

**A THREE-DIMENSIONAL FINITE-DIFFERENCE
TIME-DOMAIN FORMULATION FOR NONLINEAR
MATERIALS WITH THE FREQUENCY-DEPENDENT
ELECTRIC CONDUCTIVITY AND POLARIZATION**

S. Joe Yakura and David Dietz

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Final Report

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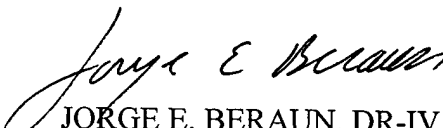
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**A Three-Dimensional Finite-Difference Time-Domain Formulation
For Nonlinear Materials with the Frequency-Dependent Electric Conductivity and Polarization**

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Abstract

In this paper, we present a three-dimensional finite-difference time-domain (FDTD) algorithm that is used to evaluate the propagation of electromagnetic waves in conductive and dispersive materials that exhibit the frequency-dependent electric conductivity and polarization. We consider a case where the electric conductivity has the linear property, specifically through the first-order (linear) electric conductivity function, and the electric polarization has both linear and nonlinear properties, specifically through the first-order (linear) and third-order (nonlinear) electric susceptibility functions. The resulting FDTD algorithm shows that the nonlinear dispersive material with a third-order susceptibility function results in coupled nonlinear cubic equations for the three components of the electric field vector, relating the next-time-step electric field vector to the previous-time-step electric field vector. This contrasts the usual algorithm of the linear conductive and dispersive material, which has a simple linear relationship between the next-time-step electric field and the previous-time-step electric field. Consequently, the coupled nonlinear cubic equations must be solved at each time step to simulate the behavior of the electric field vector in the nonlinear dispersive material that contains both frequency-dependent electric conductivity and polarization.

I. INTRODUCTION

There has been considerable interest in understanding the transient behavior of an ultrafast laser pulse that interacts with a nonlinear dispersive material. In the last several years many experimentalists have made use of newly developed Kerr lens mode-locked titanium-sapphire lasers to perform well-controlled experiments to obtain accurate measurements of the transient behavior of ultrafast laser pulses in simple molecular liquids and solids which are known to exhibit nonlinear optical behavior [1]. To better understand the details of nonlinear processes that are observed in the experiments, numerical simulations have been used extensively to reproduce observed nonlinear effects. Until recently most computer simulation has been performed by solving an approximation to Maxwell's equations, known as the generalized nonlinear Schrödinger (GNLS) equation [2], to get information about the time evolution of the envelope of the propagating oscillating wave packet so that one can obtain the overall shape of the propagating optical pulse. Because a GNLS equation-based computer simulation does not provide any information about the details of the oscillating waves inside the envelope of the optical pulse, there is a renewed interest in solving Maxwell's equations directly without having to rely on any approximations.

With the advent of present day computers which provide very fast execution times and great quantities of computer memory, we are at the point where we have enough computational power to solve Maxwell's equations directly for nonlinear dispersive materials. Among recently investigated numerical techniques that show great promise in achieving this goal is the well-known finite-difference time-domain (FDTD) method [3]. It is based on using a simple differencing scheme in both time and space to calculate the transient behavior of electromagnetic field quantities. Because of the simplicity of the FDTD method, recent researchers have focused their attention on the numerical evaluation of the linear and nonlinear convolution integral terms which appear in one of Maxwell's equations (Ampère's Law). By properly evaluating these terms, many people have successfully modeled the response of linear and nonlinear dispersive effects [4-10].

In this paper we consider the isotropic materials that exhibit both linear and nonlinear polarization properties, specifically through the first-order (linear) and third-order (nonlinear) electric susceptibility functions, $X_p^{(1)}(t-\tau)$ and $X_p^{(3)}(t, \tau, t_1, t_2)$, respectively. For such materials the relationship between $\underline{D}(t; \underline{x})$ and $\underline{E}(t; \underline{x})$ can be expressed as [11]

$$\begin{aligned} \underline{D}(t; \underline{x}) = & \epsilon_0 \epsilon_\infty \underline{E}(t; \underline{x}) + \epsilon_0 \sum_p \int_{-\infty}^{\infty} \underline{E}(\tau; \underline{x}) X_p^{(1)}(t-\tau) d\tau \\ & + \epsilon_0 \sum_p \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \underline{E}(t_2; \underline{x}) [\underline{E}(t_1; \underline{x}) \bullet \underline{E}(\tau; \underline{x})] X_p^{(3)}(t, \tau, t_1, t_2) dt_2 dt_1 d\tau, \end{aligned} \quad (1.1)$$

where ϵ_0 is the electric permittivity of free space, ϵ_∞ is the medium permittivity at infinite frequency, and $X_\rho^{(1)}(t-\tau)$ is the ρ th term of the collection consisting of ρ_{max} time dependent, first-order electric susceptibility functions, where ρ_{max} is the maximum number of terms which we choose to consider for a particular formulation of Eq. (1.1), $X_\rho^{(3)}(t, \tau, t_1, t_2)$ is the ρ th term of the four-time dependent third-order susceptibility function which contributes to the nonlinear behavior of the material and \bullet is the notation used for the dot product of vectors. When $X_\rho^{(3)}(t, \tau, t_1, t_2)$ is reduced to the single-time dependent susceptibility function, $\chi_\rho^{(3)}(t_1-t_2)$, by making use of the following Born-Oppenheimer approximation [11]:

$$X_\rho^{(3)}(t, \tau, t_1, t_2) = \delta(\tau - t_1) \delta(t - t_2) [\chi_\rho^{(3)}(t_2 - t_1) + \delta(t_2 - t) \alpha_{0\rho}^{(3)}], \quad (1.2)$$

where $\alpha_{0\rho}^{(3)}$ is a constant and $\delta(t)$ is the Dirac delta function, we can show that Eq. (1.1) reduces to an expression that consists of sums of convolution integrals of linear and nonlinear terms; namely,

$$\begin{aligned} \underline{D}(t; \underline{x}) = & \epsilon_0 \epsilon_\infty \underline{E}(t; \underline{x}) + \epsilon_0 \sum_\rho \int_{-\infty}^{\infty} \underline{E}(\tau; \underline{x}) X_\rho^{(1)}(t - \tau) d\tau \\ & + \epsilon_0 \underline{E}(t; \underline{x}) [\underline{E}(t; \underline{x}) \bullet \underline{E}(t; \underline{x})] \sum_\rho \alpha_{0\rho}^{(3)} + \epsilon_0 \underline{E}(t; \underline{x}) \sum_\rho \int_{-\infty}^{\infty} [\underline{E}(\tau; \underline{x}) \bullet \underline{E}(\tau; \underline{x})] \chi_\rho^{(3)}(t - \tau) d\tau. \end{aligned} \quad (1.3)$$

We also consider in this paper the case where the current vector, $\underline{J}(t; \underline{x})$, which appears in Ampere's Law, is represented by two contributions: the first term is directly proportional to the electric field vector, $\underline{E}(t, \underline{x})$, with the constant conductivity coefficient, $\sigma^{(0)}$, and the second term is expressed in the linear convolution integral of $\underline{E}(t; \underline{x})$ and the first-order time dependent conductivity function, $\sigma^{(1)}(t)$. Hence, we express the current vector in the form as shown below.

$$\underline{J}(t; \underline{x}) = \sigma^{(0)} \underline{E}(t; \underline{x}) + \int_{-\infty}^{\infty} \underline{E}(\tau; \underline{x}) \sigma^{(1)}(t - \tau) d\tau. \quad (1.4)$$

Based on the above expressions, we provide a general FDTD formulation for evaluating the linear and nonlinear convolution integrals that appear in Ampere's Law. We investigate, in particular, the case in which the first-order electric susceptibility function, the third-order electric susceptibility function, and the first-order time dependent conductivity function are all expressed in the following complex exponential forms that contain complex constant coefficients:

$$X_\rho^{(1)}(t) = \text{Re} \{ \alpha_\rho^L \exp(-\gamma_\rho^L t) \} U(t), \quad (1.5)$$

$$\chi_\rho^{(3)}(t) = \text{Re} \{ \alpha_\rho^{NL} \exp(-\gamma_\rho^{NL} t) \} U(t), \quad \text{and} \quad (1.6)$$

$$\sigma^{(1)}(t) = \text{Re} \{ \beta^L \exp(-\theta^L t) \} U(t). \quad (1.7)$$

where $\text{Re}\{ \}$ is used to represent the real part of a complex function, $U(t)$ is the unit step function, and α_ρ^L , α_ρ^{NL} , β^L , γ_ρ^L , γ_ρ^{NL} and θ^L are complex constant coefficients; superscripts L and NL are used to distinguish between linear and nonlinear coefficients. By making the proper choices of complex constant coefficients and performing Fourier transforms, we can readily obtain the familiar Debye and Lorentz forms of the complex conductivity and permittivity in the frequency domain.

II. FDTD FORMULATION

In light of Eqs. (1.3) and (1.4), we write Maxwell's equations inside the dispersive material as

$$\frac{\partial [\mu \underline{H}(t; \underline{x})]}{\partial t} = -\nabla \times \underline{E}(t; \underline{x}), \quad (2.1)$$

$$\frac{\partial \underline{D}(t; \underline{x})}{\partial t} = \nabla \times \underline{H}(t; \underline{x}) - \sigma^{(0)} \underline{E}(t; \underline{x}) - \underline{J}^L(t; \underline{x}), \quad (2.2)$$

with

$$\begin{aligned} \underline{D}(t; \underline{x}) = & \epsilon_{\infty} \underline{E}(t; \underline{x}) + \epsilon_0 \sum_{\rho} \underline{P}_{\rho}^L(t; \underline{x}) \\ & + \epsilon_0 \underline{E}(t; \underline{x}) \sum_{\rho} P_{\rho}^{NL}(t; \underline{x}) + \epsilon_0 \underline{E}(t; \underline{x}) [\underline{E}(t; \underline{x}) \bullet \underline{E}(t; \underline{x})] \sum_{\rho} \alpha_{\rho}^{(3)}, \end{aligned} \quad (2.3)$$

$$\underline{P}_{\rho}^L(t; \underline{x}) \equiv \int_{-\infty}^{\infty} \underline{E}(\tau; \underline{x}) \chi_{\rho}^{(1)}(t-\tau) d\tau, \quad (2.4)$$

$$P_{\rho}^{NL}(t; \underline{x}) \equiv \int_{-\infty}^{\infty} [\underline{E}(\tau; \underline{x}) \bullet \underline{E}(\tau; \underline{x})] \chi_{\rho}^{(3)}(t-\tau) d\tau, \quad (2.5)$$

$$\underline{J}^L(t; \underline{x}) = \int_{-\infty}^{\infty} \underline{E}(\tau; \underline{x}) \sigma^{(1)}(t-\tau) d\tau, \quad (2.6)$$

where $\underline{H}(t; \underline{x})$ is the magnetic field vector, μ is the magnetic permeability, $\underline{P}_{\rho}^L(t; \underline{x})$ and $[\underline{E}(t; \underline{x}) P_{\rho}^{NL}(t; \underline{x})]$ are related to the ρ th terms of linear and nonlinear polarization field vectors, respectively, and $\underline{J}^L(t; \underline{x})$ is the first-order time dependent conductivity. Using an FDTD algorithm, the above equations can be solved numerically at each time step provided we can handle $\underline{J}^L(t; \underline{x})$, $\underline{P}_{\rho}^L(t; \underline{x})$ and $P_{\rho}^{NL}(t; \underline{x})$ numerically. Therefore, the whole solution rests on the question of how to carry out the numerical evaluation of $\underline{J}^L(t; \underline{x})$, $\underline{P}_{\rho}^L(t; \underline{x})$ and $P_{\rho}^{NL}(t; \underline{x})$ at each successive time step. For that reason, the rest of this section is devoted to the discussion of numerical formulation that treats $\underline{J}^L(t; \underline{x})$, $\underline{P}_{\rho}^L(t; \underline{x})$ and $P_{\rho}^{NL}(t; \underline{x})$.

To obtain second-order accuracy in time in evaluating the convolution integrals, $\underline{E}(t; \underline{x})$ is approximated by a piecewise continuous function over the entire temporal integration range so that $\underline{E}(t; \underline{x})$ changes linearly with respect to time over a given discrete time interval $[m\Delta t, (m+1)\Delta t]$, where $m=0, 1, \dots, n$, with $n\Delta t$ being the current time step [12,13]. Thus, the mathematical expression for $\underline{E}(t; \underline{x})$ takes the following form which can be expressed in terms of the electric field values, \underline{E}_{ijk}^m and $\underline{E}_{ijk}^{m+1}$, respectively, evaluated at discrete time steps $t=m\Delta t$ and $t=(m+1)\Delta t$ where these two successive times are obtained at the same discrete spatial location $\underline{x}=(i\Delta x, j\Delta y, k\Delta z)$ with Δx , Δy and Δz being the spatial grid sizes in the x , y and z directions, respectively (we use a superscript to designate the discrete time step and a subscript for the discrete spatial location):

$$\begin{aligned} \underline{E}(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} &= \left\{ \underline{E}_{ijk}^m + \frac{(\underline{E}_{ijk}^{m+1} - \underline{E}_{ijk}^m)}{\Delta t} (t - m\Delta t) \right\} \text{ for } 0 \leq m\Delta t \leq t \leq (m+1)\Delta t \leq (n+1)\Delta t; \text{ and} \\ \underline{E}(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} &= 0 \quad \text{for } t \leq 0. \end{aligned} \quad (2.7)$$

For three-dimensional FDTD calculations in Cartesian coordinates, we need to solve the following discrete forms of Maxwell's equations which are obtained from Eqs. (2.1) and (2.2) by finite differencing in both time and space using the usual Yee algorithm [3]:

$$\mu(H_{ijk}^{n+1/2})_x - \mu(H_{ijk}^{n-1/2})_x = \left\{ \frac{\Delta t}{\Delta z} [(E_{ij(k+1/2)k}^n)_y - (E_{ij(k-1/2)k}^n)_y] - \frac{\Delta t}{\Delta y} [(E_{i(j+1/2)k}^n)_z - (E_{i(j-1/2)k}^n)_z] \right\}, \quad (2.8)$$

$$\mu(H_{ijk}^{n+1/2})_y - \mu(H_{ijk}^{n-1/2})_y = \left\{ \frac{\Delta t}{\Delta x} [(E_{(i+1/2)jk}^n)_z - (E_{(i-1/2)jk}^n)_z] - \frac{\Delta t}{\Delta z} [(E_{ij(k+1/2)}^n)_x - (E_{ij(k-1/2)}^n)_x] \right\}, \quad (2.9)$$

$$\mu(H_{ijk}^{n+1/2})_z - \mu(H_{ijk}^{n-1/2})_z = \left\{ \frac{\Delta t}{\Delta y} [(E_{i(j+1/2)k}^n)_x - (E_{i(j-1/2)k}^n)_x] - \frac{\Delta t}{\Delta x} [(E_{(i+1/2)jk}^n)_y - (E_{(i-1/2)jk}^n)_y] \right\}, \quad (2.10)$$

$$\begin{aligned} (D_{ijk}^{n+1})_x - (D_{ijk}^n)_x &= \left\{ \frac{\Delta t}{\Delta y} [(H_{i(j+1/2)k}^{n+1/2})_z - (H_{i(j-1/2)k}^{n+1/2})_z] - \frac{\Delta t}{\Delta z} [(H_{ij(k+1/2)}^{n+1/2})_y - (H_{ij(k-1/2)}^{n+1/2})_y] \right\} \\ &\quad - \sigma^{(0)} \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (E(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_x dt \right\} - \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (J^L(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_x dt \right\}, \end{aligned} \quad (2.11)$$

$$(D_{ijk}^{n+1})_y - (D_{ijk}^n)_y = \left\{ \frac{\Delta t}{\Delta x} \left[(H_{ij(k+1/2)}^{n+1/2})_x - (H_{ij(k-1/2)}^{n+1/2})_x \right] - \frac{\Delta t}{\Delta x} \left[(H_{(i+1/2)jk}^{n+1/2})_z - (H_{(i-1/2)jk}^{n+1/2})_z \right] \right\} \\ - \sigma^{(0)} \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (E(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_y dt \right\} - \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (J^L(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_y dt \right\}, \quad (2.12)$$

$$(D_{ijk}^{n+1})_z - (D_{ijk}^n)_z = \left\{ \frac{\Delta t}{\Delta x} \left[(H_{(i+1/2)jk}^{n+1/2})_y - (H_{(i-1/2)jk}^{n+1/2})_y \right] - \frac{\Delta t}{\Delta y} \left[(H_{i(j+1/2)k}^{n+1/2})_x - (H_{i(j-1/2)k}^{n+1/2})_x \right] \right\} \\ - \sigma^{(0)} \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (E(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_z dt \right\} - \left\{ \int_{n\Delta t}^{(n+1)\Delta t} (J^L(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)})_z dt \right\}. \quad (2.13)$$

To evaluate the right-hand side of Eqs. (2.11-2.13), we first begin by substituting Eq. (1.5) into Eq. (2.4) and Eq. (1.6) into Eq. (2.5) and then differentiating these integrals with respect to time to obtain the following first-order differential equations for complex functions $Q_\rho^L(t; \underline{x})$ and $Q_\rho^{NL}(t; \underline{x})$:

$$\frac{\partial Q_\rho^L(t; \underline{x})}{\partial t} + \gamma_\rho^L Q_\rho^L(t; \underline{x}) = \alpha_\rho^L \underline{E}(t; \underline{x}), \quad (2.14)$$

$$\frac{\partial Q_\rho^{NL}(t; \underline{x})}{\partial t} + \gamma_\rho^{NL} Q_\rho^{NL}(t; \underline{x}) = \alpha_\rho^{NL} [\underline{E}(t; \underline{x}) \bullet \underline{E}(t; \underline{x})]. \quad (2.15)$$

From these equations, the linear and nonlinear polarization vectors, $\underline{P}_\rho^L(t; \underline{x})$ and $[\underline{E}(t; \underline{x}) \underline{P}_\rho^{NL}(t; \underline{x})]$, can be obtained simply by taking the real parts of $Q_\rho^L(t; \underline{x})$ and $[\underline{E}(t; \underline{x}) Q_\rho^{NL}(t; \underline{x})]$, respectively. Now, solving these two equations *exactly* by using integrating factors $\exp(\gamma_\rho^L t)$ and $\exp(\gamma_\rho^{NL} t)$, respectively, and then performing the time integration from $n\Delta t$ to $(n+1)\Delta t$, we have

$$\underline{Q}_\rho^L(n\Delta t + \Delta t; \underline{x}) = \exp(-\gamma_\rho^L \Delta t) \underline{Q}_\rho^L(n\Delta t; \underline{x}) + \alpha_\rho^L \exp(-\gamma_\rho^L \Delta t) \int_{n\Delta t}^{n\Delta t + \Delta t} \underline{E}(\tau; \underline{x}) \exp[-\gamma_\rho^L(n\Delta t - \tau)] d\tau, \quad (2.16)$$

and

$$Q_\rho^{NL}(n\Delta t + \Delta t; \underline{x}) = \exp(-\gamma_\rho^{NL} \Delta t) Q_\rho^{NL}(n\Delta t; \underline{x}) \\ + \alpha_\rho^{NL} \exp(-\gamma_\rho^{NL} \Delta t) \int_{n\Delta t}^{n\Delta t + \Delta t} [\underline{E}(\tau; \underline{x}) \bullet \underline{E}(\tau; \underline{x})] \exp[-\gamma_\rho^{NL}(n\Delta t - \tau)] d\tau. \quad (2.17)$$

Based on the piecewise linear approximation which we have considered for the temporal behavior of $\underline{E}(t; \underline{x})$, we can substitute Eq. (2.7) into the right-hand side (i.e., the inhomogeneous part) of Eqs. (2.16) and (2.17) for $\underline{E}(t; \underline{x})$. Evaluating at spatial location $\underline{x}=(i\Delta x, j\Delta y, k\Delta z)$, these equations result in the following recursive relationships for $(Q_\rho^L)_{ijk}^{n+1}$ and $(Q_\rho^{NL})_{ijk}^{n+1}$ in terms of $(Q_\rho^L)_{ijk}^n$, $(Q_\rho^{NL})_{ijk}^n$, \underline{E}_{ijk}^n and $\underline{E}_{ijk}^{n+1}$:

$$\underline{Q}_\rho^L(n\Delta t + \Delta t; i\Delta x, j\Delta y, k\Delta z) \equiv (\underline{Q}_\rho^L)_{ijk}^{n+1} = \exp(-\gamma_\rho^L \Delta t) (\underline{Q}_\rho^L)_{ijk}^n + \underline{E}_{ijk}^n (\psi_{\rho,0}^L) + (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) (\psi_{\rho,1}^L), \quad (2.18)$$

and

$$Q_\rho^{NL}(n\Delta t + \Delta t; i\Delta x, j\Delta y, k\Delta z) \equiv (Q_\rho^{NL})_{ijk}^{n+1} = \exp(-\gamma_\rho^{NL} \Delta t) (Q_\rho^{NL})_{ijk}^n + [(\underline{E}_{ijk}^n \bullet \underline{E}_{ijk}^n)] (\psi_{\rho,0}^{NL}) \\ + 2 [\underline{E}_{ijk}^n \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,1}^{NL}) \\ + [(\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,2}^{NL}). \quad (2.19)$$

where

$$(\psi_{\rho,0}^L) \equiv \alpha_\rho^L \int_{n\Delta t}^{(n+1)\Delta t} \exp[-\gamma_\rho^L(n\Delta t + \Delta t - \tau)] d\tau = \alpha_\rho^L \int_0^{\Delta t} \exp(-\gamma_\rho^L \tau) d\tau = \frac{\alpha_\rho^L}{\gamma_\rho^L} [1 - \exp(-\gamma_\rho^L \Delta t)], \quad (2.20)$$

$$(\psi_{\rho,1}^L) \equiv \frac{\alpha_\rho^L}{\Delta t} \int_0^{\Delta t} (\Delta t - \tau) \exp(-\gamma_\rho^L \tau) d\tau = \frac{\alpha_\rho^L}{\gamma_\rho^L} \left\{ 1 - \frac{1}{\gamma_\rho^L \Delta t} [1 - \exp(-\gamma_\rho^L \Delta t)] \right\}, \quad (2.21)$$

$$(\psi_{\rho,0}^{NL}) \equiv \alpha_{\rho}^{NL} \int_0^{\Delta t} \exp(-\gamma_{\rho}^{NL} \tau) d\tau = \frac{\alpha_{\rho}^{NL}}{\gamma_{\rho}^{NL}} [1 - \exp(-\gamma_{\rho}^{NL} \Delta t)], \quad (2.22)$$

$$(\psi_{\rho,1}^{NL}) \equiv \frac{\alpha_{\rho}^{NL}}{\Delta t} \int_0^{\Delta t} (\Delta t - \tau) \exp(-\gamma_{\rho}^{NL} \tau) d\tau = \frac{\alpha_{\rho}^{NL}}{\gamma_{\rho}^{NL}} \left\{ 1 - \frac{1}{\gamma_{\rho}^{NL} \Delta t} [1 - \exp(-\gamma_{\rho}^{NL} \Delta t)] \right\}, \quad (2.23)$$

$$(\psi_{\rho,2}^{NL}) \equiv \frac{\alpha_{\rho}^{NL}}{(\Delta t)^2} \int_0^{\Delta t} (\Delta t - \tau)^2 \exp(-\gamma_{\rho}^{NL} \tau) d\tau = \frac{\alpha_{\rho}^{NL}}{\gamma_{\rho}^{NL}} \left\{ 1 - \frac{2}{\gamma_{\rho}^{NL} \Delta t} \left[1 - \frac{1}{\gamma_{\rho}^{NL} \Delta t} [1 - \exp(-\gamma_{\rho}^{NL} \Delta t)] \right] \right\}. \quad (2.24)$$

When Eqs. (2.18) and (2.19) are used in Eq. (2.3) to obtain discrete forms of Eq. (2.3) at two successive times $t=n\Delta t$ and $t=(n+1)\Delta t$ and at specific spatial location $\underline{x}=(i\Delta x, j\Delta y, k\Delta z)$, we can express \underline{D}_{ijk}^n and $\underline{D}_{ijk}^{n+1}$, respectively, in the following forms:

$$\underline{D}_{ijk}^n = \epsilon_0 \epsilon_{\infty} \underline{E}_{ijk}^n + \epsilon_0 \sum_{\rho} \text{Re} \{ (\underline{Q}_{\rho}^L)_{ijk}^n \} + \epsilon_0 \underline{E}_{ijk}^n \sum_{\rho} \text{Re} \{ (Q_{\rho}^{NL})_{ijk}^n \} + \epsilon_0 \underline{E}_{ijk}^n [\underline{E}_{ijk}^n \bullet \underline{E}_{ijk}^n] \sum_{\rho} \alpha_{0\rho}^{(3)}, \quad (2.25)$$

and

$$\begin{aligned} \underline{D}_{ijk}^{n+1} = & \epsilon_0 \epsilon_{\infty} \underline{E}_{ijk}^{n+1} + \epsilon_0 \sum_{\rho} \text{Re} \{ [\exp(-\gamma_{\rho}^L \Delta t)] ((\underline{Q}_{\rho}^L)_{ijk}^n] + \underline{E}_{ijk}^n (\psi_{\rho,0}^L) + (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) (\psi_{\rho,1}^L) \} \\ & + \epsilon_0 \sum_{\rho} \text{Re} \{ \underline{E}_{ijk}^{n+1} \exp(-\gamma_{\rho}^{NL} \Delta t) ((Q_{\rho}^{NL})_{ijk}^n + \underline{E}_{ijk}^{n+1} [(\underline{E}_{ijk}^n \bullet \underline{E}_{ijk}^n)] (\psi_{\rho,0}^{NL}) \\ & + 2 \underline{E}_{ijk}^{n+1} [\underline{E}_{ijk}^n \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,1}^{NL}) + \underline{E}_{ijk}^{n+1} [(\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,2}^{NL}) \} \\ & + \epsilon_0 \underline{E}_{ijk}^{n+1} [\underline{E}_{ijk}^{n+1} \bullet \underline{E}_{ijk}^{n+1}] \sum_{\rho} \alpha_{0\rho}^{(3)}. \end{aligned} \quad (2.26)$$

Subtracting Eq. (2.25) from Eq. (2.26), we obtain the following expression for the left-hand side of Eqs. (2.11-2.13) in terms of $(\underline{Q}_{\rho}^L)_{ijk}^n$, $(Q_{\rho}^{NL})_{ijk}^n$, \underline{E}_{ijk}^n and $\underline{E}_{ijk}^{n+1}$:

$$\begin{aligned} \underline{D}_{ijk}^{n+1} - \underline{D}_{ijk}^n = & \epsilon_0 \epsilon_{\infty} (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) \\ & + \epsilon_0 \sum_{\rho} \text{Re} \{ [\exp(-\gamma_{\rho}^L \Delta t) - 1] ((\underline{Q}_{\rho}^L)_{ijk}^n] + \underline{E}_{ijk}^n (\psi_{\rho,0}^L) + (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) (\psi_{\rho,1}^L) \} \\ & + \epsilon_0 \sum_{\rho} \text{Re} \{ [\underline{E}_{ijk}^{n+1} \exp(-\gamma_{\rho}^{NL} \Delta t) - \underline{E}_{ijk}^n] ((Q_{\rho}^{NL})_{ijk}^n + \underline{E}_{ijk}^{n+1} [(\underline{E}_{ijk}^n \bullet \underline{E}_{ijk}^n)] (\psi_{\rho,0}^{NL}) \\ & + 2 \underline{E}_{ijk}^{n+1} [\underline{E}_{ijk}^n \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,1}^{NL}) + \underline{E}_{ijk}^{n+1} [(\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) \bullet (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)] (\psi_{\rho,2}^{NL}) \} \\ & + \epsilon_0 [\underline{E}_{ijk}^{n+1} [(\underline{E}_{ijk}^{n+1} \bullet \underline{E}_{ijk}^{n+1})] - \underline{E}_{ijk}^n [(\underline{E}_{ijk}^n \bullet \underline{E}_{ijk}^n)]] \sum_{\rho} \alpha_{0\rho}^{(3)}. \end{aligned} \quad (2.27)$$

To evaluate the second term of the right-hand side of Eqs. (2.11-2.13), we substitute Eq. (2.7) for $\underline{E}(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)}$ and obtain the following expression:

$$\sigma^{(0)} \left\{ \int_{n\Delta t}^{(n+1)\Delta t} \underline{E}(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} dt \right\} = \sigma^{(0)} \frac{\Delta t}{2} (\underline{E}_{ijk}^{n+1} + \underline{E}_{ijk}^n). \quad (2.28)$$

To evaluate the third term of the right-hand side of Eqs. (2.11-2.13), we first substitute Eq. (1.7) into Eq. (2.6) and then differentiate the integral with respect to time to obtain the following first-order differential equation for complex function $\underline{J}^L(t; \underline{x})$:

$$\frac{\partial \underline{J}^L(t; \underline{x})}{\partial t} + \theta^L \underline{J}^L(t; \underline{x}) = \beta^L \underline{E}(t; \underline{x}). \quad (2.29)$$

As in the case of linear and nonlinear polarization vectors, the current vector, $\underline{J}^L(t; \underline{x})$, can be obtained simply by taking the real part of $\underline{J}^L(t; \underline{x})$ in the above equation. Once again, we solve the above differential equation *exactly* by using integrating factor $\exp(\theta^L t)$ and then performing the time integration from $n\Delta t$ to t to get the following expression for complex function $\underline{J}^L(t; \underline{x})$:

$$\underline{J}^L(t; \underline{x}) = \exp[\theta^L(n\Delta t - t)] \underline{J}^L(n\Delta t; \underline{x}) + \beta^L \exp(-\theta^L t) \int_{n\Delta t}^t \exp(\theta^L \tau) \underline{E}(\tau; \underline{x}) d\tau \quad (2.30)$$

Again, we substitute Eq. (2.7) into the above equation for $\underline{E}(t; \underline{x})$ based on the piecewise linear approximation. Then we integrate Eq. (2.30) from $n\Delta t$ to $n\Delta t + \Delta t$, evaluated at spatial location $\underline{x} = (i\Delta x, j\Delta y, k\Delta z)$, to obtain the following expression for the third term of the right-hand side of Eqs. (2.11-2.13):

$$\begin{aligned} \int_{n\Delta t}^{(n+1)\Delta t} \underline{J}^L(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} dt &= \text{Re} \left\{ \int_{n\Delta t}^{(n+1)\Delta t} \underline{J}^L(t; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} dt \right\} \\ &= \text{Re} \left\{ \exp(\theta^L n\Delta t) \underline{J}^L(n\Delta t; i\Delta x, j\Delta y, k\Delta z) \int_{n\Delta t}^{(n+1)\Delta t} \exp(-\theta^L t) dt \right. \\ &\quad \left. + \beta^L \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^t \exp[\theta^L(\tau - t)] \underline{E}(\tau; \underline{x})_{\underline{x}=(i\Delta x, j\Delta y, k\Delta z)} d\tau dt \right\} \\ &= \text{Re} \left\{ \exp(\theta^L n\Delta t) (\underline{J}^L)_{ijk}^n \int_{n\Delta t}^{(n+1)\Delta t} \exp(-\theta^L t) dt \right. \\ &\quad \left. + \beta^L \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^t \exp[\theta^L(\tau - t)] \left[\underline{E}_{ijk}^n + \frac{(\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n)}{\Delta t} (\tau - n\Delta t) \right] d\tau dt \right\} \\ &= \text{Re} \left\{ \frac{1}{\theta^L} [1 - \exp(-\theta^L \Delta t)] (\underline{J}^L)_{ijk}^n + \underline{E}_{ijk}^n (\zeta_0^L) + (\underline{E}_{ijk}^{n+1} - \underline{E}_{ijk}^n) (\zeta_1^L) \right\}, \quad (2.31) \end{aligned}$$

where

$$(\zeta_0^L) \equiv \beta^L \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^t \exp[\theta^L(\tau - t)] d\tau dt = \frac{\beta^L \Delta t}{\theta^L} \left\{ 1 - \frac{1}{\theta^L \Delta t} [1 - \exp(-\theta^L \Delta t)] \right\}, \quad (2.32)$$

$$(\zeta_1^L) \equiv \frac{\beta^L}{\Delta t} \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^t (\tau - n\Delta t) \exp[\theta^L(\tau - t)] d\tau dt = \frac{\beta^L \Delta t}{\theta^L} \left\{ \frac{1}{2} - \frac{1}{\theta^L \Delta t} + \frac{1}{(\theta^L \Delta t)^2} [1 - \exp(-\theta^L \Delta t)] \right\}. \quad (2.33)$$

The $(\underline{J}^L)_{ijk}^n$ expression, which appears in Eq. (2.31), can be obtained in the recursive form when we solve Eq. (2.29) exactly for $\underline{J}^L(t; \underline{x})$ using integrating factor $\exp(\theta^L t)$ and then performing the time integration from $t=(n-1)\Delta t$ to $t=n\Delta t$ while making use of the piecewise linear approximation for $\underline{E}(t; \underline{x})$ to evaluate the integral, which arises from the right-hand side of Eq. (2.29). The result is that we obtain the following recursive relationship for $(\underline{J}^L)_{ijk}^n$ which is expressed in terms of the previous time step values of $(\underline{J}^L)_{ijk}^{n-1}$, $\underline{E}_{ijk}^{n-1}$ and \underline{E}_{ijk}^n :

$$(\underline{J}^L)_{ijk}^n = \exp(-\theta^L \Delta t) (\underline{J}^L)_{ijk}^{n-1} + \underline{E}_{ijk}^{n-1} (\zeta_0^L) + (\underline{E}_{ijk}^n - \underline{E}_{ijk}^{n-1}) (\zeta_1^L), \quad (2.34)$$

where

$$(\zeta_0^L) \equiv \beta^L \int_{(n-1)\Delta t}^{n\Delta t} \exp[-\theta^L(n\Delta t - \tau)] d\tau = \beta^L \int_0^{\Delta t} \exp(-\theta^L \tau) d\tau = \frac{\beta^L}{\theta^L} [1 - \exp(-\theta^L \Delta t)], \quad (2.35)$$

$$(\zeta_1^L) \equiv \frac{\beta^L}{\Delta t} \int_0^{\Delta t} (\Delta t - \tau) \exp(-\theta^L \tau) d\tau = \frac{\beta^L}{\theta^L} \left\{ 1 - \frac{1}{\theta^L \Delta t} [1 - \exp(-\theta^L \Delta t)] \right\}. \quad (2.36)$$

Finally, when Eqs. (2.27), (2.28) and (2.31) are substituted into Eqs. (2.11-2.13), we obtain the following three coupled nonlinear cubic equations which we need to solve for $\underline{E}_{ijk}^{n+1}$ [i.e., $(E_{ijk}^{n+1})_x$, $(E_{ijk}^{n+1})_y$ and $(E_{ijk}^{n+1})_z$] in terms of known quantities $(Q_\rho^L)_{ijk}^n$, $(Q_\rho^{NL})_{ijk}^n$, $(\underline{J}^L)_{ijk}^n$, \underline{E}_{ijk}^n and $\underline{H}_{ijk}^{n+1/2}$ which are calculated at previous time steps $t=n\Delta t$ and $t=(n+1/2)\Delta t$:

$$\begin{aligned} a_{0x} + a_1 (E_{ijk}^{n+1})_x + (E_{ijk}^{n+1})_x \{ a_{2x} (E_{ijk}^{n+1})_x + a_{2y} (E_{ijk}^{n+1})_y + a_{2z} (E_{ijk}^{n+1})_z \} \\ + a_3 (E_{ijk}^{n+1})_x \{ [(E_{ijk}^{n+1})_x]^2 + [(E_{ijk}^{n+1})_y]^2 + [(E_{ijk}^{n+1})_z]^2 \} = 0, \quad (2.37) \end{aligned}$$

$$a_{0y} + a_1 (E_{ijk}^{n+1})_y + (E_{ijk}^{n+1})_y \{ a_{2x} (E_{ijk}^{n+1})_x + a_{2y} (E_{ijk}^{n+1})_y + a_{2z} (E_{ijk}^{n+1})_z \} \\ + a_3 (E_{ijk}^{n+1})_y \{ [(E_{ijk}^{n+1})_x]^2 + [(E_{ijk}^{n+1})_y]^2 + [(E_{ijk}^{n+1})_z]^2 \} = 0, \quad (2.38)$$

$$a_{0z} + a_1 (E_{ijk}^{n+1})_z + (E_{ijk}^{n+1})_z \{ a_{2x} (E_{ijk}^{n+1})_x + a_{2y} (E_{ijk}^{n+1})_y + a_{2z} (E_{ijk}^{n+1})_z \} \\ + a_3 (E_{ijk}^{n+1})_z \{ [(E_{ijk}^{n+1})_x]^2 + [(E_{ijk}^{n+1})_y]^2 + [(E_{ijk}^{n+1})_z]^2 \} = 0, \quad (2.39)$$

where a_{0x} , a_{0y} , a_{0z} , a_1 , a_{2x} , a_{2y} , a_{2z} and a_3 are given by

$$a_{0x} \equiv \left\{ \frac{\Delta t}{\Delta z} [(H_{i(j+1/2)k}^{n+1/2})_y - (H_{ij(k-1/2)}^{n+1/2})_y] - \frac{\Delta t}{\Delta y} [(H_{i(j+1/2)k}^{n+1/2})_z - (H_{ij(k-1/2)}^{n+1/2})_z] \right\} + \sigma^{(0)} \frac{\Delta t}{2} (E_{ijk}^n)_x \\ + \operatorname{Re} \left\{ \frac{1}{\theta^L} [1 - \exp(-\theta^L \Delta t)] [(J^L)_{ijk}^n]_x \right\} + (E_{ijk}^n)_x \operatorname{Re} \left\{ (\xi_0^L) - (\xi_1^L) \right\} \\ - \epsilon_o \epsilon_\infty (E_{ijk}^n)_x + \epsilon_o \sum_\rho \operatorname{Re} \left\{ [\exp(-\gamma_\rho^L \Delta t) - 1] [(Q_\rho^L)_{ijk}^n]_x \right\} + \epsilon_o (E_{ijk}^n)_x \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,0}^L) - (\psi_{\rho,1}^L) \right\} \\ - \epsilon_o (E_{ijk}^n)_x \sum_\rho \operatorname{Re} \left\{ (Q_\rho^{NL})_{ijk}^n \right\} - \epsilon_o (E_{ijk}^n)_x \left[[(E_{ijk}^n)_x]^2 + [(E_{ijk}^n)_y]^2 + [(E_{ijk}^n)_z]^2 \right] \sum_\rho \alpha_{0\rho}^{(3)}, \quad (2.40)$$

$$a_{0y} \equiv \left\{ \frac{\Delta t}{\Delta x} [(H_{i+1/2)jk}^{n+1/2})_z - (H_{(i-1/2)jk}^{n+1/2})_z] - \frac{\Delta t}{\Delta z} [(H_{i(j+1/2)k}^{n+1/2})_x - (H_{ij(k-1/2)}^{n+1/2})_x] \right\} + \sigma^{(0)} \frac{\Delta t}{2} (E_{ijk}^n)_y \\ + \operatorname{Re} \left\{ \frac{1}{\theta^L} [1 - \exp(-\theta^L \Delta t)] [(J^L)_{ijk}^n]_y \right\} + (E_{ijk}^n)_y \operatorname{Re} \left\{ (\xi_0^L) - (\xi_1^L) \right\} \\ - \epsilon_o \epsilon_\infty (E_{ijk}^n)_y + \epsilon_o \sum_\rho \operatorname{Re} \left\{ [\exp(-\gamma_\rho^L \Delta t) - 1] [(Q_\rho^L)_{ijk}^n]_y \right\} + \epsilon_o (E_{ijk}^n)_y \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,0}^L) - (\psi_{\rho,1}^L) \right\} \\ - \epsilon_o (E_{ijk}^n)_y \sum_\rho \operatorname{Re} \left\{ (Q_\rho^{NL})_{ijk}^n \right\} - \epsilon_o (E_{ijk}^n)_y \left[[(E_{ijk}^n)_x]^2 + [(E_{ijk}^n)_y]^2 + [(E_{ijk}^n)_z]^2 \right] \sum_\rho \alpha_{0\rho}^{(3)}, \quad (2.41)$$

$$a_{0z} \equiv \left\{ \frac{\Delta t}{\Delta y} [(H_{i(j+1/2)k}^{n+1/2})_x - (H_{ij(k-1/2)}^{n+1/2})_x] - \frac{\Delta t}{\Delta x} [(H_{i+1/2)jk}^{n+1/2})_y - (H_{(i-1/2)jk}^{n+1/2})_y] \right\} + \sigma^{(0)} \frac{\Delta t}{2} (E_{ijk}^n)_z \\ + \operatorname{Re} \left\{ \frac{1}{\theta^L} [1 - \exp(-\theta^L \Delta t)] [(J^L)_{ijk}^n]_z \right\} + (E_{ijk}^n)_z \operatorname{Re} \left\{ (\xi_0^L) - (\xi_1^L) \right\} \\ - \epsilon_o \epsilon_\infty (E_{ijk}^n)_z + \epsilon_o \sum_\rho \operatorname{Re} \left\{ [\exp(-\gamma_\rho^L \Delta t) - 1] [(Q_\rho^L)_{ijk}^n]_z \right\} + \epsilon_o (E_{ijk}^n)_z \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,0}^L) - (\psi_{\rho,1}^L) \right\} \\ - \epsilon_o (E_{ijk}^n)_z \sum_\rho \operatorname{Re} \left\{ (Q_\rho^{NL})_{ijk}^n \right\} - \epsilon_o (E_{ijk}^n)_z \left[[(E_{ijk}^n)_x]^2 + [(E_{ijk}^n)_y]^2 + [(E_{ijk}^n)_z]^2 \right] \sum_\rho \alpha_{0\rho}^{(3)}, \quad (2.42)$$

$$a_1 \equiv \epsilon_o \epsilon_\infty + \sigma^{(0)} \frac{\Delta t}{2} + \operatorname{Re} \left\{ (\xi_1^L) \right\} + \epsilon_o \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,1}^L) \right\} + \epsilon_o \sum_\rho \operatorname{Re} \left\{ \exp(-\gamma_\rho^{NL} \Delta t) (Q_\rho^{NL})_{ijk}^n \right\} \\ + \epsilon_o \left[[(E_{ijk}^n)_x]^2 + [(E_{ijk}^n)_y]^2 + [(E_{ijk}^n)_z]^2 \right] \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,0}^{NL}) - 2(\psi_{\rho,1}^{NL}) + (\psi_{\rho,2}^{NL}) \right\}, \quad (2.43)$$

$$a_{2x} \equiv 2 \epsilon_o (E_{ijk}^n)_x \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,1}^{NL}) - (\psi_{\rho,2}^{NL}) \right\}, \quad (2.44)$$

$$a_{2y} \equiv 2 \epsilon_o (E_{ijk}^n)_y \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,1}^{NL}) - (\psi_{\rho,2}^{NL}) \right\}, \quad (2.45)$$

$$a_{2z} \equiv 2 \epsilon_o (E_{ijk}^n)_z \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,1}^{NL}) - (\psi_{\rho,2}^{NL}) \right\}, \quad (2.42)$$

$$a_3 \equiv \epsilon_o \sum_\rho \operatorname{Re} \left\{ (\psi_{\rho,2}^{NL}) \right\} + \sum_\rho \alpha_{0\rho}^{(3)}. \quad (2.43)$$

Eqs. (2.37), (2.38) and (2.39) can be solved, respectively, for $(E_{ijk}^{n+1})_x$, $(E_{ijk}^{n+1})_y$ and $(E_{ijk}^{n+1})_z$ by using any standard root-finding numerical technique for a set of nonlinear equations [14]. One technique that is suitable for our problem

is the iterative nonlinear Newton-Raphson method using $(E_{ijk}^n)_x$, $(E_{ijk}^n)_y$ and $(E_{ijk}^n)_z$ as the initial guess for the start of the iterative procedure.

In the above formulation, we only need to consider updating Eqs. (2.8-2.11), (2.18), (2.19), (2.34) and (2.37-2.39), respectively, for $H_{ijk}^{n+1/2}$, $(Q_p^L)_{ijk}^{n+1}$, $(Q_p^{NL})_{ijk}^{n+1}$, $(J^L)_{ijk}^n$ and E_{ijk}^{n+1} at each time step in order to carry out a complete three-dimensional computer simulation of the electric field response in nonlinear dispersive materials that contain both frequency-dependent electric conductivity and polarization terms.

For the purely linear dispersive case, a_{2x} , a_{2y} , a_{2z} and a_3 , as well as some terms appearing in a_{0x} , a_{0y} , a_{0z} and a_1 , turn out to be zero. In this case we can solve for E_{ijk}^{n+1} directly without having to rely on the numerical root finding technique as discussed in greater detail in the published literature [15-20].

III. CONCLUSIONS

Based on the FDTD approach we presented here, we can solve Maxwell's equations directly for the propagation of electromagnetic waves in linear and nonlinear dispersive media that exhibit the frequency-dependent electric conductivity and polarization. Because of the piecewise linear approximation we used for the time dependent part of the electric field vector, our approach provides second order accuracy in time. In addition, our approach retains all the advantages of the usual first-order discrete recursive convolution approach, such as fast computational speed and efficient use of the computer memory.

We have shown that it is critical to express the first-order (linear) conductivity, the first-order (linear) susceptibility, and the third-order (nonlinear) susceptibility functions in the exponential forms in the time domain in order to obtain the recursive feature in our FDTD algorithm. The most important result we have shown in this paper is that FDTD formulation for nonlinear dispersive materials results in having to solve three coupled nonlinear cubic equations for the three components of the electric field vector at each time step as compared to just solving the linear equations in the case of linear dispersive materials.

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