Efficient *Z*-Transform Implementation of the D-B CFS-PML for Truncating Multi-Term Dispersive FDTD Domains

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Abstract **─** Efficient *Z*-transform implementation of the Complex Frequency-Shifted Perfectly Matched Layer (CFS-PML) using the D-B formulations are proposed to truncate open region multi-term dispersive Finite-Difference Time-Domain (FDTD) lattices. These formulations are independent of material properties of the FDTD domains and hence can be used for modeling general media because of the D-B constitutive relations. A Three-Dimensional (3-D) simulation of the two-term Lorentz dispersive FDTD domain has been carried out to demonstrate the validity of the proposed formulations. Furthermore, in order to show the validity of the proposed algorithm, the second 3D inhomogeneous problem has also been used for validating the proposed formulations. It is clearly shown that the new formulations with the CFS-PML scheme are efficient in attenuating evanescent waves and reducing late-time reflections.

Index Terms **-** D-B constitutive relations, Finite-Difference Time-Domain (FDTD), multi-term Lorentz, Perfectly Matched Layer (PML) and *Z*-transform.

I. INTRODUCTION

Since 1994, the Perfectly Matched Layer (PML) concept proposed by Berenger [1], has been a highly effective absorbing-material Absorbing Boundary Condition (ABC) to terminate the Finite-Difference Time-Domain (FDTD) domains, the innovation of the PML ABC is that plane waves of arbitrary incidence, polarization and frequency are matched at the boundary between PML and the physical domain. What's more important is that the PML can be used as an absorbing boundary to terminate domains comprised of inhomogeneous, dispersive, anisotropic and even nonlinear media. Among the various implementations of PMLs, the stretched coordinate PML (SC–PML) by Chew and Weedon [2], has the advantage of simple implementation in the corners and edges of PML regions. The SC-PML [2] was proposed through mapping Maxwell's equations into a complex stretched coordinate space. As in the original Berenger's PML; however, the implementation of the SC-PML in [2] needs splitting the field components and modifying Maxwell's equations. Several unsplit-field implementations of the SC-PML formulations have been presented. These algorithms can be classified into three categories: (1) the Convolutional PML (CPML) [3] is based on applying the convolution theorem to the SC-PML formulations, (2) the Auxiliary Differential Equation (ADE) PML [4-6] is based on incorporating the ADE method into the SC-PML formulations and (3) another SC-PML

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implementation presented [7-11] is based on the *Z*-transform methods that have been successfully incorporated into the FDTD algorithm. As in the original Berenger's PML; however, the SC-PML formulations are ineffective at absorbing evanescent waves and various efforts have been attempted to overcome this limitation [12-14]. Among these, the Complex Frequency-Shifted PML (CFS-PML) [14], implemented by simply shifting the frequency dependent pole off the real axis and into the negative-imaginary half of the complex plane has drawn considerable attention, due to the fact that this PML is efficient in attenuating low-frequency evanescent waves and reducing late-time reflections. In [3, 15-17], various modified SC-PMLs based on the convolution theorem, the ADE method and the *Z*-transform methods, respectively, were presented in detail to efficiently implement the CFS-PMLs. Recently, the proposed SC-PML formulations in 2011 [18] based on the ADE method, have been presented for effectively modeling a linear multi-term Lorentz dispersive material in the 2-D simulation. However, as described in the preceding section, the SC-PML formulations are not capable of absorbing evanescent waves in the 2-D simulation and have even worse absorption performance in 3-D numerical tests. Besides, the SC-PML formulations based on the transpose direct form II proposed in [18], are difficult to extend to the case with more than two dispersive terms, because the direct form II structure [19] is extremely sensitive to parameter discretization in general and is not recommended in practical applications.

In this paper, the unsplit-field and efficient D-B CFS-PML algorithm, based on the *Z*-transform method, are proposed to truncate linear multi-term dispersive open-region FDTD domains. In the proposed formulations, an appropriate combination of the *Z*-transform methods with the D-B constitutive relations is used for truncating arbitrary media without any modifications of Maxwell's curl equations. A 3-D numerical test for a linear two-term Lorentz dispersive problem is given to validate the proposed D-B CFS-PML formulations; as the investigation on the performance of the D-B CFS-PML for linear multi-term Lorentz dispersive problem is very rare in the literature. Only the two-term Lorentz dispersive case is described in this paper, but this approach is easy to apply to any number of dispersive terms. For convenience, these PMLs including the proposed CFS and SC-PMLs and the proposed PML in [18], are referred to here as the ZT-CFS-PML, the ZT-SC-PML and the ADE-SC-PML, respectively.

II. FORMULATIONS

In Three-Dimensional (3-D) SC-PML regions, the z component of Ampere's law for the frequency-domain modified Maxwell's equations, can be written as:

$$j\omega\varepsilon_r(\omega)E_z = \frac{c_0}{S_x}\frac{\partial H_y}{\partial x} - \frac{c_0}{S_y}\frac{\partial H_x}{\partial y}, \tag{1}$$

where c_0 is the speed of the light in free space, S_x and S_y are the complex stretched coordinate metrics and for the conventional PML, they are defined as:

$$S_\eta = \kappa_\eta + \sigma_\eta / j\omega\varepsilon, \quad \eta = x \text{ or } y, \tag{2}$$

where ε is the permittivity of the FDTD domain, $\sigma_\eta \geq 0$ is the conductivity profile different from zero only in the PML region to provide attenuation for the propagating waves and $\kappa_\eta \geq 1$ is different from 1 only in the PML region to attenuate the evanescent waves.

The conventional PML has been explained for a poor absorption of evanescent waves in [12-13]. With the CFS scheme, proposed by Kuzuoglu and Mittra in [14], S_η is defined as:

$$S_\eta = \kappa_\eta + \sigma_\eta \big/ (\alpha_\eta + j\omega\varepsilon), \tag{3}$$

where κ_η is positive real and ≥ 1 and α_η is assumed to be positive real and introduced to better absorb the evanescent waves. Several algorithms with this metric have been proposed to successfully validate the capability of the CFS-PML in the absorption of evanescent waves [3, 15-17].

To make the PML completely independent of the material properties of the FDTD computational domains, (1) can be rewritten as:

$$j\omega D_z = \frac{c_0}{S_x}\frac{\partial H_y}{\partial x} - \frac{c_0}{S_y}\frac{\partial H_x}{\partial y}. \tag{4}$$

In terms of the electric flux density D defined as:

$$D_z = \varepsilon_r(\omega) E_z \,, \tag{5}$$

where $\varepsilon_r(\omega)$ is the relative permittivity of the FDTD computational domain.

Consider a linear isotropic multi-term Lorentz dispersive media with an electrical permittivity $\varepsilon_r(\omega)$ of:

$$\varepsilon_r(\omega) = \varepsilon_\infty + \sum_{k=1}^{M} \frac{G_k(\varepsilon_s - \varepsilon_\infty)\omega_{pk}^2}{(j\omega)^2 + j\omega\Gamma_k + \omega_{0_k}^2} \,, \tag{6}$$

where M is the number of dispersive terms, $\varepsilon_s = \varepsilon_r(0)$, $\varepsilon_\infty = \varepsilon_r(\infty)$, G_k is the pole amplitude, $\sum_{k=1}^{M} G_k = 1$, ω_{pk} is the plasma frequency, ω_{0k} is the resonance frequency and Γ_k is the damping factor. Substituting (6) into (5), we obtain:

$$D_z = \left[\varepsilon_\infty + \sum_{k=1}^{M} \frac{G_k(\varepsilon_s - \varepsilon_\infty)\omega_{pk}^2}{(j\omega)^2 + j\omega\Gamma_k + \omega_{0_k}^2} \right] E_z \,. \tag{7}$$

Transforming (7) from the frequency domain to the *Z*-domain [19], we obtain:

$$D_z = \varepsilon_\infty E_z + \sum_{k=1}^{M} \frac{\tilde{G}_k \exp(-\gamma_k \Delta t)\sin(\beta_k \Delta t) z^{-1}}{1 - 2\exp(-\gamma_k \Delta t)\cos(\beta_k \Delta t) z^{-1} + \exp(-2\gamma_k \Delta t) z^{-2}} E_z \,, \tag{8}$$

where $\tilde{G}_k = \Delta t \beta^{-1} G_k (\varepsilon_s - \varepsilon_\infty)\omega_{pk}^2$, $\beta_k = (\omega_{0k}^2 - \Gamma_k^2 / 4)^{1/2}$ and $\gamma_k = \Gamma_k / 2$. Consequently, this PML can be applied to truncate an arbitrary medium and all that is needed is to modify $D_z = \varepsilon_r(\omega) E_z$ under consideration. The method is available in [8] to obtain E from D.

Transforming (4) from the frequency domain to the *Z*-domain, we obtain:

$$\frac{1 - z^{-1}}{c_0 \Delta t} D_z = S_x(z) \cdot \frac{\partial H_y}{\partial x} - S_z(z) \cdot \frac{\partial H_x}{\partial y} \,, \tag{9}$$

where Δt is the time step and $S_\eta(z)$, $(\eta = x, y)$ is the *Z*-transform of $1/S_\eta$, which can be obtained by first transforming $1/S_\eta$ to the s-domain using the relation $j\omega \to s$ and then applying the bilinear *Z*-transform method [19] using the relation $s \to (2/\Delta t)(1 - z^{-1})/(1 + z^{-1})$:

$$S_\eta(z) = C_\eta \cdot \left(\frac{1 - a_\eta z^{-1}}{1 - b_\eta z^{-1}} \right) \quad (\eta = x, y) \,, \tag{10}$$

where: $a_\eta = (1 - \Delta t \alpha_\eta / 2\varepsilon_0) / (1 + \Delta t \alpha_\eta / 2\varepsilon_0)$

$b_\eta = (1 - (\Delta t / 2)(\alpha_\eta / \varepsilon_0 + \sigma_\eta / \varepsilon_0 \kappa_\eta)) / (1 + (\Delta t / 2)(\alpha_\eta / \varepsilon_0 + \sigma_\eta / \varepsilon_0 \kappa_\eta))$

$C_\eta = \kappa_\eta^{-1} (1 + \Delta t \alpha_\eta / 2\varepsilon_0) / (1 + (\Delta t / 2)(\alpha_\eta / \varepsilon_0 + \sigma_\eta / \varepsilon_0 \kappa_\eta))$.

Substituting (10) into (9), we obtain:

$$\frac{1 - z^{-1}}{c_0 \Delta t} D_z = C_x \cdot \left(\frac{1 - a_x z^{-1}}{1 - b_x z^{-1}} \right) \cdot \frac{\partial H_y}{\partial x} - C_y \cdot \left(\frac{1 - a_y z^{-1}}{1 - b_y z^{-1}} \right) \cdot \frac{\partial H_x}{\partial y} \,. \tag{11}$$

Introducing two auxiliary variables P_{zx} and P_{zy}:

$$P_{zx} = C_x \cdot \left(\frac{1}{1 - b_x z^{-1}} \right) \cdot \frac{\partial H_y}{\partial x} = b_x z^{-1} P_{zx} + C_x \cdot \frac{\partial H_y}{\partial x} \,, \tag{12}$$

$$P_{zy} = C_y \cdot \left(\frac{1}{1 - b_y z^{-1}} \right) \cdot \frac{\partial H_x}{\partial y} = b_y z^{-1} P_{zy} + C_y \cdot \frac{\partial H_x}{\partial y} \,. \tag{13}$$

Equation (11) can be written as:

$$\frac{1 - z^{-1}}{c_0 \Delta t} D_z = (1 - a_x z^{-1}) P_{zx} - (1 - a_y z^{-1}) P_{zy} \,. \tag{14}$$

Considering that the z^{-1} operator corresponds to a single-step delay in the discrete time domain, (12) – (14) can be written in the FDTD form, respectively, as (15) – (17), where:

$$P_{zx}\Big|_{i,j,k+1/2}^{n+1} = b_{x(i)} P_{zx}\Big|_{i,j,k+1/2}^{n} + \frac{C_{x(i)}}{\Delta x} \cdot \left(H_y\Big|_{i,j+1/2,k+1/2}^{n+1/2} - H_y\Big|_{i,j-1/2,k+1/2}^{n+1/2} \right) , \tag{15}$$

$$P_{zy}\Big|_{i,j,k+1/2}^{n+1} = b_{y(j)} P_{zy}\Big|_{i,j,k+1/2}^{n} + \frac{C_{y(j)}}{\Delta y} \cdot \left(H_x\Big|_{i,j+1/2,k+1/2}^{n+1/2} - H_x\Big|_{i,j-1/2,k+1/2}^{n+1/2} \right) , \tag{16}$$

$$D_z\Big|_{i,j,k+1/2}^{n+1} = D_z\Big|_{i,j,k+1/2}^{n} + c_0\Delta t\cdot[P_{zx}\Big|_{i,j,k+1/2}^{n+1} - a_{x(i)}P_{zx}\Big|_{i,j,k+1/2}^{n} - (P_{zy}\Big|_{i,j,k+1/2}^{n+1} - a_{y(j)}P_{zy}\Big|_{i,j,k+1/2}^{n})] . \quad (17)$$

To obtain E_z from D_z, we now introduce two auxiliary variables, Q_k and L_k $(k=1,2,..,M)$, so that we can solve for E_z^{n+1} by:

$$E_z\Big|_{i,j,k+1/2}^{n+1} = \frac{1}{\varepsilon_\infty}D_z\Big|_{i,j,k+1/2}^{n+1} - \frac{1}{\varepsilon_\infty}\sum_{k=1}^{M}(a_kQ_k\Big|_{i,j,k+1/2}^{n} - L_k\Big|_{i,j,k+1/2}^{n} + b_kE_z\Big|_{i,j,k+1/2}^{n}) , \quad (18)$$

$$Q_k\Big|_{i,j,k+1/2}^{n+1} = a_kQ_k\Big|_{i,j,k+1/2}^{n} - L_k\Big|_{i,j,k+1/2}^{n} + b_kE_z\Big|_{i,j,k+1/2}^{n} , \quad (19)$$

$$L_k\Big|_{i,j,k+1/2}^{n+1} = \exp(-2\gamma_k\Delta t)Q_k\Big|_{i,j,k+1/2}^{n} , \quad (20)$$

where $a_k = 2\exp(-\gamma_k\Delta t)\cos(\beta_k\Delta t)$, $b_k = \tilde{G}_k\Delta t\exp(-\gamma_k\Delta t)\sin(\beta_k\Delta t)$ and $(k=1,2,..,M)$. We can calculate E_z^{n+1}, the current value of *E* from the current of *D*, the previous value of *E* and the previous values of *Q* and *L*. The real advantage comes when we deal with more complicated materials. A similar method can be used for other regions of SC-PML.

III. NUMERICAL RESULT

To show the validity of the proposed D-B CFS-PML formulations, we implement a 3-D FDTD simulation for the linear two-term Lorentz dispersive problem in a cubic FDTD grid. A modulated Gaussian pulse with a vertically polarized point electric dipole source, was excited at the center of a $40\Delta_x\times 40\Delta_y\times 40\Delta_z$ electrically dispersive computational domain, entirely composed of a two-term Lorentz material with the following parameters: M=2, ε_∞=2, ε_s=4, G_1=0.8, $\omega_{p1}=\omega_{01}=2\pi\times 14\times 10^9$ rad/s, $\Gamma_1 = 0.06\omega_{01}$, G_2=0.2, $\omega_{p2}=\omega_{02}=2\pi\times 20\times 10^9$ rad/s and $\Gamma_2 = 0.07\omega_{02}$. The excited Gaussian pulse is given by:

$$E_z = \sin(2\pi f_c t)\exp(-(t-t_0)^2/t_w^2) , \quad (21)$$

where f_c=25 GHz, t_w=31 ps and t_0=4 t_w. The simulation is done with a $40\times 40\times 40$ grid including 10-cell thick PML layers at each edge, as shown in Fig. 1. The space is discretized with the FDTD lattice with $\Delta x=\Delta y=\Delta z=120\,\mu$m and the time step is Δt=0.324 ps. Within the PML, σ_η and κ_η are scaled using a fourth-order polynomial scaling and α_η is a constant, as in [3]. The relative reflection error (in decibels) versus time is computed at an observation point located at (48, 48, 48), using error $=20\log_{10}(|E_z(t)-E_{zref}(t)|/|E_{zref\_max}|)$, where $E_z(t)$ is the field computed using the test domain, $E_{zref}(t)$ is the reference field based on an extended lattice and E_{zref_max} is the maximum value of the reference solution over the full-time simulation. The relative reflection error of the ZT-CFS-PML is computed first over 6000 time iterations for κ_{max}=16, α_η=0.07 and σ_{max}=93.78 S/m. This same example is repeated with the ZT-SC-PML (κ_{max}=16, α_η=0, and σ_{max}=106.28 S/m) and the ADE-SC-PML (κ_{max}=10, α_η=0, and σ_{max}=112.54 S/m). These optimum parameters are chosen empirically to obtain the lowest reflection. The difference of the optimum parameters of ZT-CFS-PML and ADE-SC-PML results from different schemes (i.e., the coefficients of (15)-(17) are different from the counterpart of proposed SC-PML in [18]).

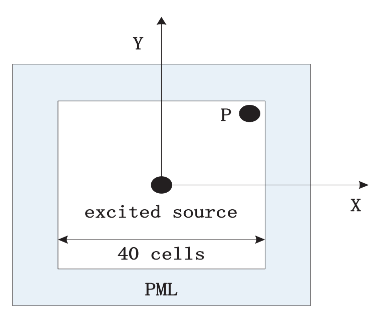

Fig.1. the FDTD grid geometry in this simulation.

These results are illustrated in Fig. 2. It is shown in Fig. 2, that the maximum relative errors of the ZT-CFS-PML, the ZT-SC-PML and the ADE-SC-PML are -78 dB, -63 dB and -63 dB, respectively. It can be concluded from Fig. 2, that the absorbing performance of the ZT-CFS-PML has 15 dB improvement in terms of the maximum relative error as compared with the ZT-SC-PML and the ADE-SC-PML and much lower reflection error for the late-time region; whereas the ZT-SC-PML and the ADE-SC-PML have comparatively high reflection errors over the entire simulation, due to the oblique incidence of the waves and low-frequency evanescent fields that are interacting with the PML interfaces.

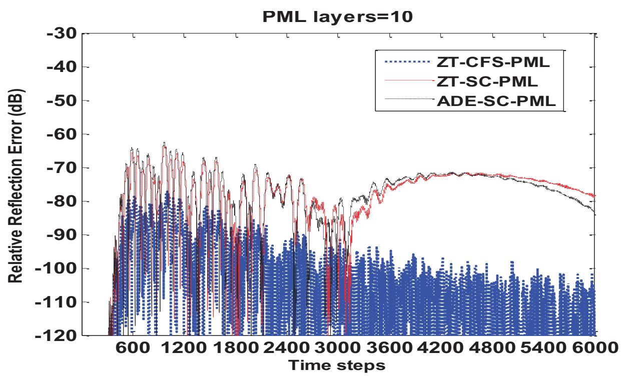

Fig. 2. Relative reflection error versus time: the ZT-CFS-PML, the ZT-SC-PML and the ADE-SC-PML, for a linear two-term Lorentz dispersive FDTD problem.

In the second example, in order to show the validity of the proposed algorithm, the second 3D inhomogeneous problem is used for validating the proposed formulations. We implement the 3D problem of the electromagnetic scattering by a highly elongated object, is studied in [20]. Particllarly, a thin 100 mm × 25 mm plate is immersed in a background media [20] with constitutive parameters ε and σ , shown in Fig. 3.

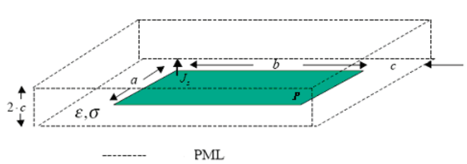

Fig. 3. The FDTD grid geometry in this simulation.

For the purposes of this study, constitutive parameters for soil are assumed, giving σ =0.273 and ε_r =7.73. The plate is illuminated by a vertically polarized electric current source placed just above one corner of the plate. The current source is given a differentiated Gaussian time signature with a 6 GHz bandwidth. The simulation is done with a $126\times51\times26$ grid, including 10-cell-thick PML layers placed only three cells from the scatter on all sides with the space steps $\Delta x=\Delta y=\Delta z=1$ mm. To study the reflection error due to the proposed ZT-CFS-PML, a reference problem is also simulated. To this end, the same mesh is extended 50 cells out in all dimensions, leading to a $226\times151\times126$ cell lattice. The fields within the lattice are then excited by an identical source and the time-dependent fields are recorded within the region representing the original lattice. The relative reflection error (in dB) versus time is computed at an observation point in the corner of the computational domain using equation in [20]. The relative reflection error is first computed over 1800 time iterations. The relative reflection error computed with 10 cells PML is recorded in Fig. 4.

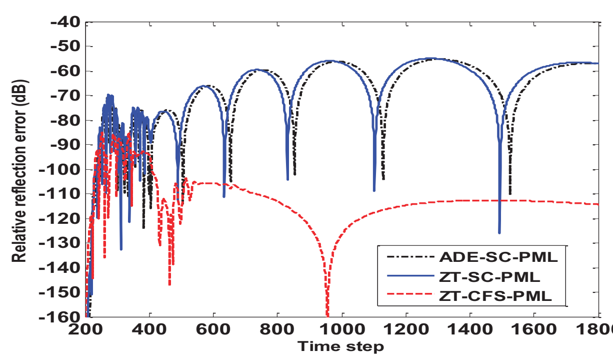

Fig. 4. Relative reflection error versus time: the ZT-CFS-PML, the ZT-SC-PML and the ADE-SC-PML.

These results are illustrated in Fig. 4. It is shown in Fig. 4, that the maximum relative errors of the ZT-CFS-PML, the ZT-SC-PML and the ADE-SC-PML are -85 dB, -54 dB and -54 dB, respectively. It can be concluded from Fig. 4, that the absorbing performance of the ZT-CFS-PML has31 dB improvement in terms of the maximum relative error, as compared with the ZT-SC-PML and the ADE-SC-PML and much lower reflection error for the late-time region; whereas the ZT-SC-PML and the ADE-SC-PML have comparatively high reflection errors over the entire simulation, due to the oblique incidence of the waves and low-frequency evanescent fields that are interacting with the PML interfaces.

IV. CONCLUSION

The D-B CFS-PML based on the unsplit-field formulations and the *Z*-transform method has been presented for truncating open-region multi-term Lorentz dispersive FDTD domains. These formulations are fully independent of the material properties of the FDTD computational domain and hence arbitrary media, like the Debye and Drude models, can be truncated without any modification and all that is needed is to modify the D-B constitutive relations under consideration. It is clearly shown in the numerical tests that the proposed formulations with the CFS-PML scheme, are efficient in the absorption of evanescent waves and in the reduction of the late-time reflections.

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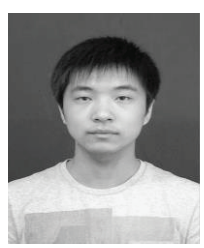

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