ENHANCING THE PML ABC FOR THE WAVE EQUATION

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Abstract: The dynamics of wave propagation and interactions in general media is described either by the system of Maxwell's equations, or by the wave equation. This paper focuses on problems modeled by the wave equation, with one or more boundaries at infinity. The computational domain is truncated by perfectly matched layer (PML) absorbing boundary conditions (ABCs) modified specifically for wave equation applications. An enhanced PML performance with reduced PML thickness is achieved within the whole frequency band of excitation in the presence of both evanescent and propagating fields.

INTRODUCTION

In time-domain electromagnetics, apart from the Finite-Difference Time-Domain (FDTD) method [1], an attractive new alternative is using the wave equation (WE), as in the time-domain wave-potential (TDWP) method [2]. It employs only two scalar quantities, the magnitudes of two collinear vector potentials $(A, F)\hat{\xi}$, to analyze an EM problem in a region of distinguished axis $\hat{\xi}$ parallel to the vector potentials. Their propagation is governed by the 3-D scalar WE. Both FDTD and TDWP methods require reliable and efficient ABCs for boundaries at infinity. Berenger's perfectly matched layer (PML) ABC [3] for the FDTD method, was recently modified for WE applications [4]. The effort to improve further the performance of PML ABCs (see e.g. [5] -[8]) continues and it is necessary, since even small numerical reflection in the time-domain response degrades the frequency-domain results, on which the CAD accuracy depends.

The overall performance of a PML absorber depends on the combined and interdependent influence of all its variables: the conductivity σ_i ($i = x, y, z$), the loss factor α_i, the reflection coefficient R_0 and its thickness δ_i. Recently it was shown ([4], [8]) that if the conductivity and the loss factor grow at different exponent rates (which adds a new degree of freedom in their definition), the PML performance improves over the whole frequency band. In [4], the conductivity is proposed to grow faster than the loss factor for the TDWP method. In [8], PML enhancement is achieved within Yee's FDTD method. There, it is shown that in the presence of strong evanescent fields, the loss factor should grow faster than the conductivity.

In this work we show that in the presence of evanescent and propagating fields, similar enhancement of the PML performance can be achieved in WE applications, without any increase in the computational load. In fact, greatly reduced PML thickness is used in comparison with the quoted in the literature, even when sources and/or discontinuities are located at one or two spatial steps from the PML interface.

Firstly, half-a-cell displacement of the PML interface is proposed, so that any PML interface passes through the position of the vector component in all directions. Such a displacement is specific for WE applications and may require modifications of Dirichlet or Neumann BCs at the terminating walls. Secondly, the performance of this enhanced PML (EPML) ABC, applied within the TDWP algorithm, is compared with Berenger's PML [3], the modified PML (MPML) [5], and the generalized PML (GPML) [6]. We demonstrate that both in 3-D open problems and in guided-wave problems, the proposed EPML offers lower reflection levels in the entire frequency spectrum. Finally, the influence of the difference β between the growth rates of the PML conductivity and the PML loss factor on the overall PML performance is discussed. Based on extensive numerical experiments, practical recommendations for the values of β are offered.

THEORY

Berenger's PML [3] added a new degree of freedom to the FDTD algorithm to improve the absorption of *propagating* waves. To accelerate the attenuation rate of *evanescent* modes, B. Chen *et al.* [5] proposed the MPML, where another degree of freedom is added by including a PML loss factor α_i. In [4], a PML ABC is developed for the 3-D scalar WE, although a thick (16-layer) absorber is used. There, the PML conductivity and loss factor grow at different exponent rates. Thus a new degree of freedom in their definition is added. The PML conductivity profile σ_i grows at higher rate than that of the PML loss factor α_i:

$$\sigma_i(\rho) = \sigma_{\max} \left(\rho_i / \delta_i \right)^{n+\beta} ; \quad \beta \in (0,3], \ i = x, y, z \tag{1}$$

while the PML loss factor α_i proposed by B. Chen *et al.* [5] remains:

$$\alpha_i(\rho) = 1 + \varepsilon_{\max} \left(\rho_i / \delta_i \right)^{n} ; \quad i = x, y, z \tag{2}$$

In [4], β is positive and no evanescent fields are considered. In this work, we propose the use of negative values of β, when strong evanescent fields are present. In (1), the parameter σ_{max} controls the attenuation of propagating waves: $\sigma_{max} = -[(n + \beta + 1)\varepsilon_0 \cdot c \cdot \ln R_0]/[2\delta_i]$. Therein, R_0 is the reflection coefficient; δ_i is the PML thickness in the i-direction ; ρ_i is the depth in PML, $0 \le \rho_i \le \delta_i$; ε_{max} is a parameter regulating the evanescent-mode-attenuation; n is the rate of growth; β is a user-defined difference in the exponent rates; ε_0 is the permittivity of vacuum; and c is the speed of light.

Two modifications of the PML ABC implementation for WE applications are proposed.

Firstly, the location of the interface plane between the internal computational domain and PML is proposed to pass through the position of the calculated variable *in all directions*. In the TDWP method, the positions of the magnetic vector potential components coincide with the positions of the electric field components within the conventional Yee's cell, see [4]. Thus, for example, for the x-component of the magnetic vector potential, $\vec{A} = \hat{x}A_x$, the interface position in the x-direction will pass through the middle of the numerical cell in the x-direction. Secondly, the above modification may require change of the location of the terminating perfect-electric-conductor (PEC) walls, e.g., the half-a-cell displacement in the x-direction for A_x requires the terminating PEC wall in the x-direction (Neumann BC) to be implemented as:

$$\partial A_x / \partial x \big|_{x=x_{max}} = 0 \ \Rightarrow \ A_x(x_{max}) = \left[4A_x(x_{max} - \triangle x) - A_x(x_{max} - 2\triangle x)\right]/3. \tag{3}$$

At the tangential PEC boundary planes (Dirichlet BC) in the y- and z-directions, the vanishing A_x remain:

$$A_x\big|_{y=y_{max}} = 0 \ \text{ and } \ A_x\big|_{z=z_{max}} = 0 \tag{4}$$

Corresponding expressions hold at $x = x_{min}$, $y = y_{min}$, and $z = z_{min}$. Off-grid perfect magnetic conductor (PMC) walls for $\vec{A}$, and off-grid PEC/PMC walls for the electric vector potential $\vec{F}$ are defined similarly.

NUMERICAL RESULTS AND DISCUSSION

To illustrate the performance of the proposed EPML ABC for WE applications, an infinitesimal dipole in open space and a rectangular waveguide are modeled by the TDWP method. The reflection magnitude is estimated using the ratio of the reflected and incident wave-potential component g_i, which has been excited:

$$R = \left| \mathcal{F}\{g_i^{refl}\} / \mathcal{F}\{g_i^{inc}\} \right| \tag{5}$$

Herein, $\mathcal{F}$ denotes Fourier transform of the respective time-domain wave-potential component.

The infinitesimal dipole in open space is modeled in a computational domain of ($150\triangle x, 150\triangle y, 150\triangle z$), where $\triangle x = \triangle y = \triangle z = 1$ mm. The magnetic potential $\vec{A} = \hat{x}A_x$ is excited by the x-directed current of the dipole, which is a Gaussian pulse in time. Fig. 1 is a comparison of the proposed EPML ($\beta = 2$) with Berenger's PML [3], the GPML [6], and the MPML [5]. The PML interfaces and PEC terminating walls of all four PMLs have locations modified as described above. A long simulation time is used so that not only the direct reflections from the PMLs but also the interferences from the reflections are included. Note that the results in Fig. 1 are for six-layer PML ABCs and the reflection level is (i) an order of magnitude lower than that for the sixteen-layer PML ABC reported in [4], (ii) below 0.01 % *in the whole frequency band* of excitation. This is an unprecedented reduction in the PML thickness.

The hollow rectangular waveguide of standard cross section 30 mm by 15 mm (cutoff frequency 5 GHz) is excited by a current sheet, which is a sinusoidal wave of frequency 7 GHz modulated by BHW function [9], so that its frequency content is from 0 to 14 GHz. Uniform mesh with $\triangle x = 1.25$ mm is used. The excitation plane is 40 steps after the front-end PML thick 30 cells. To properly measure the evanescent wave attenuation, the sampling location is only one spatial step after the excitation plane. The eight-cell thick back-end PML is located one spatial step after the sampling plane. De-embedding with longer waveguide is performed. Very long simulation time (of the order of 10^5 time steps) is necessary as noted in [10]. Because of the presence of evanescent modes, a negative value of the parameter β is proposed. Fig. 2 shows a comparison of the proposed EPML ($\beta = -1$) with Berenger's PML, the GPML, and the MPML. The reflection from the eight-cell thick EPML is comparable with the reflections from sixteen-cell thick Berenger's PML and GPML [6], [10]. We note that increasing ε_{max} improves the evanescent wave attenuation but leads to higher numerical reflections after the cutoff frequency and especially towards the high end of the frequency band. This is a common drawback of all PMLs with $\alpha_i > 1$. On the other hand, decreasing R_0 has exactly the opposite effect. The negative value of β balances these competing influences and ensures low numerical reflections in the entire frequency band of the excitation.
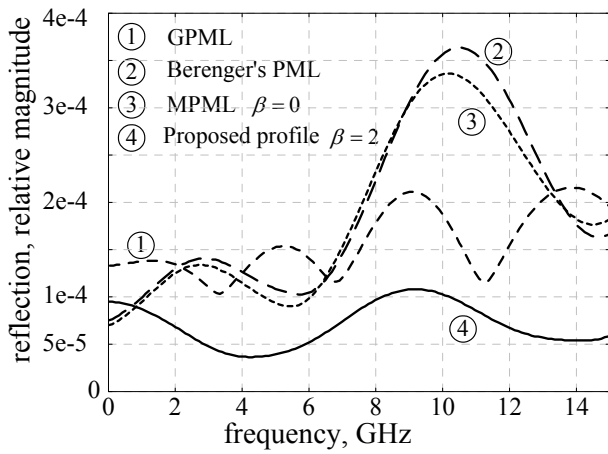
Fig. 1. Infinitesimal dipole in open space. Common PML parameters: $N_{PML} = 6$, $R_0 = 10^{-4}$, $n = 2$, $\varepsilon_{max} = 1$. (Only in Berenger's PML $\varepsilon_{max} = 0$.)
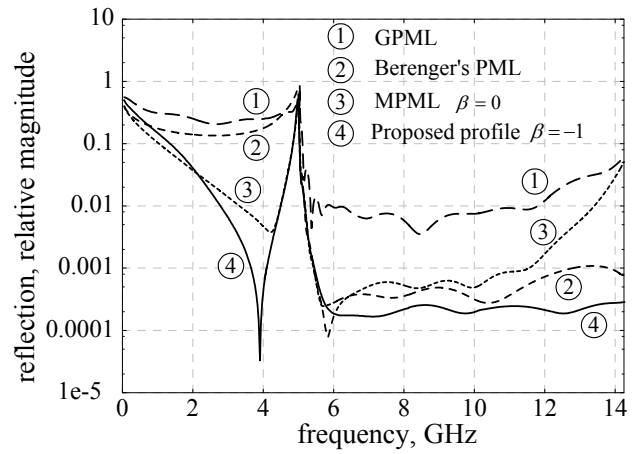
Fig. 2. Evanescent and propagating waves in waveguide. Common PML parameters: $N_{PML} = 8$, $R_0 = 10^{-5}$, $n = 3$, $\varepsilon_{max} = 8$. (Only in Berenger's PML $\varepsilon_{max} = 0$.)

CONCLUSION

For WE applications, half-a-cell displacement of the interface with the PML absorber is proposed so that it passes through the variable positions in all directions. This may require modified Neumann and/or Dirichlet BC at the terminating PEC walls. The combination of such PML interface displacement with different growth rates of the PML conductivity and PML loss factor is shown to enhance significantly the PML performance. In all major types of problems, in the presence of propagating and evanescent fields, an EPML thickness as low as 6 to 8 cells ensures reflections below 0.1 % in the whole frequency band of excitation. Where little or no evanescent energy is present, the natural choice is the PML conductivity to increase faster than the PML loss factor, i.e. $\beta > 0$. When both evanescent and propagating modes are present, a negative value of β compensates for the opposing influences of the other PML parameters. The best PML performance is usually obtained when $\beta = \pm 1$ or ± 2 in the TDWP model, and $\beta = \pm 1$ in Yee's FDTD model. Although examples only with the TDWP method are shown, it should be noted that the proposed EPML is applicable to any wave equation regardless of its specific variable.

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