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EFFICIENT EVALUATION OF CONVOLUTION INTEGRALS ARISING IN FDTD FORMULATIONS OF ELECTROMAGNETIC DISPERSIVE MEDIA

Riaz Siushansian and Joe LoVetri

Department of Electrical Engineering
The University of Western Ontario
London, Ontario
Canada N6A 5B9

Abstract–The Trapezoidal Recursive Convolution (TRC) scheme was previously used to model Nth order Lorentz type dispersive media. In this paper, the full derivation of this *quasi*-trapezoidal-based algorithm is presented and the derivation is expanded to include the Nth order Debye type dispersion as well as Sellmeyer's dispersion equation. In addition, the case of general convolution integrals is considered where any arbitrary integrand or the integral itself is represented as a sum of exponential functions, i.e. Prony's method. The technique is compared to several previously published schemes and it is shown that its performance equals or exceeds various other methods in terms of accuracy, robustness, and computational efficiency. A comparison to the exact application of trapezoidal numerical integration is made and it is shown that, for time increments encountered in typical FDTD analyses, the truncation error due to applying the quasi-trapezoidal approximation is negligible. Finally, it is shown how the skin effect phenomenon, as it applies to multiconductor transmission lines, can be modeled using a rational function approximation to the frequency dependency of the line resistance. This model is obtained by using Levy's method to curve fit the line resistance directly in the frequency domain and then the convolution integral is formulated in a form amenable to the TRC algorithm.

I. INTRODUCTION

Recently, there has been a growing interest in the numerical modeling of linear dispersive media [1–4,6,15,25,26]. Some applications, involving the study of biological tissues, are concerned with the daily human exposure to radio frequency and microwave energy [1,2], while others have considered applications of electromagnetic radiation in hyperthermia cancer therapy [3]. Also, the study of wave propagation in highly dispersive media (such as ice, snow, water, plasma, and radar-absorbing material) and the reflections from an air/dispersive medium interface have been the focus of many researchers [1,4]. Finally, modern optical technology has been demanding more accurate numerical models for pulse propagation in dispersive media. Applications in this field range from high-speed optical lines to sub-picosecond electro-optic switches and all-optical computational devices [5,6]. All of the above applications require the accurate modeling of dispersive media which is the main focus of this paper.

Generally, when a material is subjected to a time harmonic electromagnetic field, the polarization vector, P, and the permittivity are functions of the frequency of the alternating field. An important class of materials is referred to

as linear dispersive, or frequency dependent, materials [7,8]. A physical model of dispersive media can be developed by considering the forced oscillations of an electron, due to an applied electric field, in a single-electron-single-atom model. The classical equation of motion for harmonic oscillation (due to an external force) is often used to model such problems. In the frequency domain, the displacement distance of an electron, r_0, (which is the solution to the second order ordinary differential equation of harmonic oscillation) is commonly represented by a Lorentz model [7] using a pair of complex conjugate poles:

$$r_0 = \frac{K}{j\omega + \alpha + j\beta} + \frac{K^*}{j\omega + \alpha - j\beta}. \tag{1}$$

In a dispersive material, the poles essentially determine the shape and the location of the absorption bands and, hence, give each material its unique properties [9]. However, many dispersive materials contain permanent dipoles (for example water); for these materials, at low frequencies (hundreds of MHz), the external field aligns otherwise randomly oriented dipoles. This process is referred to as orientational polarization, and almost always dominates other types of polarization. In this case a first order model is often used where its solution in the frequency domain is given by the single pole

$$r_0 = \frac{A}{j\omega + \alpha}, \tag{2}$$

where both A and α are real numbers. This representation of dispersive media is referred to as the Debye model. It has been shown that an arbitrary material can be represented by N_L pairs of Lorentz complex conjugate poles and/or N_D Debye (complex) poles [9]. In section II, we briefly describe this generalization to multiple poles as it is the basis for our numerical scheme. We also note that once the generalization to an arbitrary number of multiple poles has been made, a wide variety of dispersive phenomena can be studied by modeling the dispersive behavior as a meromorphic function which then has a partial fraction expansion in the form of multiple single and/or complex conjugate poles [10]. For example, the skin effect in transmission lines is effectively modeled by assuming that the series internal impedance is modeled by [11, 12]

$$\hat{z}_i(\omega) = r_{dc} + r_{dc}\sqrt{\frac{\omega}{\omega_0}}(1 + j) \tag{3}$$

where ω_0 is the break frequency (defined as the frequency where the radius of the conductor is equal to the skin depth, that is $r_\omega = \delta$), and r_{dc} is the d.c. resistance of the conductor. In the time domain, this is approximated by a sum of exponential terms, via Prony's method, or $\hat{z}_i(\omega)$ can be approximated directly in the frequency domain as we will show in section VI.

II. Nth-ORDER DISPERSIVE MEDIA

The electromagnetic constitutive relation for a linear dispersive medium can be written as

$$\mathbf{D} = \varepsilon_0\varepsilon_\infty\mathbf{E} + \varepsilon_0\mathbf{P_L}, \tag{4}$$

where the electric polarization term, $\mathbf{P_L}$, models chromatic dispersion. As was discussed in the previous section, an arbitrary dispersive medium can be modeled using an assembly of forced harmonic oscillations; consequently, the frequency dependent permittivity is given by the Nth-order Lorentz dispersion formula

$$\varepsilon(\omega) = \frac{\mathbf{D}(\omega)}{\varepsilon_0 \mathbf{E}(\omega)} = \varepsilon_\infty + \hat{\chi}(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_{p=1}^{N} \frac{G_p \omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} \tag{5}$$

where, ε_s is the static permittivity, ε_∞ is the permittivity at infinite frequency, ω_p is the p^{th} resonant frequency, δ_p is the p^{th} damping coefficient, and $\hat{\chi}(\omega)$ is the susceptibility of the medium. To ensure causality, two complex conjugate poles exist for each term in the summation, and the relative *strength* of each term is given by G_p where the following condition must be observed [4]:

$$\sum_{p=1}^{N} G_p = 1. \tag{6}$$

On the other hand, the dispersive nature of many materials can be successfully modeled via an Nth-order Debye model [1,15,2,3]. In this case, the frequency domain expression for the permittivity is given by:

$$\varepsilon(\omega) = \frac{\mathbf{D}(\omega)}{\varepsilon_0 \mathbf{E}(\omega)} = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_{p=1}^{N} \frac{A_p}{1 + j\omega\tau_p} \tag{7}$$

where τ_p is the p^{th} relaxation time, and A_p is the relative strength of each term.

Dispersion also appears in fiber optics; an electromagnetic wave propagating in an optical cable interacts with electrons and generates a frequency dependent response in the material. This response manifests itself as the broadening of the pulse in time (i.e. chromatic dispersion), which is represented as a frequency dependent index of refraction of the fiber. The index of refraction of any material is the square root of its permittivity and, for fiber optics, it is modeled by the Lorentz dispersion equation. However, in the case of fiber optics, the resonant frequencies are often the most significant contributors to the value of permittivity. For most applications in fiber optics, and in regions far away from the resonant frequencies (where $\omega_p^2 - \omega^2 \gg 2\omega\delta_p$), the imaginary part of the permittivity is very small and can be ignored, i.e. Lorentz's equation where all damping coefficients are zero. This means that the index of refraction of any material can be modeled using Sellmeyer's equation given by [13,5]:

$$\varepsilon_r(\omega) = \eta^2(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_{p=1}^{N} \frac{G_p \omega_p^2}{\omega_p^2 - \omega^2}. \tag{8}$$

The fact that, the above equation does not provide an accurate approximation of materials' index of refraction at the resonant frequencies, is of no concern since this model of dispersive media is intended for all regions except near these resonant frequencies.

As can be seen in all the above frequency domain formulations, the linear polarization, $\mathbf{P_L}(\omega) = \hat{\chi}(\omega)\mathbf{E}(\omega)$, is modeled by a sum of first order and/or

second order poles, that is the second terms of (5) or (7). The frequency domain product of the electric field and the first-order frequency domain susceptibility function, $\hat{\chi}(\omega)$, can be represented in the time domain by a linear convolution

$$\mathbf{P_L}(t) = \int_0^t \mathbf{E}(t-\tau)\chi(\tau)d\tau \tag{9}$$

where now $\chi(\tau)$ is the time domain susceptibility of the medium and the principal of causality has been applied to simplify the limits of the above convolution integral [8]. The expression for the Lorentzian time-domain susceptibility function is obtained by taking the inverse Fourier transform of each term in (5), that is

$$\chi_p(t) = \lambda_p \sin(\beta_p t)e^{-\alpha_p t}U(t) \Leftrightarrow \frac{\lambda_p\beta_p}{(\alpha_p^2+\beta_p^2)+2j\omega\alpha_p-\omega^2}, \tag{10}$$

where $U(t)$ is the unit step function,

$$\alpha_p = \delta_p, \quad \beta = \sqrt{\omega_p^2-\delta_p^2}, \quad \text{and} \quad \lambda_p = \frac{\omega_p^2 G_p(\varepsilon_s-\varepsilon_\infty)}{\beta_p}. \tag{11}$$

The time-domain susceptibility function of a Debye medium is obtained by taking the inverse Fourier transform of the Debye term of (7)

$$\chi_p(t) = \lambda_p e^{-\alpha_p t}U(t) \Leftrightarrow \frac{\lambda_p}{(j\omega+\alpha_p)}, \tag{12}$$

where

$$\alpha_p = 1/\tau_p, \quad \lambda_p = A_p(\varepsilon_s-\varepsilon_\infty)/\tau_p. \tag{13}$$

Using these time domain susceptibility functions we now show how an efficient numerical algorithm for evaluating the convolution integrals of equation (9) can be constructed by using a numerical integration technique similar to the trapezoidal rule.

III. DERIVATION OF THE TRC SCHEME

In the standard Finite Difference Time Domain (FDTD) technique the constitutive parameters of Maxwell's equations are assumed to be constant. While this assumption is appropriate and convenient for free space and most dielectrics over a narrow band of frequencies, it is not accurate for the majority of cases, especially for highly dispersive (frequency dependent) media. The purpose of all the published extensions to the standard FDTD method which are discussed in Section IV of this paper, are to better model frequency dependent media. In this section, the derivation of the discrete Trapezoidal Recursive Convolution (TRC) [20] is presented for a general case. The derivations are developed for both an Nth-order Lorentz and an Nth-order Debye dispersive media. Consider the Maxwell-Ampere law

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \sigma \mathbf{E}, \tag{14}$$

where the time domain expression for the constitutive relation is given by (4). The above equations may be solved numerically using any of the various finite

difference methods which have been developed [4,14]. The equations can be discretized in time, where the value of a field variable at the n^{th} time step is denoted by $\mathbf{E}^n = \mathbf{E}(n\Delta t)$. If we apply this discretization to (14) we get

$$\frac{\mathbf{D}^{n+1} - \mathbf{D}^n}{\Delta t} = \nabla \times \mathbf{H}^{n+1/2} - \sigma \left(\frac{\mathbf{E}^{n+1} + \mathbf{E}^n}{2} \right), \tag{15}$$

where we have assumed that the magnetic field and the electric field components are interlaced in time. Following Luebbers [4], the discretized form of the constitutive relation (4) can be written for the difference of two consecutive time steps as

$$\mathbf{D}^{n+1} - \mathbf{D}^n = \varepsilon_0 \varepsilon_\infty (\mathbf{E}^{n+1} - \mathbf{E}^n) + \varepsilon_0 (\mathbf{P}^{n+1} - \mathbf{P}^n). \tag{16}$$

If in the convolution integral of (9) the value of the electric field over each time step is approximated as an average of the fields over two consecutive time steps, then at any point in space we have

$$\begin{aligned} \mathbf{P}(n\Delta t) &= \int_o^{n\Delta t} \mathbf{E}(n\Delta t - \tau)\chi(\tau)d\tau \\ &\cong \sum_{m=0}^{n-1} \left[\frac{\mathbf{E}^{n-m} + \mathbf{E}^{n-m-1}}{2} \right] \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau)d\tau. \end{aligned} \tag{17}$$

This is what we call the quasi-trapezoidal evaluation of the convolution integral. In general the goal is to represent the convolution term for linear polarization as a discrete function that can be evaluated recursively (at each time step). The fact that this can be accomplished is due to the exponential form of the time-domain susceptibility function we are considering. Thus, the convolution integral may be calculated by an update equation of the form $\xi^{n+1} = f(\xi^n)$.

At first sight it seems that using an average of the field components at two consecutive time points in (17) as opposed to only the $\mathbf{E}^{n-m}$ term will require two levels of back storage for the electric field values in the recursion relation (consequently requiring more memory for its implementation). However, due to the exponential nature of some of the auxiliary functions and/or variables, we will show how this discretized approximation can be implemented as a one time step recursive method. Starting with the discretized form of the constitutive relation, (16), and substituting the quasi-trapezoidal approximation, (17), we arrive at

$$\begin{aligned} \mathbf{D}^{n+1} - \mathbf{D}^n &= \varepsilon_0 \varepsilon_\infty (\mathbf{E}^{n+1} - \mathbf{E}^n) \\ &\quad + \varepsilon_0 \sum_{m=0}^{n} \left[\frac{\mathbf{E}^{n-m+1} + \mathbf{E}^{n-m}}{2} \right] \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau)d\tau \\ &\quad - \varepsilon_0 \sum_{m=0}^{n-1} \left[\frac{\mathbf{E}^{n-m} + \mathbf{E}^{n-m-1}}{2} \right] \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau)d\tau. \end{aligned} \tag{18}$$

In [4], a complex time-domain susceptibility, $\hat{\chi}_p(\tau)$, was defined such that

$$\chi_p(\tau) = Re[\hat{\chi}_p(\tau)] \tag{19}$$

and now the integral terms of (18) can be written in terms $\hat{\chi}_p(\tau)$ as

$$\hat{\chi}_p^m = \int_{m\Delta t}^{(m+1)\Delta t} \hat{\chi}_p(\tau)\partial\tau = \left(\frac{j\lambda_p}{-\alpha_p + j\beta_p}\right)\left[1 - e^{(-\alpha_p+j\beta_p)\Delta t}\right] e^{(-\alpha_p+j\beta_p)m\Delta t} \tag{20}$$

where only the real part of this expression will be used in calculations of the electric field. An important property of (20) is that at each time step, $m+1$, the value of the discrete integral of the complex time-domain susceptibility function, $\hat{\chi}_p^{m+1}$, is related to its value at the previous time step, $\hat{\chi}_p^m$, that is

$$\hat{\chi}_p^{m+1} = \hat{\chi}_p^m e^{(-\alpha_p+j\beta_p)\Delta t}. \tag{21}$$

We now consider the last two terms of (18), that is, the linear polarization terms. At this point the introduction of a complex linear polarization, $\hat{\mathbf{P}}_p^n$, is necessary due to the use of the complex susceptibility function, $\hat{\chi}_p^m$, where the subscript p denotes one pair of Lorentz poles or a single Debye pole. After some simplifications and using (21), keeping in mind that $\mathbf{E}^0 = 0$, we arrive at

$$\begin{aligned} 2(\hat{\mathbf{P}}_p^{n+1} - \hat{\mathbf{P}}_p^n) &= \mathbf{E}^{n+1}\hat{\chi}_p^0 + \sum_{m=1}^{n} \mathbf{E}^{n-m+1}\hat{\chi}_p^m - \sum_{m=0}^{n-2} \mathbf{E}^{n-m-1}\hat{\chi}_p^m \\ &= \mathbf{E}^{n+1}\hat{\chi}_p^0 + e^{(-\alpha_p+j\beta_p)\Delta t}\sum_{m=0}^{n-1} \mathbf{E}^{n-m}\hat{\chi}_p^m - \sum_{m=0}^{n-2} \mathbf{E}^{n-m-1}\hat{\chi}_p^m. \end{aligned} \tag{22}$$

The summation terms of the above equation represent discrete convolution integrals and can be evaluated recursively. In order to do so a new complex function, $\hat{\Psi}_p^n$, is defined as

$$\hat{\Psi}_p^n = \sum_{m=0}^{n-1} \mathbf{E}^{n-m}\hat{\chi}_p^m = \mathbf{E}^n\hat{\chi}_p^0 + \sum_{m=1}^{n-1} \mathbf{E}^{n-m}\hat{\chi}_p^m = \mathbf{E}^n\hat{\chi}_p^0 + e^{\delta_p\Delta t}\sum_{m=1}^{n-1} \mathbf{E}^{n-m}\hat{\chi}_p^{m-1}, \tag{23}$$

where $\delta_p = -\alpha_p + j\beta_p$. Now letting $m' = m - 1$ we get

$$\sum_{m=1}^{n-1} \mathbf{E}^{n-m}\hat{\chi}_p^{m-1} = \sum_{m'=0}^{(n-1)-1} \mathbf{E}^{(n-1)-m'}\hat{\chi}_p^{m'} = \hat{\Psi}_p^{n-1}. \tag{24}$$

Hence, we see that $\hat{\Psi}_p$ can be evaluated recursively by

$$\hat{\Psi}_p^n = \mathbf{E}^n\hat{\chi}_p^0 + e^{\delta_p\Delta p}\hat{\Psi}_p^{n-1}. \tag{25}$$

Thus, the summation terms of (22) are replaced by the recursive expression defined by (25), and we arrive at

$$2(\hat{\mathbf{P}}_p^{n+1} - \hat{\mathbf{P}}_p^n) = \mathbf{E}^{n+1}\hat{\chi}_p^0 + e^{\delta_p\Delta t}\hat{\Psi}_p^n - \hat{\Psi}_p^{n-1}. \tag{26}$$

The above equation demonstrates the "two time step" nature of our technique; this means that at each time step two previous values of $\hat{\Psi}_p^n$ must be stored. However, for most realistic problems this extra level of back-storage could mean allocation of a large block of memory that may not be available. In its place it is

possible to evaluate $\hat{\Psi}_p^{n-1}$ directly from (25), that is

$$\hat{\Psi}_p^{n-1} = (\hat{\Psi}_p^n - \mathbf{E}^n \hat{\chi}_p^0) e^{-\delta_p \Delta t}, \tag{27}$$

and hence (26) can be written as

$$2(\hat{\mathbf{P}}_p^{n+1} - \hat{\mathbf{P}}_p^n) = \mathbf{E}^{n+1} \hat{\chi}_p^0 + \mathbf{E}^n \hat{\chi}_p^0 e^{-\delta_p \Delta t} + \hat{\Psi}_p^n \left(e^{\delta_p \Delta t} - e^{-\delta_p \Delta t} \right), \tag{28}$$

This last equation requires a large amount of CPU time to evaluate the discrete polarization terms of (18) at one-half of the memory cost as compared to (26). The trade off between speed and memory is a characteristic of most numerical schemes where back-storage of variables is required. In the remainder of this paper, we will use the memory efficient formulation of the TRC scheme (28). This form can be substituted into the right hand side of equation (18) for each pole or pole pair, and subsequently into (15), where only the real part of the complex polarization vector is used. Finally, a new one time step update equation for the electric field is given by

$$\mathbf{E}^{n+1} = \frac{\mathbf{E}^n}{\varepsilon_\infty + \dfrac{\sigma \Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2}} \left[\varepsilon_\infty - \frac{\sigma \Delta t}{2\varepsilon_0} + \frac{1}{2} \sum_{p=1}^{N} Re \left[\hat{\chi}_p^0 e^{-\delta_p \Delta t} \right] \right]$$

$$+ \frac{\Delta t (\nabla \times \mathbf{H}^{n+1/2})}{\left(\varepsilon_\infty + \dfrac{\sigma \Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2} \right) \varepsilon_0} + \frac{0.5}{\varepsilon_\infty + \dfrac{\sigma \Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2}} \sum_{p=1}^{N} Re \left[(1 - e^{-2\delta_p \Delta t}) \underline{\hat{\Psi}}_p^n \right] \tag{29}$$

where an alternative form of $\underline{\hat{\Psi}}_p^n$ is defined as

$$\underline{\hat{\Psi}}_p^n = e^{\delta_p \Delta t} \hat{\Psi}_p^n, \tag{30}$$

and

$$\chi^0 = \sum_{p=1}^{N} Re[\hat{\chi}_p^0] = \sum_{p=1}^{N} Re \left[\frac{j\lambda_p}{\delta_p} \left[1 - e^{\delta_p \Delta t} \right] \right]. \tag{31}$$

The new variable, $\underline{\hat{\Psi}}_p^n$, is updated recursively using the equation

$$\underline{\hat{\Psi}}_p^n = \mathbf{E}^n \hat{\chi}_p^0 + \underline{\hat{\Psi}}_p^{n-1}. \tag{32}$$

The update equation for a Debye dispersive medium can be easily derived using a similar method. First, the integral terms in the summations of (18) are defined as

$$\chi_p^m = \int_{m\Delta t}^{(m+1)\Delta t} \chi_p(\tau) d\tau = \frac{\lambda_p}{\alpha_p} \left[1 - e^{-\alpha_p \Delta t} \right] e^{-\alpha_p m \Delta t}. \tag{33}$$

Using the property of equation (21), the time-domain susceptibility function is related to its value in the previous time step by

$$\chi_p^{m+1} = \chi_p^m e^{-\alpha_p \Delta t}. \tag{34}$$

The remainder of the derivation is identical to the one of the Lorentz medium and the final update equation for the electric field is given by:

$$\mathbf{E}^{n+1} = \frac{\mathbf{E}^n}{\varepsilon_\infty + \dfrac{\sigma\Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2}} \left[\varepsilon_\infty - \frac{\sigma\Delta t}{2\varepsilon_0} + \frac{1}{2}\sum_{p=1}^{N} \chi_p^0 e^{-\delta_p \Delta t} \right]$$

$$+ \frac{\Delta t(\nabla \times \mathbf{H}^{n+1/2})}{\left(\varepsilon_\infty + \dfrac{\sigma\Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2}\right)\varepsilon_0} + \frac{0.5}{\varepsilon_\infty + \dfrac{\sigma\Delta t}{2\varepsilon_0} + \dfrac{\chi^0}{2}} \sum_{p=1}^{N} \left[(1 - e^{-2\delta_p \Delta t}) \underline{\Psi}_p^n \right] \quad (35)$$

where

$$\underline{\Psi}_p^n = \mathbf{E}^n \chi_p^0 + \underline{\Psi}_p^{n-1}, \quad (36)$$

and

$$\chi^0 = \sum_{p=1}^{N} \chi_p^0 = \sum_{p=1}^{N} \frac{\lambda_p}{\alpha_p} \left[1 - e^{-\alpha_p \Delta t} \right]. \quad (37)$$

IV. A COMPARISON OF VARIOUS NUMERICAL SOLUTIONS

In this section a comparison of the TRC method is made with other previously published techniques. The procedure developed in [6] uses the inverse Fourier transform of the complex permittivity given by (5) or (7) to derive a second order differential equation between $\mathbf{E}(t)$ and $\mathbf{H}(t)$. A second order finite difference approximation is then derived for this equation, and an update equation for $\mathbf{E}^{n+1}$ is obtained. This scheme requires the storage of $2N-1$ real variables in addition to the field values of the standard FDTD method. The above scheme will be referred to JHT in the following discussion. Sullivan demonstrated that a Z transform technique can be employed to model dispersive media in conjunction with the FDTD method [3, 18, 19]. 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 2 poles demand 3 additional real variables beyond the current field values of the general FDTD scheme. We will denote this method as the ZT method.

Since a conventional evaluation of convolution integrals is very computationally demanding, both JHT and ZT schemes shy away from evaluating the convolution term that appears in the time domain constitutive relations of the dispersive media. However, in the convolution based schemes, the convolution terms for linear polarization is represented as a discrete function and is evaluated recursively for each time step. This method will not only eliminate the need for storage of the entire history of the electric field, but also, does not require the large number of multiplications usually associated with straight forward evaluation of convolution integrals. In the next few paragraphs we will briefly discuss three convolution based FDTD schemes.

In the Constant Recursive Convolution (CRC) method [4, 16], the convolution integral is replaced by a discrete function where all field values are assumed to be constant over each time step, Δt; hence the integral term of equation (17) is expanded as follows:

$$\mathbf{D}^n = \varepsilon_0 \varepsilon_\infty \mathbf{E}^n + \varepsilon_0 \sum_{m=0}^{n-1} \mathbf{E}^{n-m} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau) d\tau. \tag{38}$$

The above approximation is only accurate for pulses with low frequency content. However, as the slope of the electric field increases (i.e. pulses with high frequency content), the pulse approximation of the convolution integral no longer holds. Since CRC, equation (38), uses a first order accurate approximation of the convolution integral, whereas the FDTD method is a second order accurate scheme, the Piecewise Linear Recursive Convolution (PLRC) method was developed to correct this short-coming. In the PLRC scheme, the electric field of the convolution integral is represented as a piecewise linear function of time, i.e.

$$\mathbf{E}(n\Delta t - \tau) = \mathbf{E}^{n-m} + \left(\frac{\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}}{\Delta t} \right) (\tau - m\Delta t) \tag{39}$$

Thus, the constitutive relation becomes [17]

$$\begin{aligned} \mathbf{D}^n = \varepsilon_0 \varepsilon_\infty \mathbf{E}^n &+ \varepsilon_0 \sum_{m=0}^{n-1} \left[\mathbf{E}^{n-m} \int_{m\Delta t}^{(m+1)\Delta t} \chi_p(\tau) d\tau \right] \\ &+ \varepsilon_0 \sum_{m=0}^{n-1} \left[\left(\frac{\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}}{\Delta t} \right) \int_{m\Delta t}^{(m+1)\Delta t} (\tau - m\Delta t) \chi_p(\tau) d\tau \right] \end{aligned} \tag{40}$$

This scheme is theoretically more accurate than the CRC method due to its higher order of approximation of the convolution integral. However, this improvement in accuracy has its price; the electric field has to be back stored one extra time step. Also, it requires one extra complex addition and one extra complex multiplication (two real-complex multiplications) operations per-pole-per-dimension beyond the number of operations required for the update equation of the recursive function of the CRC scheme. All of the above factors will result in a more accurate solution but demand more memory and a longer computation time to obtain it.

In the TRC method described above, the convolution integral is evaluated using a quasi-trapezoidal rule of integration, that is equation (17). Although (17) is not an exact application of the trapezoidal rule; we show in the next section that for the majority of cases this formulation is as accurate as other second order accurate convolution based schemes (i.e. PLRC method). In addition, the general simplification of the TRC method allows for a one time level recursive evaluation of the convolution integral i.e. no additional memory requirement as compared to the CRC scheme.

In Table 1, all the aforementioned methods of numerical modeling of dispersive media are compared for accuracy, robustness, and computational efficiency. Numerical results have been presented in [20,21]. In terms of accuracy, all of the above methods with the exception of the CRC scheme are second order schemes

(see first row of the table). In most cases the obtained experimental data can not be represented by a single term Debye or Lorentz model and multiple orders of either of the dispersive models must be utilized to accurately represent the characteristics of the material. Although it is possible to derive multiple order expressions for both the JHT and ZT method, the equations often become lengthy and cumbersome. However, as it was stated earlier, the N-th order assumption is built into the all the recursive convolution schemes. Also, both schemes require back storage of an additional 2N-1 values per dimension, that is, N-1 values of $\mathbf{D}(t)$ and N values of $\mathbf{E}(t)$ (almost twice the convolution schemes). Due to these disadvantages, the JHT and ZT schemes are not recommended for implementation in general purpose 3-dimensional FDTD codes.

The last three rows of the table state the additional computational requirements of each scheme. The number of addition and multiplication operations, as well as the memory requirements for each scheme are given for a one dimensional problem per order of dispersion for Lorentz type dispersive media. Overall, the TRC scheme appears to be the most efficient and is the one we have implemented in our 3-dimensional general purpose FDTD code.

scheme	CRC	TRC	PLRC	JHT	ZT
accuracy	1st	2nd	2nd	2nd	2nd
Nth-order	Y	Y	Y	-	-
multiplication operations	6N	4N	8N	4N	4N
addition operations	4N	4N	8N	3N	3N
additional variables	2N	2N	2N+1	4N-1	4N-1

Table 1. Comparison of different schemes with the standard FDTD for Lorentz type dispersive medium.

V. THE TRUNCATION ERROR DUE TO THE TRC SCHEME

In this section we compare the quasi-trapezoidal integration to the PLRC scheme which is an exact application of the trapezoidal rule as given in (40). Denoting the polarization using that method as $\mathbf{P}_{PLRC}$ we can write:

$$\mathbf{P}_{diff} = \mathbf{P}_{PLRC} - \mathbf{P}_{TRC} \tag{41}$$

for the difference between the two methods of evaluating the convolution integral (for N=1), where the polarization due to the TRC approximation is given by (17). Thus we have:

$$\mathbf{P}_{diff} = \sum_{m=0}^{n-1} \mathbf{E}^{n-m} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau)d\tau + \sum_{m=0}^{n-1} \left(\frac{\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}}{\Delta t} \right) \int_{m\Delta t}^{(m+1)\Delta t} (\tau - m\Delta t)\chi(\tau)d\tau - \sum_{m=0}^{n-1} \left(\frac{\mathbf{E}^{n-m} + \mathbf{E}^{n-m-1}}{2} \right) \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau)d\tau. \quad (42)$$

Once more, the complex susceptibility function is used to evaluate linear polarization terms of (40), that is,

$$\mathbf{P}_{diff} = \sum_{m=0}^{n-1} \mathbf{E}^{n-m}\hat{\chi}^m + \sum_{m=0}^{n-1} \left(\frac{\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}}{\Delta t} \right) \int_{m\Delta t}^{(m+1)\Delta t} (\tau - m\Delta t)\hat{\chi}(\tau)d\tau - \sum_{m=0}^{n-1} \left(\frac{\mathbf{E}^{n-m} + \mathbf{E}^{n-m-1}}{2} \right) \hat{\chi}^m \quad (43)$$

where the discrete complex susceptibility function, $\hat{\chi}^m$, is defined by:

$$\hat{\chi}^m = \int_{m\Delta t}^{(m+1)\Delta t} \hat{\chi}_p(\tau)d\tau = \left(\frac{\Gamma}{\delta} \right) \left[e^{\delta\Delta t} - 1 \right] e^{\delta m\Delta t}, \quad (44)$$

and the time domain complex susceptibility function is $\hat{\chi}(\tau) = \Gamma e^{\delta\tau}$. Following the substitution of (44) in (43) and after much simplification, the truncation error due to the TRC approximation is given by:

$$\mathbf{P}_{diff} = Re \left[\left(\frac{1}{2} + \frac{1}{\delta\Delta t} - \frac{e^{\delta\Delta t}}{e^{\delta\Delta t} - 1} \right) \sum_{m=0}^{n-1} (\mathbf{E}^{n-m} - \mathbf{E}^{n-m-1})\hat{\chi}^m \right], \quad (45)$$

where for Lorentz type media

$$\delta = -\alpha + j\beta, \quad \Gamma = -j\lambda, \quad (46)$$

and for the case of Debye media,

$$\delta = -A, \quad \Gamma = -\lambda, \quad (47)$$

as given in equations (11) and (13). Further analysis of the above difference expression, (45), has revealed that the TRC scheme performs well at frequencies near the resonant frequency (i.e. when $\Delta t \leq 1/\pi\omega_0$ where ω_0 is the largest resonant frequency, or $\omega_0 = 1/\tau_0$ where τ_0 is the smallest relaxation time of the medium). However, large numerical errors (dissipation) are observed for values of Δt corresponding to the waveforms with low frequency content (as compare to the highest resonant frequency of the dispersive medium). Since no physical dispersion occurs at such low frequencies, the standard FDTD formulation may be used for the cases of waveforms with low frequency content propagating in dispersive media.

VI. TRC FORMULATION OF ARBITRARY FUNCTIONS

So far we have concentrated our efforts on the recursive formulation of the convolution integral as it appears in the Maxwell's equations. Earlier, it was shown that these equations are only applicable to the cases of either Lorentz or Debye type dispersive media. However, convolution relations are typical of time domain formulations of frequency dependent phenomenon and may arise in a variety of applications such as modeling of the skin effect in transmission lines. Hence, it is only logical to develop the above TRC scheme for convolution integrals of any arbitrary function, that is, the convolution of any set of arbitrary time domain functions can be approximated by

$$\int_0^t F(t-\tau)\chi(\tau)d\tau \cong \sum_{m=0}^{n-1}\left[\left[\frac{F^{n-m}+F^{n-m-1}}{2}\right]\int_{m\Delta t}^{(m+1)\Delta t}\chi(\tau)d\tau\right], \quad (48)$$

where $\chi(t)$ is the arbitrary function used to describe the time domain behavior of the frequency dependent material, and $F(t)$ is the unknown variable. The general derivation of such schemes follows the same procedure outlined in section III. However, in order to use the recursive evaluation properties of the auxiliary variable/functions of the TRC scheme, the kernel of the integral of equation (48) must be in the form of an exponential function. Hence, some type of procedure must be employed to represent the kernel or its integral in the desired exponential fomm. This can be accomplished either in the time or the frequency domain using either Prony's or Levy's method [23, 24].

In the frequency domain, the kernel can be evaluated at various frequencies and by using the weighted least squares curve fitting procedure, introduced by Levy, the frequency domain kernel can be represented as a meromorphic function which has partial fraction expansion in the form of multiple single and/or complex conjugate poles, (1) and (2),

$$\chi(\omega) \cong \sum_{p=1}^{P_D}\frac{A_p}{j\omega+\alpha_p} + \sum_{p=1}^{P_L/2}\left(\frac{K_p^*}{j\omega+\alpha_p+j\beta_p}+\frac{K_p}{j\omega+\alpha_p-j\beta_p}\right) \quad (49)$$

where each summation term represents either a single Debye pole or a pair of complex conjugate poles (note that α_p of the two summation terms represent different poles). The inverse Fourier transform of the expansion terms is known and thus the inverse Fourier transform of (49) is given by (note that $K = |K|\angle\theta$):

$$\chi(t) = \sum_{p=1}^{P_D} A_p e^{-\alpha_p t} + \sum_{p=1}^{P_L/2} 2|K_p|e^{-\alpha_p t}\cos(\beta_p t+\theta). \quad (50)$$

Since a recursive evaluation of the integral of the above terms is essential to the efficiency of the algorithm, a complex time domain function, similar to (19), is defined for the second term of (50), that is,

$$\chi(t) = Re(\hat{\chi}(t)) = Re\left[\sum_{p=1}^{P_D} A_p e^{-\alpha_p t} + \sum_{p=1}^{P_L/2} 2|K_p|e^{j\theta}e^{(-\alpha_p+j\beta_p)t}\right]. \quad (51)$$

where A_p, α_p, K_p, and $-\alpha_p + j\beta_p$ are the coefficients in Levy's approximation of $\chi(\omega)$, P_D are the number of Debye type terms and $P_L/2$ are the number of Lorentz type terms required for an accurate approximation of the function. Now, the integral of the kernel can be solved analytically, and is evaluated recursively for each term of the expansion,

$$\int_{m\Delta t}^{(m+1)\Delta t} \hat{\chi}_p(\tau)d\tau = \hat{\chi}_p^m = \hat{\chi}_p^{m-1} e^{-\delta_p \Delta t}, \tag{52}$$

$$\hat{\chi}_p^0 = \frac{a_p}{\delta_p}(1 - e^{-\delta_p \Delta t}), \tag{53}$$

where $\delta_p = -\alpha_p$ or $\delta_p = -\alpha_p + j\beta_p$ and $a_p = A_p$ or $a_p = 2|K|e^{j\theta}$ depending on which summation of (51) we're talking about.

After substitution of (52) in (48), the time domain convolution integral is given by

$$\int_0^t F(t-\tau)\chi(\tau)d\tau \cong Re\left[\sum_{p=1}^{P}\sum_{m=0}^{n-1}\left(\frac{F^{n-m} + F^{n-m-1}}{2}\right)\hat{\chi}_p^m\right], \tag{54}$$

where now $P = P_D + P_L/2$ and once again, the auxiliary function $\hat{\Psi}_p^n(i)$ is defined as

$$\hat{\Psi}_p^n = \sum_{m=0}^{n-1} F^{n-m}\hat{\chi}_p^m \tag{55}$$

where an updated equation for its recursive evaluation can be obtained using a similar approach to the one outlined in section III. i.e.

$$\hat{\Psi}_p^n = F^n \hat{\chi}_p^0 + e^{-\delta_p \Delta t}\hat{\Psi}_p^{n-1}. \tag{56}$$

Finally, the update equation for the convolution integral can be derived in terms of the previously defined functions/variables, that is

$$\hat{\Psi}_p^n = Re\left[\frac{1}{2}\sum_{p=1}^{P}\left[\hat{\chi}_p^0 F^{n+1} + (e^{-\delta_p \Delta t} + 1)\hat{\Psi}_p^n\right]\right]. \tag{57}$$

For the time domain case, Prony' s method is utilized to approximate the time domain integral of equation (48), that means

$$\int_{m\Delta t}^{(m+1)\Delta t} \hat{\chi}(\tau)d\tau \cong \sum_{p=1}^{P}\hat{\chi}_p^m = \sum_{p=1}^{P} a_p e^{-\delta_p m\Delta t}. \tag{58}$$

Although this approximation requires recalculations of all the coefficients using Prony's approximation, the update equations of (56) and (57) remain the same. The only change appears in the value of $\hat{\chi}_p^0$ given by

$$\hat{\chi}_p^0 = a_p. \tag{59}$$

This new procedure allows us to obtain FDTD update equations (of a frequency dependent phenomena) for time domain electromagnetic problems in formulations

other than Maxwell's equations. An example of such phenomenon is the modeling of the skin effect in Multiconductor Transmission Lines (MTL). Consider one of the MTL equations in the frequency domain

$$\frac{\partial}{\partial x}\hat{V}(x,\omega) + [j\omega L + \hat{Z}(\omega)]\hat{I}(x,\omega) = 0, \tag{60}$$

where L is the low frequency inductance and $\hat{Z}(\omega)$ is the impedance of the line, given by

$$\hat{Z}(\omega) = r_{dc} + \frac{r_{dc}}{\sqrt{\pi f_0}}\sqrt{j\omega}, \tag{61}$$

in which f_0 is the break frequency. Denoting $B = r_{dc}/\sqrt{\pi f_0}$ and $R = r_{dc}$, (60) can be written as

$$\frac{\partial}{\partial x}\hat{V}(x,\omega) + j\omega L\hat{I}(x,\omega) + R\hat{I}(x,\omega) + B\sqrt{j\omega}\hat{I}(x,\omega) = 0 \tag{62}$$

and taking the inverse Fourier transform of the above equation

$$\frac{\partial}{\partial x}\hat{V}(x,t) + L\frac{\partial}{\partial t}I(x,t) + RI(x,t) + B\int_0^t \chi(\tau)F(x,t-\tau)d\tau = 0. \tag{63}$$

where

$$\chi(t) \Leftrightarrow \frac{1}{\sqrt{j\omega}} \quad \text{and} \quad F(t-\tau) = \frac{\partial I(x,t-\tau)}{\partial(t-\tau)} \tag{64}$$

and $F(x,t)$ is the derivative of current with respect to second argument. Now the term $(j\omega)^{-1/2}$ can be approximated directly in the frequency domain, via Levy's method by the rational polynomial approximation [24]

$$\frac{1}{\sqrt{j\omega}} \cong \sum_{p=1}^{P} \frac{a_p}{j\omega + \delta_p}. \tag{65}$$

The best fit was obtained using a ninth order, $p = 9$, polynomial approximation of the above function over a frequency range of $\omega = 1 \rightarrow 100$ Mrad/s. The coefficients of the fitted rational function are given in Table 2. Also a comparison of the approximated polynomial with the original function is shown in Figure 1.

Now the losses in the MTL equations, due to the skin effect, which were previously implemented using the CRC method can now be approximated by the quasi-trapezoidal approximation of the convolution integral, i.e. the TRC method [22]. This will increase the accuracy of the obtained numerical solution at no cost to memory requirement.

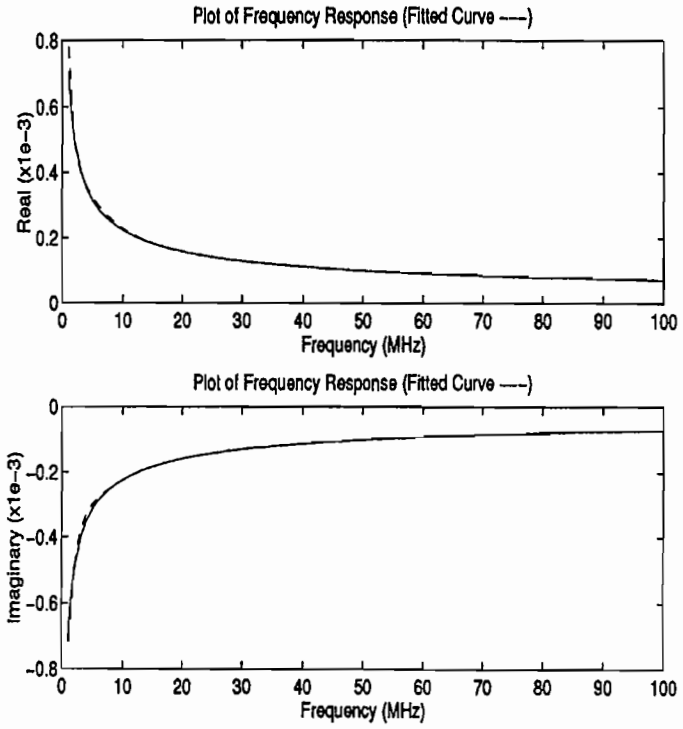

Figure 1. A comparison between the original function, $\frac{1}{\sqrt{j\omega}}$, and a ninth order fitted polynomial.

Table 2: Coefficients of the Levy's Approximation of $1/\sqrt{j\omega}$

i	$a_p \times 10^4$	$\delta_p \times 10^9$
1	−5.3019	3.3584
2	1.2165	−0.2462
3, 4	$-0.0002 \pm 0.00004j$	$0.0112 \pm 0.0672j$
5, 6	$0.0003 \pm 0.0005j$	$-0.0090 \pm 0.0597j$
7	0.3192	−0.0408
8	0.1749	−0.0075
9	0.0926	−0.0006

Table 2. Coefficients of the Levy's approximation of $\frac{1}{\sqrt{j\omega}}$.

VII. CONCLUSION

In this paper the full derivation of the TRC technique was presented for general dispersive media. It was also shown that the FDTD update equation obtained using a quasi-trapezoidal approximation of the convolution integral has similar accuracy as the piecewise linear approximation method for time steps typically encountered in FDTD analyses. A comparison of the TRC method with other published schemes showed TRC to outperform all the others in terms of accuracy, required memory, and other computer resources. The application of this method to general convolution integrals encountered in dispersive electromagnetic problems was also described and the specific case of the skin effect problem in multiconductor transmission lines was discussed.

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Riaz Siushansian received the B.E.Sc. and M.E.Sc. degrees in Electrical Engineering from The University of Western Ontario, London, Ontario, Canada, in 1993 and 1995, respectively. Since then he has been pursuing a Ph.D. degree at The University of Western Ontario and has been spending work times at the Communications Research Centre in Ottawa, Canada. His present research interests are in time domain modeling of electromagentic wave propagation in dispersive media as well as non-orthogonal FDTD techniques.

Joe LoVetri was born in Enna, Italy, in 1963. He received the B.Sc. (with distinction) and M.Sc. degrees, both in Electrical Engineering, from the University of Manitoba in 1984 and 1987 respectively. From 1984 to 1986 he was EMI/EMC engineer at Sperry Defence Division in Winnipeg, Manitoba. From 1986 to 1988 he held the position of TEMPEST engineer at the Communications Security Establishment in Ottawa. From 1988 to 1991 he was a Research Officer at the Institute for Information Technology of the National Research Council of Canada. He received the Ph.D. degree in Electrical Engineering from the University of Ottawa in 1991. He is currently an Associate Professor in the Department of Electrical Engineering at The University of Western Ontario where he has been since 1991. His main interests lie in time domain computational electromagnetics. His specific research interests are in time domain modeling of electromagnetic compatibility problems such as multiconductor transmission line networks and other electromagnetic interactions.