# An Exponential Time Differencing Algorithm for the FDTD-PML Analysis of Nonlinear PBG Structures

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***Abstract*—An exponential time differencing (ETD) algorithm is presented for the analysis of photonic band gap (PBG) structures comprising the third-order nonlinear materials. Compared with the well-known Z-transform (ZT) method and auxiliary differential equation (ADE) method for incorporating the nonlinearity, the proposed ETD algorithm has the least memory requirement and shows the same accuracy. The stretched coordinates perfectly matched layer (SC-PML) with the complex frequency shifted (CFS) variable implemented by using the ETD algorithm is applied to terminate the linear and nonlinear PBG structures. Compared with the conventional PML and the convolution PML (CPML), the proposed implementation can significantly improve the absorbing performance with similar memory requirement.**

***Index Terms*—Boundary conditions, finite difference methods, nonlinear optics.**

## I. Introduction

IN this study, we propose an exponential time differencing (ETD) algorithm to incorporate the Raman scattering effect of the third-order nonlinearity requiring only one auxiliary variable per cell per coordinate direction while both the ZT [1] and the ADE [2] methods need no less than three variables. Furthermore, the ETD method has the simplest updating procedure, and can directly lead to FDTD implementations. The ETD implementation of a series of material independent D-H formulations of the stretched coordinates PML (SC-PML), referred to as EPML, is applied to terminate the linear and nonlinear photonic band gap (PBG) structures. The EPML can improve the absorbing performance substantially with similar memory requirement when compared with the conventional SC-PML and the convolution PML (CPML). We have also found that by using appropriate parameters, the performance of conventional PML can be significantly improved without retaining the periodic pattern of PC in [1].

## II. Formulations

Taking the $x$-projection of the Ampere's law as an example, the material-independent modified Maxwell's curl equation in the SC-PML regions [3] can be written as

$$j\omega D_x = \frac{1}{s_y}\frac{\partial}{\partial y}H_z - \frac{1}{s_z}\frac{\partial}{\partial z}H_y \tag{1}$$

If the CFS-PML [4] is adopted, the stretching variable $s_i$ will be

$$s_i = \kappa_i + \frac{\sigma_i}{\alpha_i + j\omega\varepsilon_0},\, i = x,\, y,\, z. \tag{2}$$

Substituting (2) into (1), we obtain

$$j\omega D_x = \left(\frac{1}{\kappa_y} + \frac{u_y}{j\omega + v_y}\right)\frac{\partial}{\partial y}H_z - \left(\frac{1}{\kappa_z} + \frac{u_z}{j\omega + v_z}\right)\frac{\partial}{\partial z}H_y \tag{3}$$

where $u_i = -\sigma_i / \left(\kappa_i^2 \varepsilon_0\right)$ and $v_i = (\alpha_i + \sigma_i/\kappa_i)/\varepsilon_0\ (i = y, z)$. Here we introduce two auxiliary variables defined at the same FDTD grid position as the field component $D_x$, given as

$$F_{xy} = \frac{u_y}{j\omega + v_y}\frac{\partial}{\partial y}H_z \tag{4}$$

and

$$F_{xz} = \frac{u_z}{j\omega + v_z}\frac{\partial}{\partial z}H_y. \tag{5}$$

Substituting (4) and (5) into (3), we obtain

$$j\omega D_x = \frac{1}{\kappa_y}\frac{\partial}{\partial y}H_z + F_{xy} - \frac{1}{\kappa_z}\frac{\partial}{\partial z}H_y - F_{xz} \tag{6}$$

This equation can easily be written in the FDTD updating form. Following the way proposed in [5], the updating equation for $F_{xy}$ can be obtained as

$$\begin{aligned} F_{xy}^{n+1/2} &= e^{-v_y\Delta t}F_{xy}^{n-1/2} \\ &+ \tfrac{u_y}{v_y^2\Delta t}\left(v_y\Delta t - 1 + e^{-v_y\Delta t}\right)\tfrac{\partial}{\partial y}{H_z}^{n+1/2} \\ &+ \tfrac{u_y}{v_y^2\Delta t}\left(1 - v_y\Delta t e^{-v_y\Delta t} - e^{-v_y\Delta t}\right)\tfrac{\partial}{\partial y}{H_z}^{n-1/2} \end{aligned} \tag{7}$$

The updating equation for $F_{xz}$ can be obtain in the same way. By using a temporary variable which is a word of memory instead of a matrix to store the value of $\frac{\partial}{\partial y}{H_z}^{n-1/2}$, this ETD implementation of the SC-PML has the same memory requirement as the CPML.

The nonlinear polarization [1] can be expressed as

$$\mathbf{P}_K\left(t\right) = \varepsilon_0\chi_0^{(3)}\alpha\mathbf{E}^3\left(t\right) \tag{8}$$

and

$$\mathbf{P}_R\left(t\right) = \varepsilon_0\chi_0^{(3)}\left(1-\alpha\right)\mathbf{E}\left(t\right)\mathbf{S}_R\left(t\right) \tag{9}$$

with

$$\mathbf{S}_R\left(t\right) = \int_0^t g_R\left(t-\tau\right)\mathbf{E}^2\left(\tau\right)d\tau \tag{10}$$

where $\mathbf{P}_K$ denotes the Kerr effect, $\mathbf{P}_R$ represents the Raman scattering and $\mathbf{S}_R$ is an auxiliary variable for convenience. The

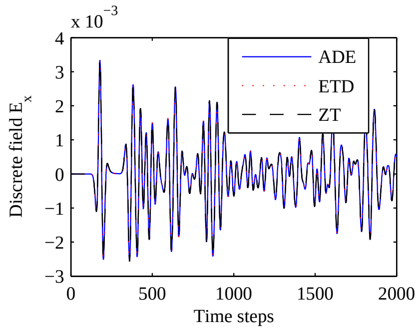


Fig. 1. Calculated results of the discrete field $E_x$ by using the ADE method, the ZT method, and the proposed ETD method.

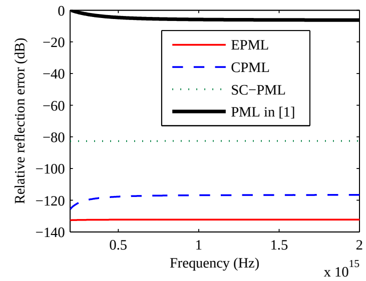


Fig. 2. Relative reflection errors of the PML used in [1], the conventional SC-PML, the CPML with $\kappa_{\max} = 20$, $\alpha_{\max} = 0.3$, $\sigma_{\max} = 6/(150\pi\Delta x)$, and the EPML with $\kappa_{\max} = 1$, $\alpha_{\max} = 1200$, $\sigma_{\max} = 6/(150\pi\Delta x)$ (all parameters are polynomial scaled) when applied to the nonlinear PBG structure.

difference equation for (8) can be obtained through taking a Taylor series expansion of $\mathbf{E}^3(t)$, given as

$$\mathbf{P}_K^{n+1} = \varepsilon_0\chi_0^{(3)}\alpha\left(3[\mathbf{E}^n]^2\mathbf{E}^{n+1} - 2[\mathbf{E}^n]^3\right) \tag{11}$$

For the Raman nonlinearity, the frequency domain equation of (10) is

$$\mathbf{S}_R(\omega) = \frac{\omega_R^2}{\omega_R^2 + 2j\omega\delta_R - \omega^2}\cdot\mathbf{FFT}\left[\mathbf{E}^2(t)\right] \tag{12}$$

where $\omega_R$ and $\delta_R$ are the corresponding coefficients, and **FFT** represents the Fourier transform. (12) can be written as

$$\mathbf{S}_R(\omega) = \frac{a_R}{j\omega + c_R}\mathbf{FFT}\left[\mathbf{E}^2(t)\right] + \frac{a_R^*}{j\omega + c_R^*}\mathbf{FFT}\left[\mathbf{E}^2(t)\right] \tag{13}$$

where $a_R = j\omega_R^2/\left(2\sqrt{\omega_R^2 - \delta_R^2}\right)$, $c_R = \delta_R + j\sqrt{\omega_R^2 - \delta_R^2}$, $a_R^*$ and $c_R^*$ are the complex conjugates of $a_R$ and $c_R$, respectively. Here we introduce an auxiliary variable $\mathbf{J}_R$, given as

$$\mathbf{J}_R = \frac{a_R}{j\omega + c_R}\mathbf{FFT}\left[\mathbf{E}^2(t)\right] \tag{14}$$

Transforming (14) into the time domain, we obtain

$$\frac{\partial}{\partial t}\mathbf{J}_R(t) + c_R\mathbf{J}_R(t) = a_R\mathbf{E}^2(t) \tag{15}$$

In a similar way as that for $F_{xy}$, we can get the updating equation for $\mathbf{J}_R$, given as

$$\mathbf{J}_R^{n+1} = e^{-c_R\Delta t}\mathbf{J}_R^n + \frac{a_R}{c_R}\left(1 - e^{-c_R\Delta t}\right)(\mathbf{E}^n)^2 \tag{16}$$

Then we obtain the updating equation for $\mathbf{P}_R$, given as

$$\mathbf{P}_R^{n+1} = 2\varepsilon_0\chi_0^{(3)}(1-\alpha)\,\mathbf{E}^{n+1}\mathrm{Re}\left(\mathbf{J}_R^{n+1}\right) \tag{17}$$

The updating equation for the electric field will be

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} + 2\varepsilon_0\chi_0^{(3)}\alpha[\mathbf{E}^n]^3}{\varepsilon_0\varepsilon_\infty + 3\varepsilon_0\chi_0^{(3)}\alpha[\mathbf{E}^n]^2 + 2\varepsilon_0\chi_0^{(3)}(1-\alpha)\,\mathrm{Re}\left(\mathbf{J}_R^{n+1}\right)} \tag{18}$$

It can be seen that for the Raman nonlinearity, the ETD algorithm needs only one auxiliary variable and only one updating step (16) while the ZT method [1] and the ADE method [2] need at least three variables and a three-step updating procedure since variables of two time steps before are involved.

## III. Numerical Results and Discussions

To validate the ETD algorithm, a two-dimensional (2-D) $\mathrm{TE}_z$ wave interacted with the Kerr and Raman nonlinear medium is considered. The discrete electric field $E_x$ of an observation point, which is at 10 cells away from the source in the two coordinate directions, is calculated. It can be seen in Fig. 1 that results of the ADE method, the ZT method, and the proposed ETD method coincide well with each other.

To show the efficiency of the EPML, we consider a $\mathrm{TM}_z$ wave propagating through a PBG structure consisting of a $9\times9$ square lattice in air background of linear dielectric circular rods with the one line in the middle made of the Kerr and Raman medium. The computational domain is truncated by using 10 cells different PMLs, respectively. It can be observed in Fig. 2 that the EPML has significant improvements in the absorbing performance over the CPML and the conventional SC-PML. It should be noted in Fig. 2 that the conventional SC-PML greatly improves the absorbing performance when compared with the PML in [1] which is actually also a conventional PML. In this study, the conductivity for the SC-PML is $\sigma_{\max} = 6/(150\pi\Delta x)$ which is different from that used in [1]. That is to say by using appropriate parameters instead of retaining the periodic pattern of the PC in the conventional PML regions in [1], performance of the conventional PML can be much more significantly improved. This will further reduce the memory requirement and make the use of thinner PML possible which also results in memory saving.

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