Frequency Dependence of the Constitutive Parameters of Causal Perfectly Matched Anisotropic Absorbers

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Abstract— **Perfectly matched layers (PML's), which are employed for mesh truncation in the finite-difference time-domain (FDTD) or in finite element methods (FEM's), can be realized by artificial anisotropic materials with properly chosen permittivity and permeability tensors. The tensor constitutive parameters must satisfy the Kramers-Kronig relationships, so that the law of causality holds. These relations are used to relate the real and imaginary parts of the constitutive parameters of the PML media to deduce the asymptotic behaviors of these parameters at low and high frequencies.**

I. Introduction

The PERFECTLY matched layer (PML) concept, introduced by Berenger [1], is an efficient method for truncating the unbounded spatial domain in electromagnetic radiation and scattering problems. Although the PML approach was originally introduced in the context of the finite-difference time-domain (FDTD) method [1], it has been found useful [2] in mesh truncation in the finite element method (FEM) as well. It has recently been verified that artificial anisotropic media, with properly designed permittivity and permeability tensors, can absorb electromagnetic waves irrespective of their frequency and angle of incidence [3]. This idea has been generalized for designing conformal PML's, which provides an efficient FEM mesh truncation, especially for problems involving electrically large antennas and scatterers [4], [5].

In this letter, we report the results of an investigation of the causality issues in PML's and deduce their low- and high-frequency asymptotic behaviors. Although the PML's are artificial anisotropic media introduced primarily for the purpose of mesh truncation in finite methods, it is necessary to investigate the dispersion relations satisfied by the constitutive parameters of this medium to ensure that they satisfy the conditions of linearity, time-invariance, and causality. The principal objective of this letter, therefore, is to discuss the conditions that should be taken into account in designing the permittivity and permeability tensors of the PML media.

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II. Constitutive Relations in PML Media

In [3], it has been shown that PML's can be realized as anisotropic media that satisfies the following constitutive relations:

$$\vec{D}(\omega) = \bar{\bar{\varepsilon}}(\omega)\vec{E}(\omega) \quad \vec{B}(\omega) = \bar{\bar{\mu}}(\omega)\vec{H}(\omega) \tag{1}$$

where ω is the angular frequency and the permittivity and permeability tensors, $\bar{\bar{\varepsilon}}(\omega)$ and $\bar{\bar{\mu}}(\omega)$ are defined by

$$\bar{\bar{\varepsilon}}(\omega) = \varepsilon_0[\Lambda](\omega) \quad \bar{\bar{\mu}}(\omega) = \mu_0[\Lambda](\omega). \tag{2}$$

In (2), $[\Lambda](\omega)$ is a 3×3 tensor, whose entries must be chosen such that an incident electromagnetic wave is absorbed by the PML half-space without any reflection, and the transmitted wave in the PML is attenuated in the direction normal to the free space-PML interface. In [3], a planar interface between the free space and PML absorber has been investigated for the cartesian coordinate system (x, y, z), where the z-variable is normal to the interface. It has been shown that the tensor $[\Lambda](\omega)$ must be of the form

$$[\Lambda](\omega) = \begin{bmatrix} a(\omega) & 0 & 0 \\ 0 & a(\omega) & 0 \\ 0 & 0 & 1/a(\omega) \end{bmatrix} \tag{3}$$

where the complex parameter $a(\omega)$ is defined as

$$a(\omega) = 1 - j\frac{\sigma}{\omega\varepsilon_0}. \tag{4}$$

For a curved interface between free space and the PML, a local coordinate system (ξ, η, ν) can be defined at any point P on the interface, such that the (ξ, η)-plane is tangent to the curved surface at P and ν is the normal direction along which the wave transmitted should attenuate. To realize a PML medium, $[\Lambda]_{(\xi,\eta,\nu)}(\omega)$, which is the representation of $[\Lambda](\omega)$ in the local coordinate system, must still have the form [4]

$$[\Lambda]_{(\xi,\eta,\nu)}(\omega) = \begin{bmatrix} a(\omega) & 0 & 0 \\ 0 & a(\omega) & 0 \\ 0 & 0 & 1/a(\omega) \end{bmatrix} \tag{5}$$

where $a(\omega) = 1 - j\frac{\sigma(\nu)}{\omega\varepsilon_0}$. For this case, σ is no longer a constant, but is a nondecreasing function of ν, such that $\sigma(0) = 0$. The representation of $[\Lambda](\omega)$ in the global (x, y, z) coordinate system, reads

$$[\Lambda](\omega) = a(\omega)[\Lambda]_1 + \frac{1}{a(\omega)}[\Lambda]_2 \tag{6}$$

where $[\Lambda]_1$ and $[\Lambda]_2$ are tensors that are functions of the space coordinates, but they are independent of ω. The coefficients $a(\omega)$ and $1/a(\omega)$ determine the frequency dependence of $[\Lambda](\omega)$. In FEM applications, the solutions are obtained at a single frequency and, hence, the approach developed so far, is totally valid. However, the variation of $a(\omega)$ (and $1/a(\omega)$) over the entire spectrum [i.e., for $\omega \in (-\infty, \infty)$] cannot be defined arbitrarily. As shown in the next section, the real and imaginary parts of $a(\omega)$ are not independent and they can be determined from each other in a unique way.

III. Causality and Dispersion Relations in PML Media

Let us consider the constitutive relationship $\vec{D}(\omega) = \bar{\bar{\varepsilon}}(\omega)\vec{E}(\omega)$. This relationship can be interpreted as one that relates the input and output of a linear, time-invariant system, whose transfer function matrix is $\varepsilon_0[\Lambda](\omega)$. The matrix $[\Lambda](\omega)$ (which is a diagonal matrix in a local coordinate system), must satisfy [6]

1) $$[\Lambda](\omega) = [\Lambda]^*(-\omega) \tag{7}$$

   where * denotes complex conjugation.

2) $$\mathrm{Re}([\Lambda](\omega) - I) = \frac{2}{\pi} P \int_0^\infty \frac{x}{x^2 - \omega^2} \mathrm{Im}([\Lambda](x)) dx \tag{8}$$

   and

   $$\mathrm{Im}([\Lambda](\omega)) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{1}{x^2 - \omega^2} \mathrm{Re}([\Lambda](x) - I) dx \tag{9}$$

   where I is the identity matrix and P denotes the Cauchy principal value.

The condition (7) arises from the fact that both $\vec{E}(t)$ and $\vec{D}(t)$, which are inverse Fourier transforms of $\vec{E}(\omega)$ and $\vec{D}(\omega)$, respectively, are real signals. Equations (8) and (9) are known as Kramers-Kronig relations, and they must be satisfied if the system is to be causal. Specifically, this means that $\vec{D}(t)$ depends only on $\vec{E}(t')$ if the time t' precedes t. Another important consequence of (8) and (9) is that the real and imaginary parts of the tensor $[\Lambda](\omega)$ are related to each other, i.e., they are not independent. Since the frequency dependence of $[\Lambda](\omega)$ is determined by $a(\omega)$ (and $1/a(\omega)$), the conditions (7) and (8) must be satisfied by these functions.

Let $a(\omega) = a_r(\omega) + j a_i(\omega)$. Condition (7) implies that $a_r(\omega)$ and $a_i(\omega)$ are even and odd functions of ω, respectively. Thus, for $a(\omega)$, the Kramers-Kronig relations can be written as

$$a_r(\omega) - 1 = \frac{2}{\pi} P \int_0^\infty \frac{x a_i(x)}{x^2 - \omega^2} dx \tag{10}$$

$$a_i(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{a_r(x) - 1}{x^2 - \omega^2} dx. \tag{11}$$

An important consequence of (11) is that if $a_r(\omega) = 1$ for $\omega \in [0, \infty)$, then $a_i(\omega)$ must vanish for $\omega \in [0, \infty)$, which is consistent with the fact that for a dispersionless medium there can be no absorption. It can be seen from (10) and (11) that there can be dispersion only if the medium has some absorption. Hence, it is impossible to realize a causal PML medium by choosing $\mathrm{Re}(a(\omega))$ as unity over the entire frequency spectrum.

Let us now discuss how $a(\omega)$ can be defined properly, such that conditions (10) and (11) are satisfied. We postulate the frequency dependence of $a(\omega)$ to be

$$a(\omega) = 1 + \frac{f(x,y,z)}{1 + j\alpha\omega} \tag{12}$$

where α is a constant and f is a function of position such that it reduces to zero at the free space–PML interface and is a nondecreasing function in the direction normal to the boundary. At an arbitrary fixed point (x_0, y_0, z_0) within the PML region, let $f(x_0, y_0, z_0) = \beta$. Then, at that point, $a(\omega)$ can be written as

$$a(\omega) = 1 + \frac{\beta}{1 + j\alpha\omega}. \tag{13}$$

It is straightforward to verify that $a(\omega)$ satisfies (10) and (11), owing to the special form of the ω dependence [6]. Now, let us consider the term $1/a(\omega)$, which can be written as

$$\frac{1}{a(\omega)} = 1 - \frac{\beta}{(1+\beta) + j\alpha\omega}. \tag{14}$$

It is also possible to show that (14) satisfies the Kramers-Kronig relations. Hence, the tensor $[\Lambda](\omega)$, which is defined in terms of $a(\omega)$ and $1/a(\omega)$, can be used to realize a causal PML medium. Since $[\Lambda](\omega)$ appears in the expressions of both $\bar{\bar{\varepsilon}}(\omega)$ and $\bar{\bar{\mu}}(\omega)$, the electromagnetic wave propagation within the PML obeys the law of causality if the expression of $a(\omega)$ is given by (12).

Finally, let us consider the low and high frequency limits of $a(\omega)$. Equation (12) can be rewritten as

$$a(\omega) = \frac{1 + \alpha^2\omega^2 + f(x,y,z)}{1 + \alpha^2\omega^2} - j\frac{\alpha\omega f(x,y,z)}{1 + \alpha^2\omega^2} \tag{15}$$

1) Low-frequency limit: If $\alpha\omega \ll 1$, (15) becomes

$$a(\omega) \approx 1 + f(x,y,z). \tag{16}$$

2) High-frequency limit: If $\alpha\omega \gg 1$, (15) becomes

$$a(\omega) \approx 1 - j\frac{f(x,y,z)}{\alpha\omega}. \tag{17}$$

It is interesting to note that $a(\omega)$, given by (17), has been used in PML applications in FEM or FDTD formulations. Therefore, it is not surprising to find that there are difficulties [7] associated with the performance of the PML chosen as above as the frequency of operation becomes very low.

IV. Conclusion

The tensor constitutive parameters of a perfectly matched anisotropic medium must satisfy certain conditions, such that the linear, time-invariant dynamical system governed by the constitutive relations is causal. This, in turn, introduces certain restrictions on the material properties of the PML medium. It is possible, however, to express the frequency dependence of the parameters such that not only they satisfy the causality condition, but also provide expressions for limiting cases of low and high frequencies.

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