A Comparison of Numerical Techniques for Modeling Electromagnetic Dispersive Media

Riaz Siushansian and Joe LoVetri

Abstract—**A comparison of various time domain numerical techniques to model material dispersion is presented. Methods that model the material dispersion via a convolution integral as well as those that use a differential equation representation are considered. We have shown how the convolution integral arising in the electromagnetic constitutive relation can be approximated by the trapezoidal rule of numerical integration and implemented using a newly derived one-time-step recursion relation. The superiority of the new method, in terms of accuracy and computer resources, over four previously published techniques is demonstrated on the problem of a transient electromagnetic plane wave propagating in a dispersive media. All of the methods considered are easily incorporated into 3-D codes where the requirement for efficiency is very important.**

I. Introduction

It is well known that in the time domain a dispersive medium exhibits electromagnetic memory and can be modeled via a convolution integral [1]. Recently, several numerical schemes have been suggested to model material dispersion in the time domain [2]–[7]. In this letter, the first approach we consider is the method by Joseph *et al.* where the constitutive relation relating the electric flux density $\boldsymbol{D}(\boldsymbol{x},t)$ to the electric field $\boldsymbol{E}(\boldsymbol{x},t)$ is expressed via a second-order ordinary differential equation [4]. The second technique we consider is that of Luebbers and Hunsberger (and later on by Kelley and Luebbers) in which the constitutive relation for a general Nth order Lorentz dispersive medium is represented as a recursive convolution integral [5], [6]. Finally, Sullivan formulates the constitutive relation using the Z transform and obtains a recursive relation between electric flux density and the electric field [7]. Other schemes have been published, but these three seem to be the most popular. We then summarize our new higher-order convolution scheme, which was described in [8], and give comparative results from applying all the schemes on a sample problem.

II. Nth Order Lorentz Dispersion

A commonly used mathematical model to account for the presence of dispersive material is to relate the electric flux density to the electric field in the frequency domain by a frequency-dependent constitutive relation. Specifically, an order-M Lorentz dispersion relation

$$\varepsilon(\omega)=\frac{D(\omega)}{\varepsilon_0 E(\omega)}=\varepsilon_\infty+(\varepsilon_s-\varepsilon_\infty)\sum_{p=1}^{N}\frac{G_p\omega_p^2}{\omega_p^2+2j\omega\delta_p-\omega^2} \tag{1}$$

can be used to model a wide variety of material where, in general, the $M=2N$ complex conjugate poles in the summation model the natural resonances exhibited by the medium. In (1) ω_p represents the pth resonant frequency, δ_p the pth damping coefficient, ε_∞ is the high-frequency permittivity, and ε_s the static permittivity. The time domain equivalent can be represented as a convolution integral, as described in [1], [5], or by taking the inverse Fourier transform of (1) as a second-order ordinary differential equation, as was done for $M=2$ in [4].

III. Review of Numerical Approximations for Dispersion

In all the numerical methods described, Maxwell's curl equations are solved by the standard FDTD method, but the frequency-dependent nature of the constitutive relation must now also be approximated. The procedure developed in [4] uses the inverse Fourier transform of the complex permittivity given by (1) to derive a second-order differential equations between $E(\boldsymbol{x},t)$ and $H(\boldsymbol{x},t)$. A second-order finite difference approximation is then derived for this equation and an update equation for E^{n+1} is obtained. This scheme requires the storage of $2M-1$ real variables in addition to the field values of the general FDTD method. The above scheme will be referred to as JHT in the following discussion.

The procedure described in [5] approximates the convolution integral by a (0th order) discrete summation and then derives a recursive method for implementation. This method will be referred to as the Constant Recursive Convolution (CRC) method and is summarized in [5]. For an order-M medium, M additional complex variables are required to be stored over the standard FDTD method, i.e. for a general dispersive material with P poles, a total of P real variables are required in addition to the field values of the FDTD scheme.

Recently a new method was presented by Kelley and Luebbers [6] in which the electric field in the convolution integral is represented as a piecewise linear function of time. This Piecewise Linear Recursive Convolution (PLRC) has shown significant improvement over the CRC scheme. However, this new method requires one extra level of back storage of the electric field, E^{n-1}, in addition to the CRC scheme.

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The authors are with the Department of Electrical Engineering, The University of Western Ontario, London, Ontario N6A 5B9, Canada.
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Finally, Sullivan demonstrated that a Z transform technique can be employed to model dispersive media in conjunction with the FDTD method [7]. The convolution integral of the constitutive relation is represented by a recursive relation obtained from its Z Transform and is incorporated into a new update equation for the electric field. The FDTD calculations of a dispersive medium with two poles demand three additional real variables beyond the current field values of the general FDTD method. We will denote this method as the ZT method.

IV. Discrete Trapezoidal Convolution Method

The main computational advantage of the convolution method CRC over the ordinary differential equation method (JHT) and the Z transform method (ZT) is that only one level of back storage is required for the auxiliary variable $\hat{\psi}^n$ used in the method. The reason the CRC scheme requires only one time level of back storage is that the electric field is assumed to be "constant" over each Δt interval in the discretized convolution (this being the 0th-order integration approximation). At first sight it seems that if we try to increase the order of the integration to the first-order "trapezoidal rule" instead of the "constant" approximation, we would require two time levels of back storage (thus sacrificing memory requirement for accuracy). This idea of using a piecewise linear approximation to approximate the convolution integral was recently used by Kelley and Luebbers in order to obtain better accuracy [6]. Our trapezoidal rule is also a piecewise linear approximation of the convolution integral, but we've been able to implement it using a one time step recursive scheme given by [8]

$$\begin{aligned} E_y^{n+1}(i) = {} & \frac{E_y^n(i)}{\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2}} \left[-\varepsilon_\infty + \sum_{p=1}^{n} \right. \\ & \left. \cdot \operatorname{Re}\left[\frac{\hat{\chi}_p^0}{2e^{(-\alpha_p + j\beta_p)\Delta t}} \right] \right] \\ & - \frac{1}{\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2}} \sum_{p=1}^{N} \\ & \cdot \operatorname{Re}\left[\left(\frac{e^{2(-\alpha_p + j\beta_p)\Delta t} - 1}{2e^{(-\alpha_p + j\beta_p)\Delta t}} \right) \hat{\psi}_p^n \right] \\ & - \frac{\Delta t}{\left(\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2} \right) \varepsilon_0 \Delta x} \\ & \cdot \left[H_z^{n+(1/2)}\left(i + \frac{1}{2}\right) - H_z^{n+(1/2)}\left(i - \frac{1}{2}\right) \right] \end{aligned} \tag{2}$$

where

$$\alpha_p = \delta_p, \beta_p = \sqrt{\omega_p^2 + \delta_p^2}$$

and the discrete auxiliary function $\hat{\psi}_p^n$ is found by the recursive procedure

$$\hat{\psi}_p^n = E_y^n(i)\hat{\chi}_p^0 + e^{(-\alpha_p + j\beta_p)\Delta t}\hat{\psi}_p^{n-1}. \tag{3}$$

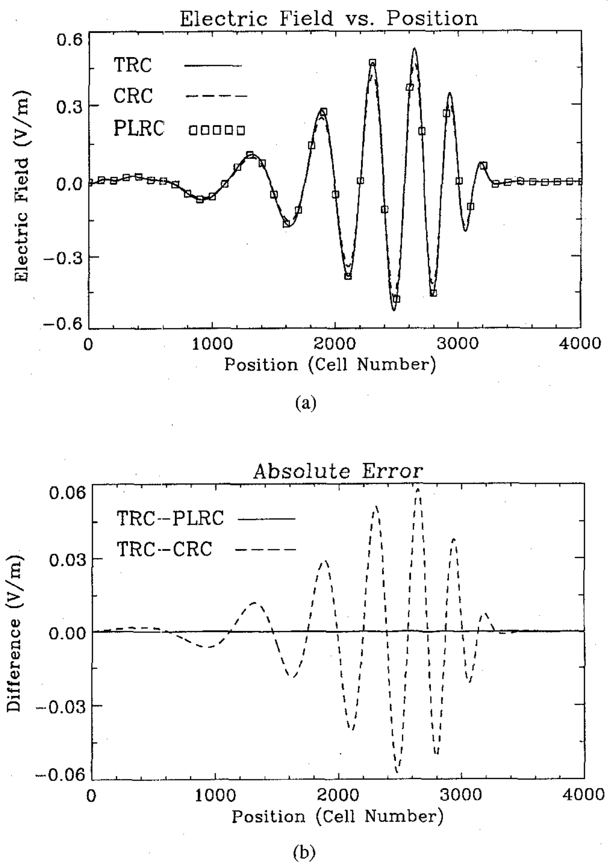


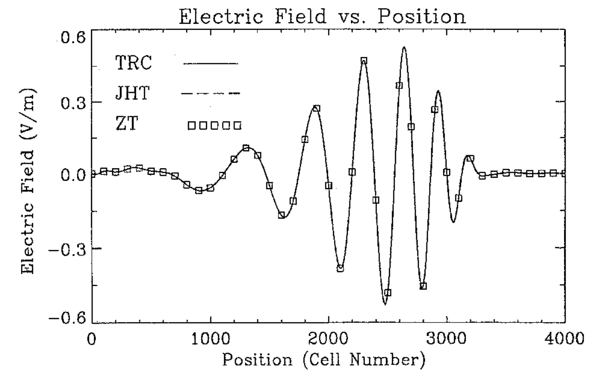
Fig. 1. (a) Electric field and (b) difference between methods of a hyperbolic secant envelope with carrier in a second-order dispersive medium after 5000 time steps using TRC, CRC, and PLRC.

In the remaining discussion we will refer to this new method as the TRC method. This scheme is more accurate than the CRC scheme when the slope of the electric field in one Δt differs appreciably from a constant (i.e. for waveforms with high frequency content).

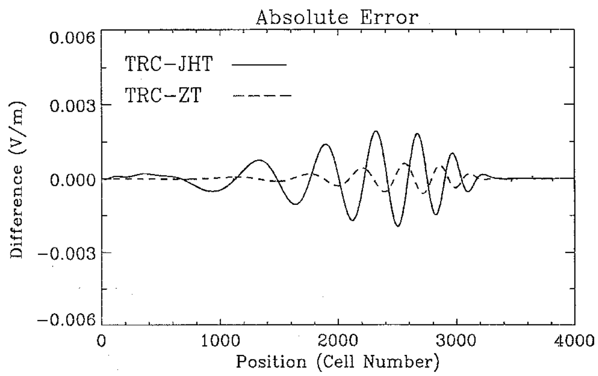
V. Experimental Results

We give results comparing all five methods on the linear dispersive problem proposed in [4]. A sinusoidal carrier of frequency $f = 1.37 \times 10^{14}$ Hz is modulated by a hyperbolic secant envelope with time constant of 14.6 fs and propagated in a second-order dispersive medium (where $\varepsilon_s = 5.25, \varepsilon_\infty = 2.25, \omega_1 = 4.0 \times 10^{14}, \delta_1 = 1.0 \times 10^9, \Delta t = 2.25 \times 10^{-17}\,\mathrm{s}, \Delta x = 5$ nm). Results after 5000 time steps using all three recursive convolution schemes are shown in the first plot of Fig. 1. The absolute difference between the TRC and CRC methods as well as between the TRC and PLRC methods are shown in the second plot of Fig. 1. It is evident that our higher-order convolution method TRC is more accurate than the original constant convolution method CRC and also our earlier claim of interchangeability of PLRC and TRC schemes is also supported by Fig. 1.

Next, we compared our TRC scheme with the other, nonconvolution-based schemes, i.e. JHT and ZT. A small, yet significant, difference was observed between the results



(a)



(b)

Fig. 2. (a) Electric field and (b) difference between methods of a hyperbolic secant envelope with carrier in a second-order dispersive medium after 5000 time steps using TRC, JHT, and ZT.

obtained by the different schemes, as can be seen in Fig. 2. The numerical dissipation produced by the schemes is the least for the TRC method followed by PLRC, ZT, JHT, and CRC.

In terms of computational efficiency, the CPU times per cell per time step are shown in Table I. We see that using our new TRC requires only an 8% increase in computation time over the CRC and requires the same amount of storage space.

TABLE I
CPU TIME FOR THE DIFFERENT SCHEMES

Scheme	RC	JHT	TRC	PLRC	ZT
μs/cell/step	2.6	2.7	2.8	3.4	3.4
% increase	0	4%	8%	31%	31%

VI. CONCLUSION

We have described a new higher-order convolution scheme, TRC, which is based on the trapezoidal rule, and have derived a *one* time step recursive scheme to compute it. This new method has been compared to four previously published techniques and the results show the TRC method to be superior in terms of accuracy and required computer resources. This new method is a general method capable of modeling order-M dispersive media whereas the JHT and ZT schemes have been derived only for a second-order dispersive media. Furthermore, the PLRC method requires the storage of one more real variable per electric field component than the TRC scheme. This will be very important in 3-D applications.

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