Transformation Optics PML and quasi-mode analysis: application to diffraction gratings

Benjamin Vial[a,b], André Nicolet[a], Frédéric Zolla[a], Guillaume Demésy[a], Mireille Commandré[a] and Stéphane Tisserand[b]

[a]Institut Fresnel UMR CNRS 6133, Aix-Marseille Universite, Ecole Centrale de Marseille, Campus de Saint-Jerôme, 13013 Marseille, France,
[b]Silios Technologies, France

Abstract. This paper presents the Perfectly Matched Layers (PMLs) in the framework of transformation optics as a complex-valued change of coordinates. PMLs provide the suitable operator extensions required for the leaky mode computation of open waveguides and the quasi-mode computation of scattering problems. Quasi-modes of diffraction gratings are considered here together with a numerical use of this spectral analysis.

Keywords: finite element method, quasi-modes, leaky modes, transformation optics, perfectly matched layer(PML), diffraction gratings.
PACS: 41.20.Jb, 42.25.Bs,78.20.Bh,42.79.Dj,02.70.Dh

PML and Transformation Optics

The introduction of Perfectly Matched Layers (PMLs) by Bérenger in 1994 [1] has been a major breakthrough to ensure Outgoing Wave Conditions (OWC) in the computation of open electromagnetic wave problems using domain methods such as the Finite Difference method and the Finite Element Method (FEM). PMLs have been soon revisited by Chew et al. [2] as a complex valued stretch of the coordinates. Transformation Optics (TO) has set up a general framework to deal with quite arbitrary changes of coordinates (including complex valued ones) in a very convenient way where the geometrical transformations are translated into equivalent material properties [3]. For instance, in an electromagnetic problem, if initial coordinates x_1,x_2,x_3 are transformed into new coordinates u_1,u_2,u_3, it is equivalent to transform the permittivity tensor using the formula :

$$\underline{\underline{\varepsilon'}} = \mathbf{J}^{-1}\underline{\underline{\varepsilon}}\mathbf{J}^{-T}det(\mathbf{J}) \tag{1}$$

where $\mathbf{J}$ is the Jacobian matrix associated to the change of coordinates ($J_{ij} = \frac{\partial x_i}{\partial u_j}$), $\mathbf{J}^{-1}$ its inverse, $\mathbf{J}^{-T}$ the transpose of its inverse, and a similar formula for the permeability μ. The interpretation of this equivalence principle is the following one: solve your electromagnetic problem (e.g. numerically) with the new material properties but just as if you were still in the original coordinate system x_1,x_2,x_3 (usually Cartesian) and you get the solution in the new u_1,u_2,u_3 system. Of course, the values of the electromagnetic field depend on the coordinate system but the translation from one system to the other is straightforward. Transformation optics is a unifying point of view for several applications and techniques: invisibility cloaking, perfect lenses, special geometries such as twisted structures [4], and PMLs. Indeed PMLs can be set up as a complex valued change of coordinates:

$$r'(r_c) = \int_0^{r_c} s_r(\rho)d\rho \tag{2}$$

where r' is a complex coordinate such that $\mathfrak{Re}(r') = r$ is the original coordinate (corresponding to the initial "physical" coordinate system). r' is expressed as a function of the new r_c coordinate. The function s_r is a complex valued function depending on a real variable. This relation is usually described in the integral form (2) because it is the derivative, given directly by s_r, that is explicitly involved in the Jacobian matrix. The subscript c indicates that r_c is the "complex" coordinate, however it is a real-valued parameter that can be manipulated as usual in the geometrical description of a numerical problem. The application of formula (1) provides the equivalent permittivity and permeability (complex valued tensors) corresponding to the PML. In practice, the change of coordinates is chosen to be the identity in the region of interest (where the fields have therefore directly their "physical" values) and the complex stretch is limited to a surrounding layer. The PML region is theoretically an open domain but the exponential decrease of the field allows a safe truncation at a finite distance.

Leaky Modes of Waveguides

If PMLs have been a dramatic progress in the finite element/finite difference analysis of open domain wave scattering problems, they are also fundamental tools in

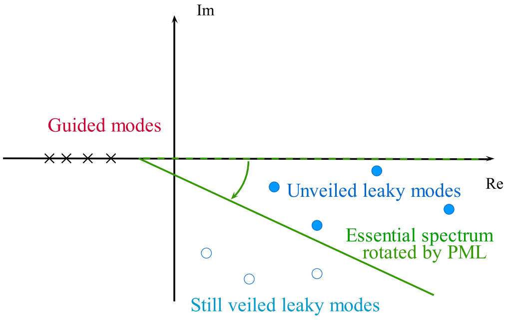

FIGURE 1. Guided modes, essential spectrum and leaky modes in an open waveguide.

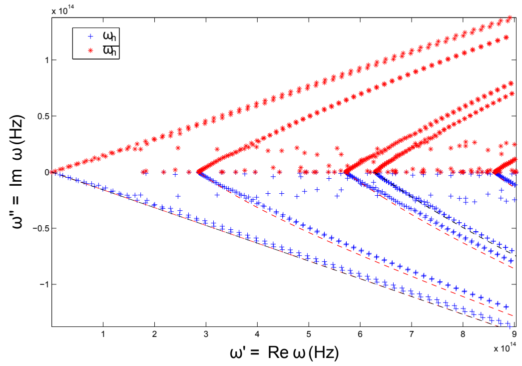

FIGURE 2. Quasi-modes of a grating with PML: "leaky modes" (individual $+$), essential spectrum (dashed lines) and its discrete numerical approximation ($+$ closed to dashed lines), and their complex conjugates ($*$ in upper half plane).

the numerical study of open dielectric waveguides. In some cases it is very important to determine leaky modes corresponding to complex propagation constant (quasi-modes). It can be shown that the corresponding EM eigenfields are not of finite energy and even increase exponentially towards infinity. In this case, PMLs provide an efficient tool to circumvent the difficulty. Fig. 1 shows the principle of the use of PMLs in spectral analysis. Consider an open waveguide (with non dissipative media). The spectrum is real valued and may contain discrete eigenvalues associated to guided modes but also a continuum called the essential spectrum [5] and corresponding to a real half line. The introduction of the PMLs rotates this essential spectrum in the complex plane (since the operator involved in the problem is now a non self-adjoint extension of the original self-adjoint operator). The effect is not only to turn the essential spectrum into complex values but it also unveils the leaky modes is the region swept by the rotation of this essential spectrum [6]. Leaky modes are discrete modes associated to a complex propagation constant (or frequency) and they are intrinsically associated to the open structure. Indeed, a correct choice of the PML allows to compute some of them (depending on the choice of the parameters of the PML) but their values do not depend on the particular PML. Fig. (1) corresponds to the case where s_r in equation (2) is a constant but for more general choices, the transformed essential spectrum may be a curve. This technique has been applied to compute the influence of the torsion of a microstructured optical fibre on the leaky modes and especially on the losses. Transformation optics has allowed a natural combination of helical coordinates and PMLs as a composition of the two coordinate transformations [7].

Spectral Analysis of Diffraction Gratings

Another interesting problem is the spectral analysis of diffraction gratings (periodic along one direction or bi-periodic along two directions). For spectral filtering applications, one should determine the line shape of the transmission or reflection spectra in order to fit the required features. To avoid the calculation of diffracted efficiencies for a wide range of wavelengths, resonances of the structures should be found. The computational domain is open and these resonances correspond to quasi-modes. Of course, there is no incident field in the spectral problem but the angle of incidence shows through the coefficient of quasi-periodicity in Floquet-Bloch conditions: the spectral problem is then labeled by this coefficient. In this case too, the quasi-modes are determined numerically using the FEM with PMLs [8]. We consider here the 2D case for the sake of simplicity but everything can be quite straightforwardly extended to the 3D case (and possibly with anisotropic materials) [9]. We define the following operator:

$$\mathscr{L}_{\xi,\chi} = \mathrm{div}(\xi\,\mathrm{grad}(u)) + k_0^2 \chi u \qquad (3)$$

In the p-polarisation case, $\xi = \varepsilon^{-1}$, $\chi = \mu$, and $u = H_z(x,y)$. The diffraction grating problem is defined by the material properties: ε and μ are uniform in an upper half-plane called the superstrate and in a lower half-plane called the substrate (but usually with a different medium from the superstrate). The horizontal band between the superstrate and the substrate, named the groove region, contains non-uniform ε and μ both periodic along this band. The diffraction grating is illuminated conventionally from above by a plane wave u_0 and the problem is to find u satisfying: $\mathscr{L}_{\xi,\chi}(u) = 0$ together with a diffracted field $u_d = u - u_0$ satisfying OWC and Floquet-Bloch quasi-periodic conditions. Placing PMLs in the superstrate and in the substrate allows to deal with OWC in the FEM. Nevertheless, in this problem, the scattering obstacle is of infinite extent since the substrate is different from the superstrate and, in this case, the equivalent sources necessary for the computation of the diffracted field are also of infinite extent. In order to circumvent this difficulty, we have set up a new method [9, 10]: consider ε_1 and μ_1 a distribution of material properties similar to the one of the initial problem but where the groove region has been replaced by the same material as in the superstrate. The new problem associated with this configuration (and still with incident field u_0) is very simple. It can be solved in a closed form and this solution is named u_1. The initial problem for u can be set up the following way: Define $u_{2d} = u - u_1$ and find;

$$\mathscr{L}_{\xi,\chi}(u_2^d) = -\mathscr{L}_{\xi,\chi}(u_1) \equiv \mathscr{S}_1 \qquad (4)$$

with u_2^d satisfying OWC and $\mathscr{S}_1$ an equivalent source computed in closed form and with its support contained within the groove region. This formulation also allows an analysis of the resonances of the gratings: find the (ω_n, v_n) such that:

$$\mathscr{M}_\xi(v_n) \equiv -\text{div}(\xi\,\text{grad}(v_n)) = \omega_n^2 \chi v_n / c^2 \qquad (5)$$

In the case of lossless materials, the operator is self-adjoint and the corresponding FEM matrices are Hermitian with only real eigenvalues. We have an open problem and we are interested in the quasi-modes corresponding to complex eigenvalues ω_n. Here again, *the PMLs provide the requested extension of $\mathscr{M}_\xi$ to a suitable non self-adjoint operator $\mathscr{M}_\xi^{PML}$*. Fig. 2 shows the eigenvalues computed for a simple grating made of slits in a *Ge* layer with an air superstrate and a *ZnS* substrate. Even if there is no incident field in the modal problem, there is a reminiscence of the incidence angle of the plane wave in the choice of the Floquet-Bloch conditions: to a particular grating corresponds indeed a one-parameter family of problem depending on the quasi-periodic condition. On the Fig. 2, the "leaky" modes appear in a band along the real axis and they do not depend on the choice of the PMLs but for their unveiling while the modes corresponding to the discretization of the essential spectrum are close to the theoretical curves (dashed curves), both depending on the particular choice of the PMLs. The knowledge of the modes provide a very useful frequency characterization of the diffraction grating that can be used for instance in the design of filters. The information contained in the eigenfields v_n is also extremely useful because it allows an efficient computation of the solutions of scattering problems. Since the considered operator $\mathscr{M}_\xi^{PML}$ is not self-adjoint, its eigenfields v_n are not orthogonal but if you consider the adjoint $\overline{\mathscr{M}_\xi^{PML}}$, its eigenvalues are the complex conjugates $\overline{\omega_n}$ of the ω_n and its eigenfields w_n form a bi-orthogonal system with the v_n with respect to the following scalar product: $\int_{\mathbb{R}^2} \chi v_n \overline{w_m} dx\,dy = \delta_{nm}$ (after normalization). In practice, if the FEM matrix associated to $\mathscr{M}_\xi^{PML}$ is A, the one corresponding to $\overline{\mathscr{M}_\xi^{PML}}$ is $\overline{A}^T$, the complex conjugate transpose, and the w_n are easily obtained. Given an incident field, the corresponding equivalent source $\mathscr{S}_1$ is first computed (see Eq. (4)) and the solution to the scattering problem can be computed as $u \simeq \sum_{n=1}^N P_n(\omega) v_n(x,y)$ with the coefficients

$$P_n(\omega) = \frac{c^2}{\omega_n^2 - \omega^2} \int_\Omega \mathscr{S}_1 \overline{w_n} dx\,dy \qquad (6)$$

where Ω is the support of $\mathscr{S}_1$ contained in the groove region. Theoretically, the sum extends to infinity (and is even an integral for the essential spectrum [5]) but in practice only a finite number N of modes is considered. Fig. 3 shows the reconstruction of a scattered field using this method with 500 quasi-modes.

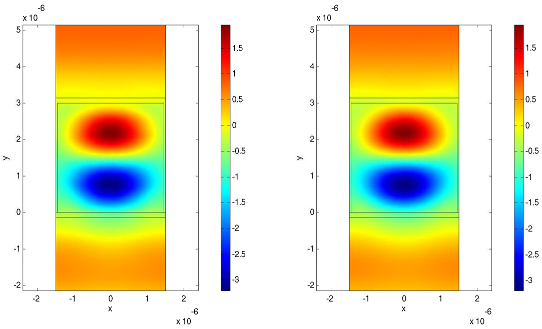

FIGURE 3. The scattered field computed using the modal method with 500 eigenvalues (left) is compared with the direct computation of the scattering problem (right). The maximum discrepancy is locally of the order of a few percent.

REFERENCES

1. J.-P. Berenger, Journal of Computational Physics **114**, 185 (1994), ISSN 0021-9991.
2. W. Chew and W. Weedon, Microwave and optical technology letters **7**, 599 (1994).
3. A. Nicolet, F. Zolla, Y. Agha, and S. Guenneau, COMPEL: Int J for Computation and Maths. in Electrical and Electronic Eng. **27**, 806 (2008).
4. A. Nicolet, F. Zolla, and S. Guenneau, The European Physical Journal Applied Physics **28**, 153 (2004).
5. G. Hanson and A. Yakovlev, *Operator theory for electromagnetics: an introduction* (Springer Verlag, 2002).
6. B. Goursaud, Ph.D. thesis (2010).
7. A. Nicolet, F. Zolla, Y. Ould Agha, and S. Guenneau, Waves in Random and Complex Media p. 559 (2007).
8. B. Vial, M. Commandré, F. Zolla, A. Nicolet, and S. Tisserand, in *AIP Conference Proceedings* (2011), vol. 1398.
9. G. Demésy, F. Zolla, A. Nicolet, and M. Commandré, J. Opt. Soc. Am. A **27**, 878 (2010).
10. G. Demésy, F. Zolla, A. Nicolet, M. Commandré, and C. Fossati, Opt. Express **15**, 18089 (2007).