An Efficient Higher Order Numerical Convolution for Modelling Nth-Order Lorentz Dispersion

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Abstract

Results of using a higher order numerical convolution technique to model Nth-order, Lorentz type, dispersive media are presented. The convolution integral arising in the electromagnetic constitutive relation is approximated by the *trapezoidal rule* of numerical integration and implemented using a newly derived *one time step* recursion relation. This new method is compared to previously published techniques on the problem of a transient electromagnetic plane wave propagating in a dispersive media. All the methods considered solve the first order wave equations using the standard finite difference time domain technique. The results presented show that the new method performs the same or better than the other methods in terms of accuracy, robustness, and memory requirements.

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 media with Lorentz type dispersion in the time domain. One approach is the method proposed by Joseph *et al.* (JHT), where the constitutive relation relating the electric flux density $\boldsymbol{D}(x, t)$ to the electric field $\boldsymbol{E}(x, t)$ is expressed via a second order differential equation [2]. The second, more general, technique is that of Luebbers and Hunsberger (LH) in which the constitutive relation for a general Nth order Lorentz dispersive medium is represented as a convolution integral [3]. Other schemes have been published, but these two seem to be the most popular. We first consider the (LH) and then summarize our new higher order convolution scheme and give results arising from the two convolution schemes on a sample problem.

II. Nth-Order Lorentz Dispersion

When considering time-varying electromagnetic fields, 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 given by the Nth-order Lorentz dispersion, that is

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

where, in general, two complex conjugate poles exist for each term in the summation. These poles model the natural resonances exhibited by the medium. The time domain equivalent can be represented as a convolution integral, as in [1, 3].

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III. Numerical Approximation

In numerical computations, Maxwell's curl equations can be approximated by the standard FDTD method (for $\boldsymbol{D}(x,t)$ and $\boldsymbol{E}(x,t)$) and the new frequency dependent constitutive relation must also be approximated. The procedure described in [3] approximates the convolution integral by a (0th order) discrete summation and then derives a recursive method for implementation. This method, which will be referred to as (LH), is summarized by the new electric field update equation given by

$$E_y^{n+1}(i) = \frac{\varepsilon_\infty}{\frac{\sigma(i)\Delta t}{\varepsilon_0}+\varepsilon_\infty+\chi^0}E_y^n(i) + \frac{1}{\frac{\sigma(i)\Delta t}{\varepsilon_0}+\varepsilon_\infty+\chi^0}\sum_{p=1}^{N} Re\left[\hat{\psi}_p^n(i)\right]$$

$$-\frac{\Delta t}{\left(\frac{\sigma(i)\Delta t}{\varepsilon_0}+\varepsilon_\infty+\chi^0\right)\varepsilon_0\Delta x}\left[H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2}\right)-H_z^{n+\frac{1}{2}}\left(i-\frac{1}{2}\right)\right] \tag{2}$$

where the discrete function $\hat{\psi}_p^n(i)$ is calculated recursively as

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

For a detailed description of the meaning of all the variables we refer the reader to [3, 4].

IV. Discrete Trapezoidal Convolution Method

The main computational advantage of the convolution method (LH) over the ordinary differential equation method (JHT) is that only one level of backstorage is required for any of the variables and/or fields [2, 3]. The reason the (LH) scheme only requires one time level of backstorage 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 then we would require two time levels of backstorage (thus sacrificing memory requirement for accuracy). We have been able to incorporate the "trapezoidal rule" approximation into a one time step recursive scheme where the discrete function $\hat{\psi}_p^n(i)$ is found by the recursive procedure

$$\hat{\psi}_p^n(i) = E_y^n(i)\ \hat{\chi}_p^0 + e^{(-\alpha_p+j\beta_p)\Delta t}\ \hat{\psi}_p^{n-1}(i) \tag{4}$$

and the update equation for the electric field is given by (5) below.

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

$$
\begin{aligned}
E_y^{n+1}(i) = {} & \frac{E_y^{\,n}(i)}{\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2}} \sum_{p=1}^{N} Re\left[\frac{\hat{\chi}_p^0 - 2\varepsilon_\infty e^{(-\alpha_p + j\beta_p)\Delta t}}{2e^{(-\alpha_p + j\beta_p)\Delta t}}\right] \\
& - \frac{1}{\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2}} \sum_{p=1}^{N} Re\left[\left(\frac{e^{2(-\alpha_p + j\beta_p)\Delta t} - 1}{2e^{(-\alpha_p + j\beta_p)\Delta t}}\right)\hat{\psi}_p^n\right] \\
& - \frac{\Delta t}{\left(\frac{\sigma(i)\Delta t}{\varepsilon_0} + \varepsilon_\infty + \frac{\chi^0}{2}\right)\varepsilon_0 \Delta x}\left[H_z^{\,n+\frac{1}{2}}\left(i+\tfrac{1}{2}\right) - H_z^{\,n+\frac{1}{2}}\left(i-\tfrac{1}{2}\right)\right]
\end{aligned}
\tag{5}
$$

V. Comparison on Two Test Problems

We first give results comparing the (LH) and (TC) methods on the linear dispersive problem proposed in [3], where a plane Gaussian pulse is launched in a free space region and impinges normally onto a dispersive media ($\varepsilon_s = 3.0$, $\varepsilon_\infty = 1.5$, $\omega_1 = 40\pi \times 10^9$, $\omega_2 = 100\pi \times 10^9$, $\delta_1 = 0.1\omega_1$, $\delta_2 = 0.1\omega_2$, $G_1 = 0.4$, $G_2 = 0.6$, $\Delta t = 0.125$ [ps], $\Delta x = 37.5$ [μm]). Figure 1 includes plots of the results for the (LH) and (TC) methods and their difference after 1300 time steps. Next, we reduce the width of the Gaussian pulse by half, and therefore, approximately double its frequency content. The results of such a pulse are shown in Figure 1. As can be seen, and as expected, the methods agree better in the first test problem than the second problem due to the lower frequency content of the pulse.

We have also obtained similar results by comparing the schemes for a modulated femtosecond pulse in a linear dispersive problem proposed in [2]. The absolute error (after 5000 time steps) between (JHT) and (TC) were minimal when compared to the absolute difference between the results of (LH) and either (JHT) or (TC) [5].

VI. Conclusion

We have given a new higher order convolution scheme based on the trapezoidal rule and have derived a one time step recursive scheme to compute it. This new method has been compared to two previously published techniques and the results are favorable, especially when the frequency content of the electric field is high.

References

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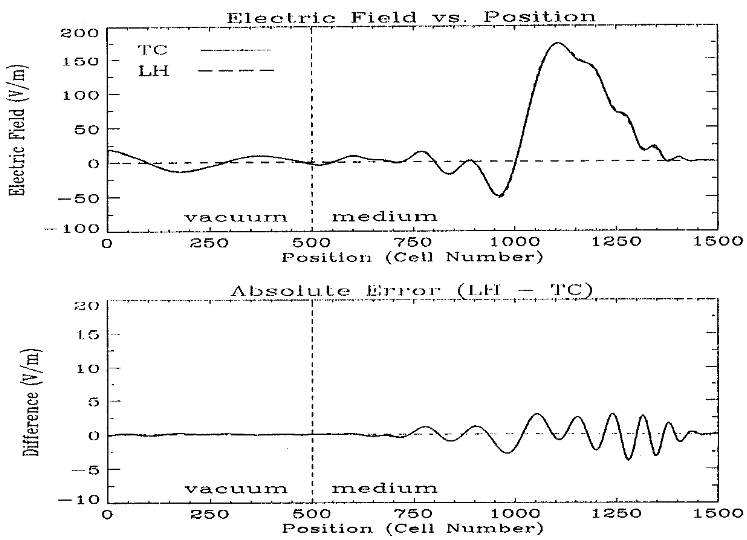

Figure 1. **Electric field and difference between methods for a Gaussian pulse propagating in a fourth-order dispersive medium after 1300 time steps using (LH) and (TC) methods.**

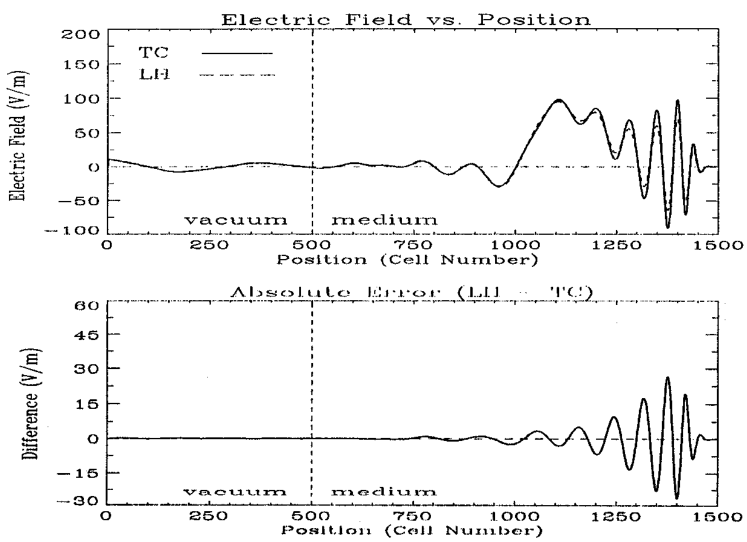

Figure 2. **Electric field and difference between methods for a Gaussian pulse with higher frequency content propagating in a fourth-order dispersive medium after 1300 time steps.**