Nonlinear FDTD Formulations Using Z Transforms

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***Abstract*—An implementation of the FDTD method for nonlinear optical simulation is described. This method draws on ideas from digital filtering theory by formulating the nonlinearities using Z transforms. This provides a means of directly calculating the nonlinear polarizations in a straightforward manner. Further, an analytic expression for the reflection coefficient from a nonlinear dielectric is described and used to confirm the accuracy of the nonlinear FDTD formulation. Finally, a one-dimensional nonlinear FDTD simulation is used to calculate soliton propagation in nonlinear media.**

I. Introduction

THE FINITE-DIFFERENCE time-domain (FDTD) method has been proven capable of modeling electromagnetic interactions in a wide variety of applications [1]. In particular, developments over the past few years have allowed for the accurate modeling of frequency dependent materials [2]–[9]. These methods have been brought to bear on the problem of modeling an optical pulse [10]. It has even been demonstrated that an FDTD formulation can model the nonlinear effects which induce soliton propagation [11], [12]. Recent developments have included the modeling of soliton propagation in two-dimensional dielectric waveguides [13]. However, the simulation of nonlinear effects has lead to more elaborate, and therefore, more complicated mathematical formulations.

A previous paper [14] advocated the use of the Z transform for a more concise formulation of dispersive effects in the FDTD paradigm. In the present paper, a direct formulation of the nonlinearities using the FDTD method is suggested which again draws on Z transforms for a more efficient calculation.

Along with the problem of developing methods to implement nonlinear calculations comes the difficulty of verifying their accuracy. In Section III of this paper, a method is described to calculate the reflection coefficient from a nonlinear dielectric slab. This calculation is used to verify the accuracy of a simple one-dimensional implementation of the nonlinear FDTD method.

Finally, the results of simulating a pulse in a nonlinear medium are described. The dynamics of the nonlinearities are demonstrated by using pulses of different amplitudes and plotting the results in both the time and frequency domains. Specifically, soliton propagation can be observed, in keeping with the previous results of Goorjian, Taflove, and Joseph [11]–[13].

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II. Nonlinear FDTD Formulation

A. Overview

Starting with the one-dimensional Maxwell's equations in the time domain

$$\frac{\partial D_x}{\partial t} = \frac{\partial H_y}{\partial z} \tag{1a}$$

$$\varepsilon_0 \varepsilon_\infty E_x = D_x - P_L - P_{NL} \tag{1b}$$

$$\frac{\partial \mu_0 H_y}{\partial t} = \frac{\partial E_x}{\partial z} \tag{1c}$$

the linear polarization is given by a linear convolution of E_x with the susceptibility function $\chi^{(1)}(t)$

$$P_L(t) = \varepsilon_0 \int_0^t \chi^{(1)}(t-\tau) \cdot E(\tau)\, d\tau \tag{2}$$

where $\chi^{(1)}(t)$ is usually a second order Lorentz linear dispersion characterized by

$$\chi^{(1)}(\omega) = \frac{(\varepsilon_s - \varepsilon_\infty)}{1 + j2\delta_L\left(\frac{\omega}{\omega_L}\right) - \left(\frac{\omega}{\omega_L}\right)^2}. \tag{3}$$

The nonlinear polarization P_{NL} will be described by

$$\begin{aligned} P_{NL}(t) &= \varepsilon_0 \chi_0^{(3)} E(t) \int_0^t [(\alpha\delta(t-\tau) \\ &\quad + (1-\alpha) g_R(t-\tau)] \cdot E^2(\tau)\, d\tau \\ &= \varepsilon_0 \chi_0^{(3)} \alpha E^3(t) + \varepsilon_0 \chi_0^{(3)} (1-\alpha) E(t) \\ &\quad \cdot \int_0^t g_R(t-\tau) \cdot E^2(\tau)\, d\tau. \end{aligned} \tag{4}$$

$\chi_0^{(3)}$ is the nonlinear coefficient, a constant, and α is a constant which dictates the relative strengths of the two nonlinearities. The first term on the right is the "Kerr effect"

$$P_K(t) = \varepsilon_0 \chi_0^{(3)} \alpha E^3(t). \tag{5}$$

The second term is due to the Raman scattering

$$\begin{aligned} P_R(t) &= \varepsilon_0 \chi_0^{(3)} (1-\alpha) E(t) \cdot \int_0^t g_R(t-\tau) \\ &\quad \cdot E^2(\tau)\, d\tau \end{aligned} \tag{6}$$

where

$$g_R(\omega) = \frac{1}{1 + j2\delta_{NL}\left(\frac{\omega}{\omega_{NL}}\right) - \left(\frac{\omega}{\omega_{NL}}\right)^2}. \tag{7}$$

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It will be advantageous to separate the two nonlinearities, so (1b) can be rewritten as

$$E_x = \frac{1}{\varepsilon_0 \varepsilon_\infty}(D_x - P_L - P_K - P_R). \tag{8}$$

The implementation of (1a) and (1c) into the FDTD formulation is straightforward. The interesting part of the problem is (1b) because the linear and nonlinear polarizations, P_L and P_{NL} are often frequency dependent, which leads to a complicated convolution in the time domain. In recent years, numerous satisfactory approaches have been developed for the linear frequency dependencies. Solutions to the nonlinear polarization are complicated by the fact that P_{NL} contains terms of E_x^2 or E_x^3. Equation (1b) will be posed as a digital filtering problem to draw on techniques from signal processing and system theory which expedite the formulation. The FDTD formulations of the three polarization terms P_L, P_R and P_K, are the subject of the next three subsections.

B. Formulation of the Linear Polarization $P_L(t)$

The linear polarization was given in (2).

$$P_L(t) = \varepsilon_0 \int_0^t \chi^{(1)}(t-\tau) \cdot E(\tau)\, d\tau. \tag{2}$$

A previous paper [14] demonstrated the use of digital filtering theory to solve complicated frequency dependent problems using the FDTD method. This was accomplished by use of the Z transform. Taking the Z transform of (2) (see (9) at the bottom of the page) where

$$\alpha_L = \omega_L \cdot \delta_L \tag{10a}$$

$$\beta_L = \omega_L \cdot \sqrt{1-\delta_L^2} \tag{10b}$$

$$\gamma_L = \frac{\omega_L \cdot (\varepsilon_s - \varepsilon_\infty)}{\sqrt{1-\delta_L^2}} \tag{10c}$$

z^{-1} is an operator that indicates a delay of one time step. Defining a new variable

$$S_L(z) = \frac{\gamma_L \cdot \delta t \cdot e^{-\alpha_L \cdot \delta t} \cdot \sin(\beta_L \cdot \delta t) \cdot E(z)}{1 - 2 \cdot e^{-\alpha_L \cdot \delta t} \cdot \cos(\beta_L \cdot \delta t) \cdot z^{-1} + e^{-2\alpha_L \cdot \delta t} \cdot z^{-2}} \tag{11}$$

(9) becomes

$$P_L(z) = \varepsilon_0 z^{-1} \cdot S_L(z) \tag{12a}$$

$$S_L(z) = c1 \cdot z^{-1} S_L(z) - c2 \cdot z^{-2} S_L(z) + c3 \cdot E(z) \tag{12b}$$

where

$$\begin{aligned} c1 &= 2 \cdot e^{-\alpha_L \cdot \delta t} \cdot \cos(\beta_L \cdot \delta t) \\ c2 &= e^{-2\alpha_L \cdot \delta t} \\ c3 &= \gamma_L \cdot \delta t \cdot e^{-\alpha_L\, \delta t} \cdot \sin(\beta_L \cdot \delta t). \end{aligned} \tag{13}$$

Rewriting (12a) and (12b) in an FDTD formulation gives

$$P_L^n = \varepsilon_0 S_L^{n-1} \tag{14a}$$

$$S_L^n = c1 \cdot S_L^{n-1} - c2 \cdot S_L^{n-2} + c3 \cdot E^n. \tag{14b}$$

C. Formulation of the Raman Scattering $P_R(t)$

The Raman scattering was given by (6)

$$P_R(t) = \varepsilon_0 \chi_0^{(3)}(1-\alpha) E(t) \cdot \int_0^t g_R(t-\tau) \cdot E^2(\tau)\, d\tau. \tag{6}$$

Begin by defining an integral

$$I_R(t) = \varepsilon_0 \chi_0^{(3)}(1-\alpha) \int_0^t g_R(t-\tau) \cdot E^2(\tau)\, d\tau. \tag{15}$$

Note that $g_R(t)$ is also a second order Lorentz, so it should not be surprising that the solution to the integral will be similar to the linear polarization. Taking the Z transform (see (16) at the bottom of the page) where

$$\alpha_R = \omega_{NL} \cdot \delta_{NL} \tag{17a}$$

$$\beta_R = \omega_{NL} \cdot \sqrt{1-\delta_{NL}^2} \tag{17b}$$

$$\gamma_R = \frac{\omega_{NL} \cdot \chi_0^{(3)} \cdot (1-\alpha)}{\sqrt{1-\delta_{NL}^2}} \tag{17c}$$

and once more, defining a new term

$$S_R(z) = \frac{\gamma_R \cdot \delta t \cdot e^{-\alpha_R \cdot \delta t} \cdot \sin(\beta_R \cdot \delta t) \cdot E^2(z)}{1 - 2 \cdot e^{-\alpha_R \cdot \delta t} \cdot \cos(\beta_R \cdot \delta t) \cdot z^{-1} + e^{-2\alpha_R \cdot \delta t} \cdot z^{-2}} \tag{18}$$

then

$$I_R(z) = \varepsilon_0 z^{-1} S_R(z) \tag{19a}$$

$$S_R^n = cnl1 \cdot S_R^{n-1} - cnl2 \cdot S_R^{n-2} + cnl3 \cdot (E^2)^n \tag{19b}$$

where

$$cnl1 = 2e^{-\alpha_R T} \cos(\beta_R \cdot \delta t) \tag{20a}$$

$$cnl2 = e^{-2\alpha_R t} \tag{20b}$$

$$cnl3 = \gamma_R \cdot \delta t \cdot e^{-\alpha_R \cdot \delta t} \cdot \sin(\beta_R \cdot \delta t) \tag{20c}$$

$$\begin{aligned} P_L(z) &= \varepsilon_0 \chi^{(1)}(z) \cdot E(z) \cdot \delta t \\ &= \varepsilon_0 \frac{\gamma_L \cdot \delta t \cdot e^{-\alpha_L \cdot \delta t} \cdot \sin(\beta_L \cdot \delta t) \cdot z^{-1}}{1 - 2 \cdot e^{-\alpha_L \cdot \delta t} \cdot \cos(\beta_L \cdot \delta t) \cdot z^{-1} + e^{-2\alpha_L \cdot \delta t} \cdot z^{-2}} \cdot E(z) \end{aligned} \tag{9}$$

$$I_R(z) = \varepsilon_0 \frac{\gamma_R \cdot \delta t \cdot e^{-\alpha_R \cdot \delta t} \cdot \sin(\beta_R \cdot \delta t) \cdot z^{-1}}{1 - 2 \cdot e^{-\alpha_R \cdot \delta t} \cdot \cos(\beta_R \cdot \delta t) \cdot z^{-1} + e^{-2\alpha_R \cdot \delta t} \cdot z^{-2}} \cdot E^2(z) \tag{16}$$

or rewriting as finite difference terms

$$I_R^n = \varepsilon_0 S_R^{n-1}. \tag{21}$$

Going back to (6) and inserting (15)

$$P_R(t) = \varepsilon_0 E(t) \cdot I_R(t). \tag{22}$$

Changing to the finite difference notation,

$$P_R^n = \varepsilon_0 E^n \cdot I_R^n$$

and substituting in S_{NL}^{n-1} from (21)

$$P_R^n = \varepsilon_0 E^n \cdot S_R^{n-1} \tag{23}$$

$$S_R^n = cnl1 \cdot S_R^{n-1} - cnl2 \cdot S_R^{n-2} + cnl3 \cdot (E^n)^2 \tag{19b}$$

gives a method of calculating P_R^n. Note that in (23), P_R^n is calculated from the *previous* value of S_R, i.e., S_R^{n-1}. Then in (19b), the new value of S_R, i.e., S_R^n, is calculated from $(E^n)^2$.

D. Formulation of the Kerr Effect $P_K(t)$

Finally, what is lacking is a method to calculate the Kerr effect,

$$P_K(t) = \varepsilon_0 \chi_0^{(3)} \alpha E^3(t). \tag{24}$$

In calculating the linear dispersion and the Raman scattering, the Z transform of the second order Lorentz provided a delay operator z^{-1} in the numerator ((9) and (16)) which meant that only the previous value of $E(t)$ or $E^2(t)$ was needed to calculate the new value of $P_L(t)$ or $P_R(t)$. No such formulation is available now; in order to calculate the new value of $P_K(t)$, the new value of $E^3(t)$ is needed. Start by taking a Taylor series expansion of $E^3(t)$ around the point $t = t_{n-1}$ and evaluating it at the point $t = t_n$

$$\begin{aligned} E^3(t_n) &\approx E^3(t_{n-1}) + \frac{d}{dt}(E^3(t_{n-1})) \cdot (t_n - t_{n-1}) \\ &= E^3(t_{n-1}) + 3 \cdot E^2(t_{n-1}) \\ &\quad \cdot \left(\frac{E(t_n) - E(t_{n-1})}{t_n - t_{n-1}}\right)(t_n - t_{n-1}) \\ &= E^3(t_{n-1}) + 3 \cdot E^2(t_{n-1}) \\ &\quad \cdot (E(t_n) - E(t_{n-1})) \\ &= 3E^2(t_{n-1}) \cdot E(t_n) - 2 \cdot E^3(t_{n-1}). \end{aligned} \tag{25}$$

Naturally, it will be assumed that the times t_{n-1} and t_n correspond to times in the FDTD formulation, so (25) will be written

$$(E^n)^3 \cong 3 \cdot (E^{n-1})^2 \cdot (E^n) - 2 \cdot (E^{n-1})^3. \tag{26}$$

And finally, substituting this approximation for $(E^n)^3$ into (24)

$$P_K^n(t) = \varepsilon_0 \chi_0^{(3)} \alpha [3 \cdot (E^{n-1})^2 \cdot (E^n) - 2 \cdot (E^{n-1})^3]. \tag{27}$$

Note that the new value of $P_K^n(t)$ is calculated, in part, from the new value of E^n, as well as $(E^{n-1})^2$ and $(E^{n-1})^3$.

E. Calculation of the E Field from the Polarizations

Now the three polarization terms will be used to calculate E. Going back to (8)

$$\varepsilon_0 \varepsilon_\infty E^n = D^n - P_L^n - P_R^n - P_K^n. \tag{8}$$

Substituting (14a), (23), and (27) for the P terms

$$\begin{aligned} \varepsilon_0 \varepsilon_\infty E^n = {}& D^n - \varepsilon_0 S_L^{n-1} - \varepsilon_0 \chi_0^{(3)} (1-\alpha) \\ & \cdot E^n \cdot S_R^{n-1} \\ & - \varepsilon_0 \chi_0^{(3)} \alpha \cdot [3 \cdot (E^{n-1})^2 \cdot (E^n) \\ & - 2 \cdot (E^{n-1})^3]. \end{aligned} \tag{28}$$

Now collect all terms containing E^n on the left

$$\begin{aligned} & \varepsilon_0 \varepsilon_\infty E^n + \varepsilon_0 \chi_0^{(3)} (1-\alpha) \cdot E^n \cdot S_R^{n-1} \\ & \quad + \varepsilon_0 \chi_0^{(3)} \alpha 3 \cdot (E^{n-1})^2 \cdot E^n \\ & \quad = D^n - S_L^{n-1} + \varepsilon_0 \chi_0^{(3)} \alpha \cdot [2 \cdot (E^{n-1})^3] \end{aligned} \tag{29}$$

or

$$E^n = \frac{\frac{1}{\varepsilon_0} D^n - S_L^{n-1} + \chi_0^{(3)} \alpha \cdot [2 \cdot (E^{n-1})^3]}{\varepsilon_\infty + \chi_0^{(3)} (1-\alpha) \cdot S_R^{n-1} + \chi_0^{(3)} \alpha 3 \cdot (E^{n-1})^2} \tag{30}$$

$$S_L^n = c1 \cdot S_L^{n-1} - c2 \cdot S_L^{n-2} + c3 \cdot E^n \tag{14b}$$

$$S_R^n = cnl1 \cdot S_R^{n-1} - cnl2 \cdot S_R^{n-2} + cnl3 \cdot (E^n)^2. \tag{19c}$$

The new value of E is calculated from the new value of D and the previous values of E^2, E^3, S_L, and S_R. Then the new values of S_L and S_R can be calculated from this new value of E.

III. Analytic Formulation of the Reflection Coefficient

The accuracy of the method described in the last section will be evaluated by calculating the reflection coefficient from a nonlinear dielectric slab. To do this, an analytic expression for the dielectric constant at a certain frequency and amplitude will be developed. From this dielectric constant, the reflection coefficient can be calculated.

Assume we are dealing with a signal of the form

$$e(t) = E_1 \cos(2\pi \cdot f_1 \cdot t) \tag{31}$$

the Fourier transform (F.T.) is given by

$$F[e(t)] = E(f) = \frac{E_1}{2} \cdot [\delta(f + f_1) + \delta(f - f_1)]. \tag{32}$$

Next we need the F.T. of $e^2(t)$. Since a multiplication in the time domain, i.e., $e(t)$ times $e(t)$ leads to a convolution in the frequency domain

$$\begin{aligned} F[e^2(t)] &= E(f) \otimes E(f) \\ &= E_1^2 \cdot [\tfrac{1}{4}\delta(f + 2f_1) + \tfrac{1}{2}\delta(f) \\ &\quad + \tfrac{1}{4}\delta(f - 2f_1)]. \end{aligned} \tag{33}$$

Similarly, the Fourier transform of $e^3(t)$ is the convolution of $E(f)$ with $E^2(f)$,

$$\begin{aligned} F[e^3(t)] &= E(f) \otimes E^2(f) \\ &= E_1^3 \cdot [\tfrac{1}{8}\delta(f+3f_1) + \tfrac{3}{8}\delta(f+f_1) \\ &\quad + \tfrac{3}{8}\delta(f-f_1) + \tfrac{1}{8}\delta(f-3f_1)]. \end{aligned} \tag{34}$$

(Note that $E^2(f)$ and $E^3(f)$ represent the F.T. of $e^2(t)$ and $e^3(t)$, respectively, and *not* the square or cube of the F.T. of $e(t)$!.)

In the previous section, we derived an FDTD formulation of the following nonlinearity

$$D_x(t) = \varepsilon_0\varepsilon_\infty E(t) + P_L(t) + P_K(t) + P_R(t). \tag{35}$$

The Fourier tranform of (35)

$$D_x(f) = \varepsilon_0\varepsilon_\infty E(f) + P_L(f) + P_K(f) + P_R(f) \tag{36}$$

is obtained by taking the F.T. of each polarization. In the frequency domain, the linear polarization is just $E(f)$ times $\chi^{(1)}(f)$

$$\begin{aligned} P_L(f) &= \varepsilon_0\chi^{(1)}(f) \cdot E(f) \\ &= \varepsilon_0\chi^{(1)}(f) \cdot \frac{E_1}{2} \cdot [\delta(f+f_1) + \delta(f-f_1)] \\ &= \varepsilon_0 \frac{E_1}{2} \cdot [\chi^{(1)}(-f_1) \cdot \delta(f+f_1) \\ &\quad + \chi^{(1)}(f_1)\delta(f-f_1)] \end{aligned} \tag{37}$$

i.e., the convolution of $E(f)$ and $\chi^{(1)}$ is just $\chi^{(1)}(f)$ evaluated at $+f_1$ and $-f_1$, times $E_1/2$. The F.T. of the Kerr polarization is just a constant times the F.T. of $e^3(t)$.

$$\begin{aligned} P_K(f) &= \varepsilon_0\alpha\chi^{(3)} \cdot E^3(f) \\ &= \varepsilon_0\alpha\chi_0^{(3)} \cdot E_1^3 \cdot [\tfrac{1}{8}\delta(f+3f_1) + \tfrac{3}{8}\delta(f+f_1) \\ &\quad + \tfrac{3}{8}\delta(f-f_1) + \tfrac{1}{8}\delta(f-3f_1)]. \end{aligned} \tag{38}$$

The F.T. of $P_R(t)$ is more complicated because it is the multiplication of $E(t)$ with a convolution of $g_R(t)$ and $E^2(t)$. Therefore, in the frequency domain, $E(f)$ must be convolved with $G_R(f)$ times $E^2(f)$.

$$P_R(f) = \varepsilon_0 E(f) \otimes [G_R(f) \cdot E^2(f)]. \tag{39}$$

Using the expression for $E^2(f)$ in (33)

$$\begin{aligned} P_R(f) &= \varepsilon_0 E(f) \otimes \left\{ G_R(f) \cdot E_1^2 \left[\frac{1}{4}\delta(f+2f_1) \right.\right. \\ &\quad \left.\left. + \frac{1}{2}\delta(f) + \frac{1}{4}\delta(f-2f_1) \right] \right\} \\ &= \varepsilon_0 E(f) \otimes \left\{ E_1^2 \left[\frac{G_R(-2f_1)}{4}\delta(f+2f_1) \right.\right. \\ &\quad \left.\left. + \frac{G_R(0)}{2}\delta(f) + \frac{G_R(2f_1)}{4}\delta(f-2f_1) \right] \right\} \\ &= \varepsilon_0 \left[\frac{E}{2}\delta(f+f_1) + \frac{E_1}{2}\delta(f-f_1) \right] \\ &\quad \otimes \left\{ E_1^2 \left[\frac{G_R(-2f_1)}{4}\delta(f+2f_1) + \frac{G_R(0)}{2}\delta(f) \right.\right. \\ &\quad \left.\left. + \frac{G_R(2f_1)}{4}\delta(f-2f_1) \right] \right\} \end{aligned} \tag{40}$$

from which we finally get

$$\begin{aligned} P_R(f) &= E_1^3 \cdot \{[\tfrac{1}{8}G(-2f_1)+] \cdot \delta(f+3f_1) \\ &\quad + [\tfrac{1}{4}G(0) + \tfrac{1}{8}G(-2f_1)] \cdot \delta(f+f_1) \\ &\quad + [\tfrac{1}{4}G(0) + \tfrac{1}{8}G(2f_1)] \cdot \delta(f-f_1) \\ &\quad + [\tfrac{1}{8}G(2f_1)+] \cdot \delta(f-3f_1)\}. \end{aligned} \tag{41}$$

Now a variable called the "effective dielectric constant" will be defined as

$$\varepsilon_{eff}(f) = \frac{D(f)}{E(f)}. \tag{42}$$

This will be evaluated at the frequency f_1 only! (see (43) at the bottom of the page).

Going back to (35), (37), (38), and (41), and taking only those terms evaluated at f_1, i.e., only those terms multiplied by $\delta(f-f_1)$ (see (44) at the bottom of the page).

Using (44), the reflection coefficient can be calculated by

$$\Gamma(E_1, f_1) = \frac{\varepsilon_{eff}(E_1, f_1) - 1}{\varepsilon_{eff}(E_1, f_1) + 1}. \tag{45}$$

Equation (45) is an expression for the reflection coefficient at one frequency. Naturally, the nonlinear material will generate numerous harmonics, so (45) is valid at f_1 only.

Note that (45) was developed assuming the input was a cosine (31). The development could just as easily have been

$$\varepsilon_{eff}(E_1, f_1) = \frac{D(f_1)}{E(f_1)} = \frac{\varepsilon_0\varepsilon_\infty E(f_1) + \varepsilon_0 P_L(f_1) + \varepsilon_0 P_K(f_1) + \varepsilon_0 P_R(f_1)}{E(f_1)} \tag{43}$$

$$\begin{aligned} \varepsilon_{eff}(E_1, f_1) &= \frac{\varepsilon_0\varepsilon_\infty \frac{E_1}{2} + \varepsilon_0 \frac{E_1}{2}\chi^{(1)}(f_1) + \varepsilon_0\chi_0^{(3)}\frac{3E_1^2}{8} + \varepsilon_0 E_1^3 \left[\frac{G_R(0)}{4} + \frac{G_R(2f_1)}{8} \right]}{E_1/2} \\ &= \varepsilon_0\varepsilon_\infty + \varepsilon_0\chi^{(1)}(f_1) + \varepsilon_0\chi_0^{(3)}\frac{3E_1^2}{4} + \varepsilon_0 E_1^2 \left[\frac{G_R(0)}{2} + \frac{G_R(2f_1)}{4} \right] \end{aligned} \tag{44}$$

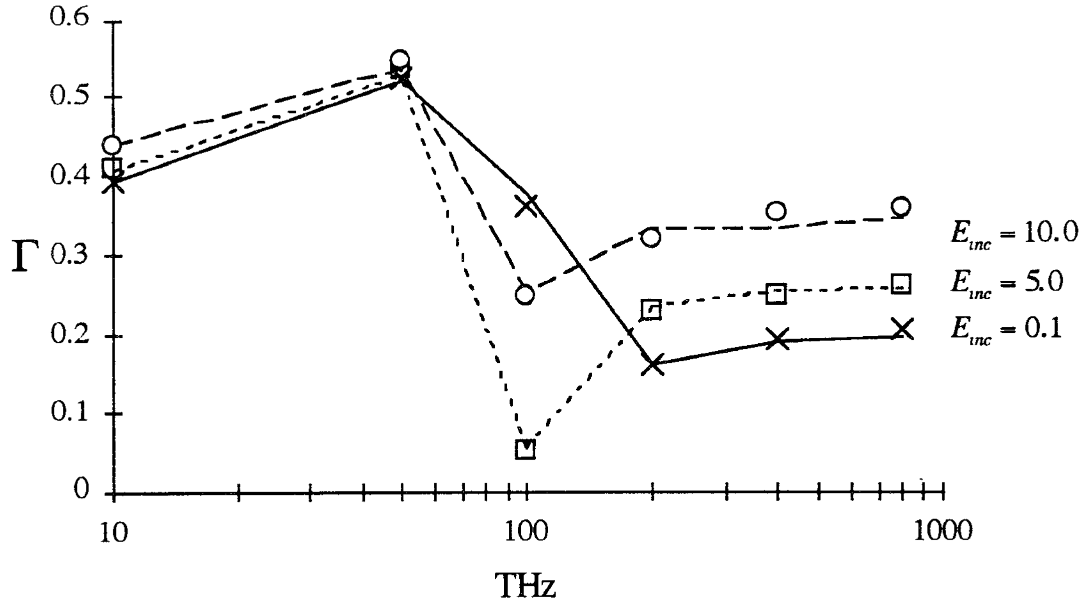

Fig. 1. Comparison of FDTD versus an analytic calculation of the magnitude of the reflection coefficient as a function of the frequency. The calculation was made from a nonlinear material with the following properties: ε_∞ = 2.25, ε_s = 5.25, f_L = 63.7 THz, δ_L = 0.00025, $\chi_0^{(3)}$ = 0.07, α = 0.7, f_{NL} = 14.8, δ_{NL} = 0.336. The lines are the analytic calculations and the symbols are the FDTD calculations.

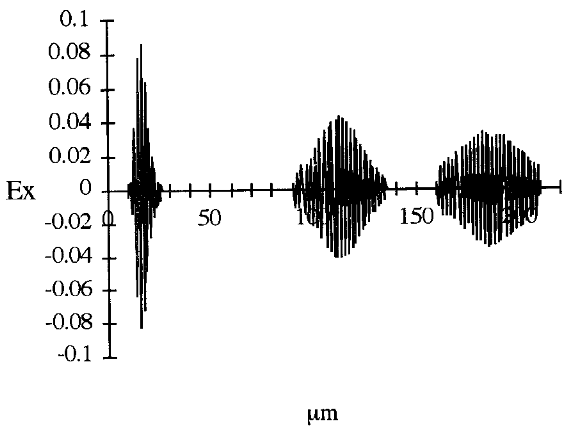

Fig. 2. Propagation of a pulse whose peak-to-peak amplitude is 0.1 V/m at three different times corresponding to 8000, 48000, and 78000 time steps.

made for a sine or for

$$E(t) = E_1 e^{-j2\pi \cdot f_1 \cdot t} = E_1[\cos(2\pi \cdot f_1 \cdot t) - j\sin(2\pi \cdot f_1 \cdot t)] \quad (46)$$

so it is valid for any single frequency expression.

Fig. 1 is a comparison of the reflection coefficient of a nonlinear material as calculated by the FDTD method described in Section II and the analytic expression described in this section. The values used were taken from [12], which were based on experimental data of silica fibers. Although most optical simulations will be pulse sources, single frequency illumination is used because the analytic results are valid for single frequencies only. The results have been calculated for 10, 50, 100, 200, 400, and 800 THz. Three different sets of calculations have been made, for incident E fields of 0.1 V/m, 5 V/m, and 10 V/m. An E field of 0.1 V/m is essentially a linear problem, since the magnitude is not great enough to

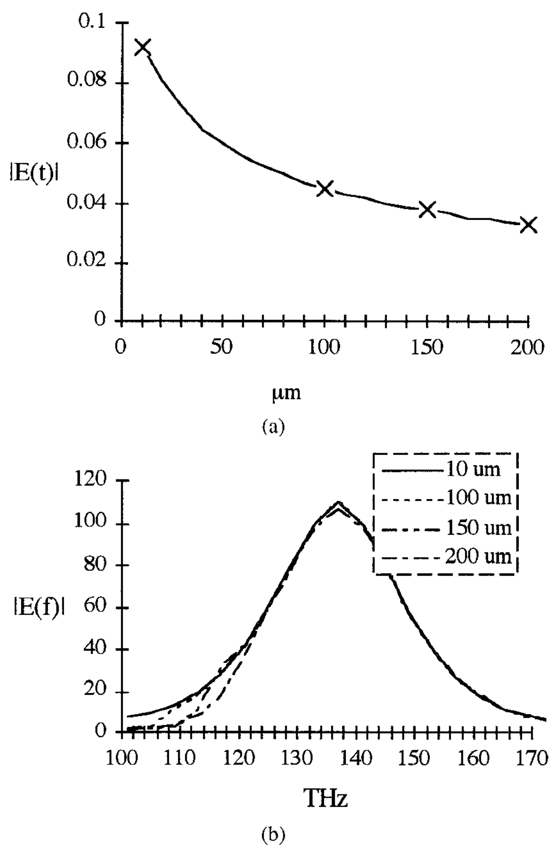

Fig. 3. Peak-to-peak amplitude (a) and frequency response (b) for a pulse whose incident amplitude was 0.1 V/m.

cause significant nonlinear terms. The FDTD program used to calculate the results in Fig. 1 was a one-dimensional program which used a cell size of 0.1 μm, and a time step of 0.0165 femtosecond. Each calculation required about 1000 time steps

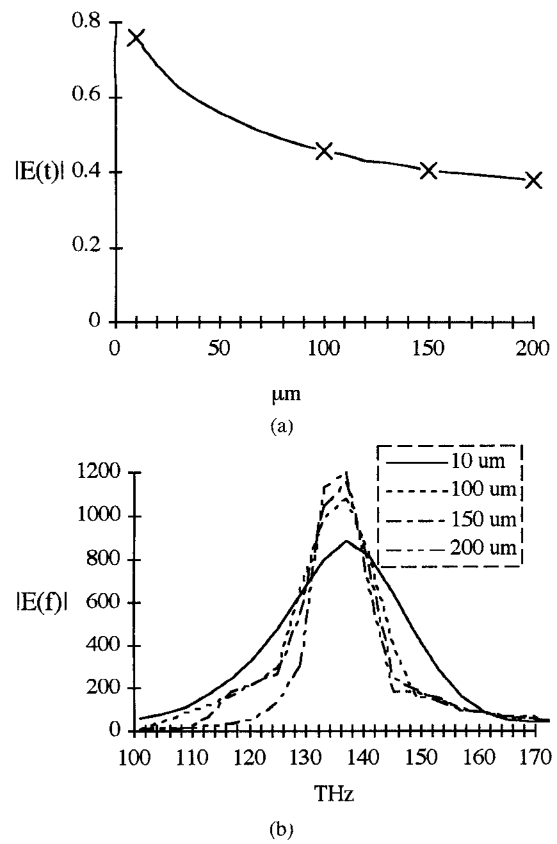

Fig. 4. Peak-to-peak amplitude (a) and frequency response (b) for a pulse whose incident amplitude was 0.8 V/m.

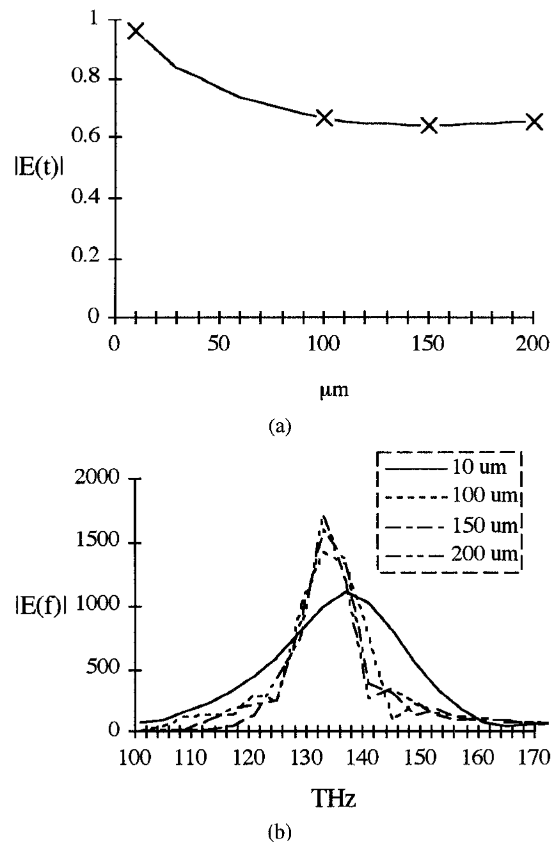

Fig. 5. Peak-to-peak amplitude (a) and frequency response (b) for a pulse whose incident amplitude was 1.0 V/m.

to converge, which took about 30 seconds on a DECstation 5000/125 workstation.

The agreement is reasonably good, demonstrating the method's ability to take into account the dispersive and nonlinear characteristics of the material over wide frequency and amplitude ranges.

IV. Soliton Propagation

The effects of the nonlinearity can be observed by simulating the propagation of pulses of various magnitudes in a media having the same parameters as the silica glass used in the previous section. The incident field is a pulse with a center frequency of 137 THz modulated by a hyperbolic secant envelope function with a characteristic time constant of 14.6 fs [10]. The source is located at $x = 0$. The FDTD cell size is 10 nm.

Fig. 2 shows a pulse with an amplitude of 0.1 V/m at three different times corresponding to 8000, 48000, and 78000 time steps. The pulse is clearly dispersing as it propagates. Fig. 3(a) is a plot of the peak-to-peak amplitude of the pulse as a function of the distance propagated through the material. Fig. 3(b) is the amplitude of the Fourier spectrum of the pulse at distances of 10, 100, 150, and 200 μm showing virtually no change as it propagates. (The X's in Fig. 3(a) show the corresponding amplitudes.) Apparently, the amplitude of this pulse was not enough to engage the nonlinear phenomena and overcome the linear dispersive effects. Fig. 4(a) is the peak-to-peak plot of another pulse with an amplitude of 0.8 V/m. It, too, continuously declines, even though Fig. 4(b) shows a shift in the frequency spectrum. The nonlinearity did have some effect, but not enough to induce soliton formation. Figs. 5(a) and 5(b) represent a pulse whose input amplitude is 1 V/m. This pulse levels off in amplitude at about 100 μm, while the frequency domain shows a decided shift, indicating soliton propagation. Fig. 6 is the time domain graph of the pulse at 8000, 48000, 68000, and 88000 times steps. These simulations were done in a one-dimensional problem space of 25 000 cells. The cells were 0.01 μm. The 88 000 iterations used about 120 CPU seconds on a Cray C90. These results, showing that a pulse with an amplitude of 1 V/m was enough to induce soliton formation, essentially confirms previous results [11], [12].

V. Summary

This paper described the implementation of nonlinear phenomena into the FDTD formulation, partly drawing on methods from digital filtering theory. The accuracy of this method was tested in simple one-dimensional calculations of the reflection coefficient, which could be verified by an analytic expression. It was demonstrated that this formulation could simulate soliton propagation.

Because of the efficiency of the described formulation, extension to the modeling of realistic three-dimensional structures should be straightforward. What will not be straightforward is the development of better analytic expressions of the nonlinearities to verify the accuracy in three dimensions.

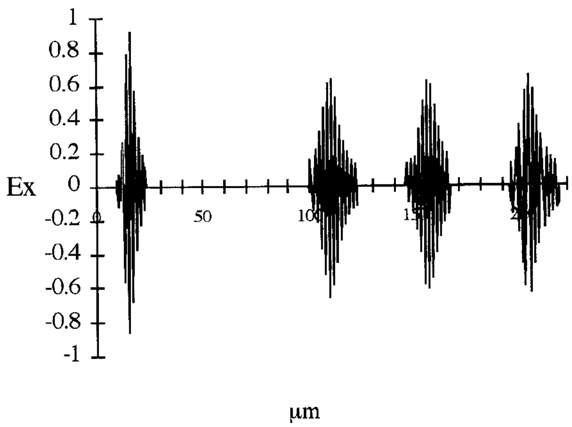

Fig. 6. Propagation of a pulse whose incident peak-to-peak amplitude is 1.0 V/m at four times corresponding to 8000, 48000, 68000, and 88000 time steps.

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