

[19] C. Geuzaine and J. F. Remacle, “Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities,” International Journal for Numerical Methods in Engineering, vol. 79, no. 11, pp. 1309–1331, 2009.

[20] P. Dular, C. Geuzaine, F. Henrotte and W. Legros, “A general environment for the treatment of discrete problems and its application to the finite element method,” IEEE Transactions on Magnetics, vol. 34, no. 5, pp. 3395–3398, 1998.

[21] F. Zolla and R. Petit, “Method of fictitious sources as applied to the electromagnetic diffraction of a plane wave by a grating in conical diffraction mounts,” JOSA A, vol. 13, no. 4, pp. 796–802, 1996.

[22] J. D. Joannopoulos, R. Meade, and J. N. Winn, Photonic Crystals Molding the Flow of Light. Princeton University Press, 1995.

[23] C. Lackner, S. Meng, and P. Monk, “Determination of electromagnetic bloch variety in a medium with frequency-dependent coefficients,” Journal of Computational and Applied Mathematics, vol. 358, pp. 359 – 373, 2019.

[24] P. Amestoy, I. Duff, A. Guermouche, J. Koster, J.-Y. L’Excellent, and S. Pralet, Multifrontal Massively Parallel Solver, (MUMPS 4.8.4), Users’ guide. CERFACS, ENSEEIHT-IRIT, and INRIA, December 2008. http://mumps.enseeiht.fr and http://graal.ens-lyon.fr/MUMPS.

[25] S. Balay, K. Buschelman, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, B. F. Smith, and H. Zhang, PETSc Users Manual, 2007.

[26] V. Hernandez, J. E. Roman, and V. Vidal, “SLEPC: A scalable and flexible toolkit for the solution of eigenvalue problems,” ACM Trans. Math. Software, vol. 31, no. 3, pp. 351–362, 2005.