Absorbing Boundary Conditions for Adjoint Problems in the Design Sensitivity Analysis With the FDTD Method

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***Abstract*—In this paper, absorbing boundary conditions (ABCs) for adjoint problems with a backward time variable are derived from first principles. It is shown that all single-layer ABCs for the adjoint backward time problem, which are based on the one-way wave equation, have the same form as for the original forward time problem. In the case of the adjoint perfectly matched layer (PML) ABC, the signs before the spatial derivatives are opposite to those in the PML ABC of the original forward time problem. To verify the theoretical findings, the numerical reflections from the adjoint ABCs are investigated in a microstrip-line example. The reflections from the ABCs of the forward- and backward time schemes are shown to be identical for the same type of ABCs.**

***Index Terms*—Absorbing boundary conditions (ABCs), adjoint problems, design sensitivity analysis, finite-difference time-domain (FDTD) method, perfectly matched layer (PML).**

I. Introduction

RECENTLY, an adjoint variable technique with the finite-difference time-domain (FDTD) method was proposed for the design sensitivity analysis of high-frequency structures [1], [2]. The adjoint electric- and magnetic-field vectors are shown to satisfy a set of coupled Maxwellian curl equations subject to homogeneous terminal value conditions. Therefore, a backward time variable is introduced $\tau = T - t$, where t is the forward time variable and T is the time at which the terminal conditions are imposed. The sensitivity information is used to perform the optimal shape design of a given structure. To solve the original and the adjoint Maxwell equations, absorbing boundary conditions (ABCs) are needed.

A direct modification of existing ABCs, developed for the original forward time scheme, as it is done in [1] and [2], might lead to incorrect results. There, the backward time variable is substituted in the perfectly matched layer (PML) equations pertinent to the forward time problem. Thus, the sign before the derivative with respect to the backward time variable changes. Consequently, an artificial choice of nonphysical negative PML conductivities is made to overcome the induced positive exponential amplitude growth in the so-defined PML medium.

In this paper, we show one possible way to derive various ABCs for adjoint problems with the backward time variable from first principles. We consider the PML ABC, as well as single-layer ABCs based on the one-way wave equation (WE).

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Firstly, we show that, for the adjoint PML ABC, only the sign before the spatial derivatives is opposite to that in the PML ABC of the original forward time problem. Secondly, we show that all single-layer ABC equations for the adjoint problem have the same form as the corresponding ones for the original problem despite the reversed time. From a physical point-of-view, this result is not surprising since these ABCs are *local* in nature. At the same time, the waves at the outer boundaries of the computational domain are *locally outgoing* in the respective coordinate systems both with forward- and backward time stepping.

II. Theory

A. Derivation of the PML ABC for the Adjoint Problem

Consider the adjoint problem for the backward time scheme [1], [2]

$$\begin{aligned} \nabla \times \vec{\bar{\lambda}}^E &= \mu \frac{\partial \vec{\bar{\lambda}}^H}{\partial \tau} \\ \nabla \times \vec{\bar{\lambda}}^H &= -\varepsilon \frac{\partial \vec{\bar{\lambda}}^E}{\partial \tau} + \vec{\bar{J}}^{\lambda}_{\mathrm{FDTD}}(T-\tau) \end{aligned} \quad (1)$$

where the backward time variable $\tau = T - t$ starts at the end of the fixed final time T for the optimal shape design problem. $\vec{\bar{J}}^{\lambda}_{\mathrm{FDTD}}(T-\tau)$ is the time-reversed pseudoelectric current density; $\vec{\bar{\lambda}}^E$ and $\vec{\bar{\lambda}}^H$ are the time-reversed adjoint electric- and magnetic-field intensity vectors. The bar above the variables denotes that they are functions of the backward time τ. Equations (1) are subject to the homogeneous terminal conditions (initial conditions with respect to τ)

$$\begin{aligned} \vec{\lambda}^E(t=T) &= \vec{\bar{\lambda}}^E(\tau=0) = 0 \\ \vec{\lambda}^H(t=T) &= \vec{\bar{\lambda}}^H(\tau=0) = 0. \end{aligned} \quad (2)$$

For the backward time adjoint equations, one can use any of the methods to define a corresponding PML medium, e.g., the stretched coordinate approach [3]. In [3], the stretched curl operator is defined as

$$\nabla_s \times = \left(\frac{1}{s_x}\frac{\partial}{\partial x}\hat{x} + \frac{1}{s_y}\frac{\partial}{\partial y}\hat{y} + \frac{1}{s_z}\frac{\partial}{\partial z}\hat{z} \right) \times \quad (3)$$

where the stretching variables are $s_\xi = \alpha_\xi + \sigma_\xi/(j\omega\varepsilon)$, $\xi = x, y, z$. Note that, in the original Berenger's PML [4], $\alpha_\xi = 1$, $\xi = x, y, z$. Later, Chen *et al.* [5] showed that the PML loss factor $\alpha_\xi > 1$ accelerates the evanescent wave absorption. In the PML medium, the requirement for a reflectionless transmission

$\sigma/\varepsilon = \sigma^m/\mu$ holds [4], where σ and σ^m are the PML electric and magnetic conductivities.

The general procedure to the definition of the PML medium given below follows the method outlined in [6]. There, the PML equations are derived for applications with the forward time WE. What makes this procedure generally applicable to any time-domain partial differential equations is the initial step of mapping them into the frequency domain where the PML derivations are made. We now apply this approach to the adjoint system of Maxwell's equations.

Firstly, the time-domain equations (1) are mapped into the frequency domain. The modified curl operator $\nabla_s\times$ is then applied as follows:

$$\nabla_s \times \vec{\overline{\lambda}}_\omega^E = j\omega\mu\vec{\overline{\lambda}}_\omega^H \quad \nabla_s \times \vec{\overline{\lambda}}_\omega^H = -j\omega\varepsilon\vec{\overline{\lambda}}_\omega^E \tag{4}$$

where the subscript ω is used to distinguish the adjoint electric- and magnetic-field vectors in the frequency domain from their time-domain counterparts in (1). The current term has been omitted, as sources are unlikely to exist in the PML. For brevity, the derivations for the x-components of the adjoint PML equations only are given hereafter. The x-components of (4) are

$$\begin{aligned} j\omega\varepsilon\overline{\lambda}_{\omega_x}^E &= -\left(\frac{1}{s_y}\frac{\partial\overline{\lambda}_{\omega_z}^H}{\partial y} - \frac{1}{s_z}\frac{\partial\overline{\lambda}_{\omega_y}^H}{\partial z}\right) \\ j\omega\mu\overline{\lambda}_{\omega_x}^H &= \left(\frac{1}{s_y}\frac{\partial\overline{\lambda}_{\omega_z}^E}{\partial y} - \frac{1}{s_z}\frac{\partial\overline{\lambda}_{\omega_y}^E}{\partial z}\right). \end{aligned} \tag{5}$$

The equations in (5) are split so that each subcomponent depends on one spatial derivative. The stretching variables and reflectionless transmission relation are then applied. Thus, the frequency-domain adjoint PML ABCs are obtained as

$$\begin{aligned} (j\omega\varepsilon\alpha_y + \sigma_y)\overline{\lambda}_{\omega_{xy}}^E &= -\frac{\partial\left(\overline{\lambda}_{\omega_{zx}}^H + \overline{\lambda}_{\omega_{zy}}^H\right)}{\partial y} \\ (j\omega\mu\alpha_y + \sigma_y^m)\overline{\lambda}_{\omega_{xy}}^H &= \frac{\partial\left(\overline{\lambda}_{\omega_{zx}}^E + \overline{\lambda}_{\omega_{zy}}^E\right)}{\partial y} \\ (j\omega\varepsilon\alpha_z + \sigma_z)\overline{\lambda}_{\omega_{xz}}^E &= \frac{\partial\left(\overline{\lambda}_{\omega_{yx}}^H + \overline{\lambda}_{\omega_{yz}}^H\right)}{\partial z} \\ (j\omega\mu\alpha_z + \sigma_z^m)\overline{\lambda}_{\omega_{xz}}^H &= -\frac{\partial\left(\overline{\lambda}_{\omega_{yx}}^E + \overline{\lambda}_{\omega_{yz}}^E\right)}{\partial z}. \end{aligned} \tag{6}$$

The last step is to map back the 12 PML equations into the time domain

$$\begin{aligned} \varepsilon\alpha_y\frac{\partial\overline{\lambda}_{xy}^E}{\partial\tau} + \sigma_y\overline{\lambda}_{xy}^E &= -\frac{\partial\left(\overline{\lambda}_{zx}^H + \overline{\lambda}_{zy}^H\right)}{\partial y} \\ \mu\alpha_y\frac{\partial\overline{\lambda}_{xy}^H}{\partial\tau} + \sigma_y^m\overline{\lambda}_{xy}^H &= \frac{\partial\left(\overline{\lambda}_{zx}^E + \overline{\lambda}_{zy}^E\right)}{\partial y} \\ \varepsilon\alpha_z\frac{\partial\overline{\lambda}_{xz}^E}{\partial\tau} + \sigma_z\overline{\lambda}_{xz}^E &= \frac{\partial\left(\overline{\lambda}_{yx}^H + \overline{\lambda}_{yz}^H\right)}{\partial z} \\ \mu\alpha_z\frac{\partial\overline{\lambda}_{xz}^H}{\partial\tau} + \sigma_z^m\overline{\lambda}_{xz}^H &= -\frac{\partial\left(\overline{\lambda}_{yx}^E + \overline{\lambda}_{yz}^E\right)}{\partial z}. \end{aligned} \tag{7}$$

The above equations give the general modified perfectly matched layer (MPML) ABC for a reversed time problem. It should be emphasized that the MPML conductivities σ_ξ and loss factors α_ξ ($\xi = x, y, z$) have positive values both for the forward and backward time schemes. The modification of the forward time PML ABC into a backward time PML ABC in [1] and [2] is mathematically unsound and leads to the physically unsound assumption that the backward time PML has negative electric conductivities and magnetic losses. As can be seen from (7), the correctly defined adjoint (backward time) PML ABC absorbs both propagating and evanescent outgoing adjoint waves. The PML equations suggested in [1] and [2] are a special case of (7) with $\alpha_\xi = 1$, $\xi = x, y, z$. Notice that the difference between the PML ABCs for the original and adjoint problems is actually in the signs in front of the spatial derivatives at the right-hand sides of the PML equations rather than the signs of the PML conductivities.

B. Derivation of ABCs Based on the One-Way WE

In some problems, especially in the case of guiding structures, in some particular (lateral) directions, there is very little electromagnetic energy to be absorbed. Other considerations may also be important, e.g., the simplicity of implementation, the minimal additional computational overhead, and the discretization possible with little or no additional memory requirements. In such cases, single-layer ABCs are preferable, e.g., Engquist–Majda's one-way WE ABC [7], Mur's ABCs [8], or the dispersive boundary conditions (DBCs) [9].

The WE corresponding to the adjoint problem is easily obtained by taking a curl of the first equation in (1) and substituting in it the time derivative with respect to the reversed time variable τ of the second equation

$$\frac{\partial^2\vec{\overline{\lambda}}^E}{\partial\tau^2} - \frac{1}{\mu\varepsilon}\nabla^2\vec{\overline{\lambda}}^E = 0. \tag{8}$$

Here, a unified approach will be described to the derivation of the above-mentioned single-layer ABCs. The WE (8) can be written in the operator form

$$\left(L^2 - v^2\nabla^2\right)\vec{\overline{\lambda}}^E = 0 \tag{9}$$

where $L = \partial/\partial\tau$ and the velocity of propagation is $v = (\mu\varepsilon)^{-1/2}$. Its one-dimensional (1-D) version in the direction of propagation (and absorption), the ξ-direction, $\xi = x, y, z$, will be

$$L^+L^-\left\{\vec{\overline{\lambda}}^E\right\} = 0 \tag{10}$$

where the wave operators L^+ and L^-, corresponding to the forward and backward wave propagation, respectively, are

$$L^+ = L + v_\xi\partial/\partial\xi \tag{11}$$

$$L^- = L - v_\xi\partial/\partial\xi. \tag{12}$$

Here, v_ξ is the velocity of propagation in the ξ-direction, $\xi = x, y, z$.

Three single-layer ABCs for the backward time-stepping algorithm are described below.

1) The one-way WE ABCs corresponding to (11) and (12) are, respectively,

$$\frac{1}{v_\xi}\frac{\partial\vec{\overline{\lambda}}^E}{\partial\tau}+\frac{\partial\vec{\overline{\lambda}}^E}{\partial\xi}\bigg|_{\xi=\xi_{\max}}=0$$
$$\frac{1}{v_\xi}\frac{\partial\vec{\overline{\lambda}}^E}{\partial\tau}-\frac{\partial\vec{\overline{\lambda}}^E}{\partial\xi}\bigg|_{\xi=\xi_{\min}}=0 \quad (13)$$

in which the first-order approximation of the velocity of propagation in the ξ-direction is used ($v_\xi = v$). The boundaries along the ξ-axis are at $\xi_{\min}$ and $\xi_{\max}$, respectively.

2) For Mur's second-order ABC for the adjoint problem, the general procedure given in [8] is used. Thus, at $\xi=\xi_{\max}$

$$\frac{\partial^2\vec{\overline{\lambda}}^E}{\partial\tau^2}=-v\frac{\partial^2\vec{\overline{\lambda}}^E}{\partial\xi\partial\tau}+\frac{v^2}{2}\left(\frac{\partial^2\vec{\overline{\lambda}}^E}{\partial\eta^2}+\frac{\partial^2\vec{\overline{\lambda}}^E}{\partial\zeta^2}\right). \quad (14)$$

3) Similarly, concatenating two one-way WEs with different propagation velocities, corresponding to different frequencies of interest, the second-order DBC for the adjoint problem can be obtained at $\xi=\xi_{\max}$ as

$$\left(\frac{1}{v_{1\xi}}\frac{\partial}{\partial\tau}+\frac{\partial}{\partial\xi}\right)\left(\frac{1}{v_{2\xi}}\frac{\partial}{\partial\tau}+\frac{\partial}{\partial\xi}\right)\left\{\vec{\overline{\lambda}}^E\right\}=0. \quad (15)$$

Note that all single-layer ABC equations for the adjoint problem are identical with the ABCs for the original problem despite the reversed time. This result is due to the *local* nature of these ABCs. At the boundaries of the respective computational domain, both with a forward and backward time scheme, the waves are locally outgoing.

III. Numerical Examples

The performance of the ABCs for the adjoint problem was tested on the example of a microstrip line of width $w=0.6$ mm printed on a dielectric substrate of relative dielectric permittivity $\varepsilon_r = 9.6$ and height $h = 0.6$ mm. The excitation is the z-component of the adjoint electric field $\overline{\lambda}_z^E$, which is normal to the strip. It is uniformly distributed in the transverse plane under the microstrip line and is a Gaussian pulse in time so that its form is the same both for the forward and backward time variables. Its spectrum covers the frequency band from 0 to 50 GHz. The size of the computational domain is (300 Δx, 76 Δy, 56 Δz) for the single-layer ABCs and (300 Δx, 46 Δy, 26 Δz) for the PML ABC, where $\Delta x=\Delta y=\Delta z=0.1$ mm. The parameters of the PML ABC are the: 1) number of layers in the absorber $N_{PML} = 8$; 2) reflection coefficient at normal incidence $R_0 = 10^{-3}$; 3) PML conductivity $\sigma(\rho)=-(n_\sigma+1)\varepsilon_0 c\ln(R_0)(\rho/\delta)^{n_\sigma}/(2\delta), 0\le\rho\le\delta, n_\sigma=4$ and $n_\sigma=3$; and 4) PML loss factor $\alpha(\rho)=1+\varepsilon_{\max}(\rho/\delta)^{n_\alpha}$, $0\le\rho\le\delta$, $n_\alpha=3$, $\varepsilon_{\max}=1$. Here, ρ is the depth inside the PML medium, δ is the thickness of the PML, and $c=(\mu_0\varepsilon_0)^{-1/2}$. The reflection is calculated using the ratio of the reflected and incident z-component of the adjoint electric field $R_{\rm dB} = 20\log_{10}|\mathfrak{F}\{\overline{\lambda}_z^{refl}\}/\mathfrak{F}\{\overline{\lambda}_z^{inc}\}|$, where $\mathfrak{F}$ denotes the Fourier transform of the respective time-dependent field component. In the cases of single-layer ABCs, the time guard between the incident and reflected field suffices to separate them. In the case of the PML, deembedding with a microstrip line of double length is used since the level of the reflections is extremely low.

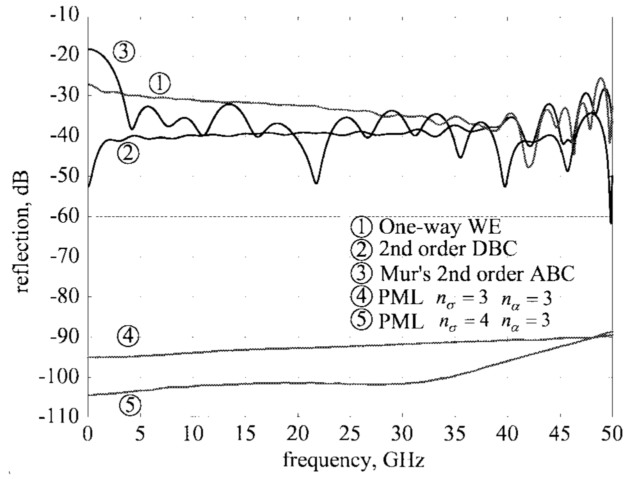

Fig. 1. Spectrum of the reflection for the adjoint problem using four different ABCs: ①: one-way WE ABC. ②: second-order DBC. ③: Mur's second-order ABC. ④: PML ABC ($N_{\rm PML} = 8$, $R_0 = 10^{-3}$, $\varepsilon_{\max} = 1$, $n_\alpha = 3$, $n_\sigma = 3$). ⑤: PML ABC ($N_{PML} = 8$, $R_0 = 10^{-3}$, $\varepsilon_{\max} = 1$, $n_\alpha = 3$, $n_\sigma = 4$).

The three-dimensional computational domain is terminated in all directions (except the ground plane) by the four types of ABCs derived in Section II: the one-way WE ABC, Mur's second-order ABC, the DBC, and the PML ABC. Their respective reflections for the reversed-time problem are shown in Fig. 1. The reflections for the same types of ABCs, when the forward time problem is considered, coincide with the ones shown in Fig. 1.

IV. Conclusion

In this paper, ABCs for adjoint problems with backward time variable are derived from first principles. It is shown that all single-layer ABCs for the adjoint problem, which are based on the one-way WE, have the same equations as for the original forward time problem, despite the reversed time. In the adjoint PML ABC case, the signs of the spatial derivatives are opposite to those in the PML ABC of the original forward time problem. These rigorously obtained results are consistent with the fact that, for both the original and adjoint problems, the waves are locally outgoing at the outer boundaries. To verify the theoretical findings, the reflections in a microstrip-line example are investigated so that metal and inhomogeneous dielectrics intersect the PML boundary. The reflections of the forward and backward time schemes are identical for the same type of ABCs.

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