A Nonlinear and Dispersive APML ABC for the FD-TD Methods

Masafumi Fujii and Peter Russer

***Abstract*—We have developed a modified anisotropic perfectly matched layer (APML) absorbing boundary condition (ABC) for the finite-difference time-domain (FD-TD) analysis of nonlinear and dispersive media. The formulation is a simple modification to the original nonsplit APML, and retains the robustness and the simple implementation in the FD-TD and the higher-order schemes. The proposed ABC has a broad area of application, and is especially suitable for the analysis of nonlinear optical waveguide problems.**

***Index Terms*—absorbing boundary conditions (ABC), finite-difference time-domain (FD-TD), nonlinear dispersive anisotropic perfectly-matched layer (APML).**

I. Introduction

TIME-DOMAIN numerical techniques have been of great importance in modeling electromagnetic and optical wave propagation, and the absorbing boundaries play an important role to enable analysis of infinite space of open structures. Among many absorbing boundaries proposed in literature [1], Berenger's perfectly matched layer (PML) absorbing boundary conditions (ABC) [2] has achieved a significantly high absorption rate, thereby reducing the area of numerical analysis. The anisotropic PML (APML) has been proposed by Gedney [3], which provides an unsplit-field formulation and simple numerical implementation.

The PML is an unique absorbing boundary that is straightforwardly applicable to the high-order finite-difference methods as well as the wavelet-based techniques [4], [5]; the one-way absorbing boundaries derived from the wave equation has difficulty in the consistent termination of the stencil of the high-order methods.

A variety of modified PMLs have been proposed for the linear dispersive media [6], [7], while only limited publication can be found for nonlinear dispersive media. Some techniques based on the Berenger's split-field PML have been proposed for nonlinear media [8], [9]; however, [8] is not applicable to dispersive media because the time retardation of the polarization requires the incorporation of the electric field while [8] formulates with the flux density. The other technique [9] is too complicated to implement in the corner of the analysis region.

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The authors are with the Institute for High Frequency Engineering, Technical University of Munich, Munich, Germany (e-mail: fujii@ei.tum.de).

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In this paper, we have extended Gedney's APML to general nonlinear dispersive media by introducing the auxiliary differential equation (ADE) techniques [10], nevertheless, in a modified manner to fit in our PML formulation, which, as in [11], does not require solving a system of equations for multipole dispersive media. The proposed absorbing boundary has been applied to the analysis of optical pulse propagation in the instantaneous Kerr nonlinearity and the linear Lorentz dispersive media; the performance of the absorption has been evaluated numerically.

II. Theory

We consider two-dimensional TE polarized wave propagation in the xz-plane of the Cartesian coordinates. Starting with a constitutive relation between the flux density D_y and the electric field E_y in the medium of frequency dependent relative dielectric constant $\mathcal{E}(\omega)$, we write in the frequency domain as in [1]

$$\tilde{D}_y(\omega) = \mathcal{E}_0 \mathcal{E}_r(\omega) \tilde{E}_y(\omega) \qquad (1)$$

where $\mathcal{E}_0$ is the dielectric constant of free space. The time-harmonic Ampère's law within the APML is written as

$$\frac{\partial \tilde{H}_x(\omega)}{\partial z} - \frac{\partial \tilde{H}_z(\omega)}{\partial x} = j\omega \mathcal{E}_0 \mathcal{E}_r(\omega) \frac{s_x s_z}{s_y} \tilde{E}_y(\omega) \qquad (2)$$

where

$$s_\xi = \kappa_\xi + \frac{\sigma_\xi}{j\omega \mathcal{E}_0} \qquad (3)$$

for $\xi = x,\ y$, and z. The APML parameters κ_ξ and σ_ξ normally have an polynomial grading.

Now, we introduce two auxiliary variables $\tilde{\mathcal{D}}_y$ and $\tilde{\mathcal{E}}_y$ defined by

$$\tilde{\mathcal{D}}_y(\omega) = \mathcal{E}_0 \mathcal{E}_r(\omega) \frac{s_x}{s_y} \tilde{E}_y(\omega) \qquad (4)$$

and

$$\tilde{\mathcal{E}}_y(\omega) = \frac{1}{\mathcal{E}_{0-}\mathcal{E}_r(\omega)} \tilde{\mathcal{D}}_y(\omega). \qquad (5)$$

The variables $\tilde{\mathcal{D}}_y$ and $\tilde{\mathcal{E}}_y$ represent the equivalent flux density and the equivalent electric field in the APML loss space, respectively. Substituting (4) into (2), and applying the usual ADE procedure of the inverse Fourier transform, i.e., replacing the factor $j\omega$ with differentiation $\partial/\partial t$, we obtain

$$\frac{\partial H_x(t)}{\partial z} - \frac{\partial H_z(t)}{\partial x} = \kappa_z \frac{\partial \mathcal{D}_y(t)}{\partial t} + \frac{\sigma_z}{\epsilon_0} \mathcal{D}_y(t). \qquad (6)$$

Equation (6) is discretized using the semi-implicit scheme for the right-hand side of the equation, yielding

$$\mathcal{D}^{n+1}_{y,\,i,\,k} = \frac{2\mathcal{E}_0\kappa_z - \sigma_z\Delta t}{2\mathcal{E}_0\kappa_z + \sigma_z\Delta t}\mathcal{D}^{n}_{y,\,i,\,k} + \frac{2\mathcal{E}_0\Delta t}{2\mathcal{E}_0\kappa_z + \sigma_z\Delta t}\mathcal{H}^y \quad (7)$$

where $\mathcal{H}^y$ is the spatial difference approximation

$$\mathcal{H}^y = \frac{H^{n+1/2}_{x,i,k+1/2} - H^{n+1/2}_{x,i,k-1/2}}{\Delta z} - \frac{H^{n+1/2}_{z,i+1/2,k} - H^{n+1/2}_{z,i-1/2,k}}{\Delta x} \quad (8)$$

which can be replaced by the high-order finite-difference scheme or the wavelet-based schemes [4], [5].

Then, the instantaneous Kerr nonlinearity and the linear Lorentz dispersion properties are implemented by the ADE technique, nevertheless, with a slight modification from [11] to fit in our PML media. From (5), we can write

$$\begin{aligned}\tilde{\mathcal{D}}_y(\omega) &= \mathcal{E}_0\mathcal{E}_r\tilde{\mathcal{E}}_y(\omega)\\ &= \mathcal{E}_0\mathcal{E}_\infty\tilde{\mathcal{E}}_y(\omega) + \tilde{\mathcal{P}}_L(\omega) + \tilde{\mathcal{P}}_{NL}(\omega)\end{aligned} \quad (9)$$

where $\tilde{\mathcal{P}}_L$ and $\tilde{\mathcal{P}}_{NL}$ denote the linear and the nonlinear polarization, and $\mathcal{E}_\infty$ is the relative delectric constant in the limit of infinite frequency. By applying the inverse Fourier transform, the expression in the time domain is obtained as

$$\mathcal{D}_y(t) = \mathcal{E}_0\mathcal{E}_\infty\mathcal{E}_y(t) + \mathcal{P}_L(t) + \mathcal{P}_{NL}(t). \quad (10)$$

The polarization of the linear Lorentz dispersive media is given by

$$\tilde{\mathcal{P}}_L(\omega) = \mathcal{E}_0\chi_p(\omega)\tilde{\mathcal{E}}_y(\omega) = \frac{\mathcal{E}_0\Delta\mathcal{E}_p\omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2}\tilde{\mathcal{E}}_y(\omega) \quad (11)$$

where χ_p denotes the electric susceptibility, ω_p is the Lorentz resonant frequency, $\Delta\mathcal{E}_p$ is the difference of the relative dielectric constant caused by the resonance, and δ_p is the damping factor. This is transformed into the differential equation by replacing $j\omega$ with $\partial/\partial t$, and $-\omega^2$ with $\partial^2/\partial t^2$

$$\omega_p^2\mathcal{P}_L(t) + 2\delta_p\frac{\partial\mathcal{P}_L(t)}{\partial t} + \frac{\partial^2\mathcal{P}_L(t)}{\partial t^2} = \epsilon_0\Delta\epsilon_p\omega_p^2\mathcal{E}_y(t) \quad (12)$$

which leads to the time difference form of $\mathcal{P}_L$ as

$$\mathcal{P}_L^{n+1} = a_L\mathcal{P}^n + b_L\mathcal{P}^{n-1} + c_L\mathcal{E}_y^n \quad (13)$$

with the coefficients

$$\begin{aligned}a_L &= \frac{2 - \omega_p^2\Delta t^2}{1 + \delta_p\Delta t}\\ b_L &= -\frac{1 - \delta_p\Delta t}{1 + \delta_p\Delta t}\\ c_L &= \frac{\mathcal{E}_0\Delta\mathcal{E}_p\Delta t^2\omega_p^2}{1 + \delta_p\Delta t}.\end{aligned} \quad (14)$$

The polarization of the instantaneous Kerr nonlinear media is simply given by

$$\mathcal{P}_{NL}(t) = \mathcal{E}_0\chi_0^{(3)}\mathcal{E}_y(t)^3 \quad (15)$$

where $\chi_0^{(3)}$ is the strength of the nonlinearity related to the linear part of the refractive index n_0 and the nonlinear part to the refractive index n_2 ($\mathrm{m}^2/\mathrm{V}^2$) by $\chi_0^{(3)} = 2n_0n_2$. The time difference expression is given by

$$\mathcal{P}_{NL}^{n+1} = \mathcal{E}_0\chi_0^{(3)}(\mathcal{E}_y^{n+1})^3. \quad (16)$$

By substituting (13) and (16) into (10), and solving with respect to $\mathcal{E}^{n+1}$, we obtain the nonlinear equation

$$\mathcal{E}_y^{n+1} = \frac{\mathcal{D}_y^{n+1} - a_L\mathcal{P}_L^n - b_L\mathcal{P}_L^{n-1} - c_L\mathcal{E}_y^n}{\mathcal{E}_0\mathcal{E}_\infty + \mathcal{E}_0\chi_0^{(3)}\left(\mathcal{E}_y^{n+1}\right)^2}. \quad (17)$$

Equation (17) can be solved by a simple iteration method as in [12]. Because we model the dispersive media by the relation between the polarization and the electric field, one can solve the nonlinear equation (17) with including arbitrary number of polarization factors without solving a system of equations [11].

Finally, from (4) and (5), we have

$$\tilde{\mathcal{E}}_y(\omega) = \frac{s_x}{s_y}\tilde{E}_y(\omega). \quad (18)$$

Substituting (3) to (18) leads to

$$\tilde{\mathcal{E}}_y(\omega)\left(\kappa_y + \frac{\sigma_y}{j\omega\mathcal{E}_0}\right) = \tilde{E}_y(\omega)\left(\kappa_x + \frac{\sigma_x}{j\omega\mathcal{E}_0}\right). \quad (19)$$

By the inverse Fourier transformation and discretizing the resulting differential equation, we obtain

$$\begin{aligned}E^{n+1}_{y,\,i,\,k} &= \frac{2\kappa_x\mathcal{E}_0 - \sigma_x\Delta t}{2\kappa_x\mathcal{E}_0 + \sigma_x\Delta t}E^n_{y,\,i,\,k} + \frac{1}{2\kappa_x\mathcal{E}_0 + \sigma_x\Delta t}\\ &\cdot\left[(2\kappa_y\mathcal{E}_0 + \sigma_y\Delta t)\mathcal{E}^{n+1}_{y,\,i,\,k} - (2\kappa_y\mathcal{E}_0 - \sigma_y\Delta t)\mathcal{E}^n_{y,\,i,\,k}\right].\end{aligned} \quad (20)$$

To summarize, computing (7), (17), (13), and (20) in sequence completes the update of the electric field. The magnetic fields can be updated by the standard APML algorithm for nonmagnetic media.

III. Numerical Experiments

The performance of the modified APML has been evaluated by analyzing pulse propagation in a 2.5 × 2.5-μm-square region. The space step is $\Delta x = \Delta z = 0.0125$ μm. In order to reduce the computational region, the boundary conditions are set to be the perfect magnetic conductor (PMC) walls at $x = z = 0$ μm, and the interface between the real domain and the PML has been placed at $x = z = 2.5$ μm. The APML conductance has fourth-order polynomial grading with the maximum value of $\sigma_{\max} = 1/(30\pi\sqrt{\epsilon_\infty}\Delta x)$ [3].

The carrier frequency of the excitation pulse is 231 THz, i.e., the free-space wavelength is $\lambda_0 = 1.3$ μm; the time envelope is a raised cosine function having approximately ten carrier cycles in it, which corresponds to the −20-dB bandwidth of approximately 80 THz. The transverse profile of the pulse is a hyperbolic secant function with its full width at half magnitude (FWHM) of 0.65 μm. The media has a instantaneous Kerr nonlinearity of $\chi_0^{(3)} = 2.0\times10^{-20}$ $\mathrm{m}^2/\mathrm{V}^2$, and a linear Lorentz dispersion of $\omega_p = 9.0\times10^{14}$ rad/s, $\delta_p = 5.0\times10^9$ 1/s, $\Delta\mathcal{E}_p = 3.0$, and $\mathcal{E}_\infty = 6.05$.

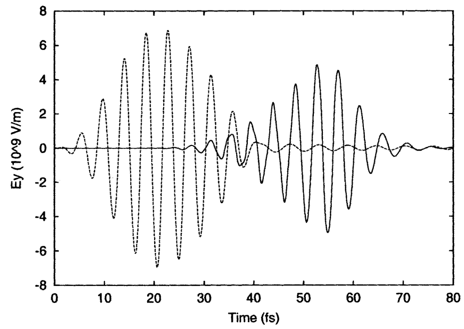

Fig. 1. Time series data for the large signal excitation (7×10^9 V/m). - - -: excitation; —: at one cell in front of the APML interface.

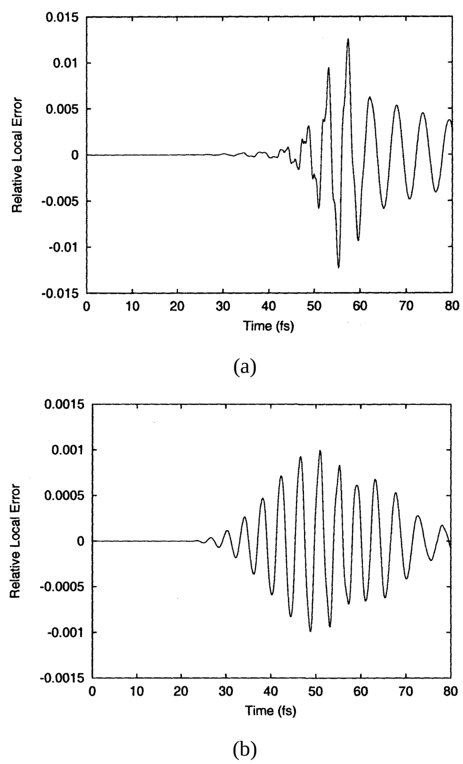

Fig. 2. Relative local reflection errors of the five-layer modified APML. (a) For large-signal excitation 7×10^9 V/m and (b) for small-signal excitation 2×10^9 V/m.

With this choice, the numerical dispersion of the finite difference-time domain (FD-TD) lattice is sufficiently smaller than the Lorentz dispersion, and the carrier frequency is in the range of anomalous dispersion of the Lorentz media; the group velocity dispersion parameter β_2 ranges from -100 to -5 ps^2/m over the -20-dB bandwidth from 190 to 270 THz, where temporal soliton pulse can be formed by an excitation with sufficient intensity. Two cases of the excitation pulse amplitude 7×10^9 V/m and 2×10^9 V/m have been tested for comparison; the former is of enough strength for the soliton formation, while the latter is not. The pulse is excited such that it propagates along the z-direction, and the time signal is detected one cell in front of the PML interface. The reference structure has 7.5×7.5-μm region terminated with perfect electric conductor (PEC) walls instead of PML.

The time series data for the large excitation amplitude is shown in Fig. 1; it is noted that the pulse waveform exhibits the symptom of triangular soliton pulse formation.

The ratio of local reflection errors to the maximum of the reference time data is plotted in Fig. 2(a) and (b) for the large and the small excitation amplitudes, respectively. The APML has five layers in all the cases. For the small signal, the absorption is good, i.e., approximately -60 dB or less reflection is achieved, while for the large signal, the absorption is about one order of magnitude worse. When ten-layer APML was used, some improvement was observed for the small signal absorption, while little improvement was observed for the large signal.

The signal amplitude dependence of the absorption may be due to the fact that the time stepping scheme of the FD-TD has been developed for the linear response of the electric field, while the third-order nonlinearity causes more rapid response, which leads to less accurate solution. Preliminary experiments have shown that when the linear APML is applied for this nonlinear pulse, more than 10% of reflection occurs; the modified version in this paper exhibits much better performance.

IV. Conclusion

A modified APML absorbing boundary condition has been developed for the FD-TD analysis of nonlinear and dispersive media. The performance of the APML was investigated numerically and found that the absorption depends on the strength of the nonlinearity; typically -35 to -60 dB reflection has been obtained with a five-layer APML.

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