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Validation and Demonstration of Frequency Approximation Methods for Modeling Dispersive Media in FDTD

by

John H. Beggs
Mississippi State University
Department of Electrical and Computer Engineering
Box 9571
Mississippi State, MS 39762

Abstract

Recently, digital signal processing techniques were used to design, analyze and implement discrete models of polarization dispersion for the Finite-Difference Time-Domain (FDTD) method. The goals of the present work are to illustrate the FDTD update equations for these techniques and to validate and demonstrate these techniques for one-dimensional problems involving reflections from dispersive dielectric half-spaces. Numerical results are compared with several other dispersive media FDTD implementations.

1 Introduction

The Finite-Difference Time-Domain (FDTD) method is an accurate and robust method for the numerical solution of Maxwell's time-dependent curl equations directly in the time domain. Transient electromagnetic field propagation, coupling and scattering is directly simulated by approximating Maxwell's equations with discrete-time equations. The FDTD method has been applied successfully to a wide variety of problems including those involving the complex interaction of electromagnetic fields with materials. These materials include (but are not limited to) biological tissues, optical materials and ferrites; all of which exhibit dispersion. The strength and usefulness of FDTD for these problems depends on an accurate treatment of the material dispersion. There have been many different implementations for modeling dispersion in FDTD, and these usually fall into three separate categories: recursive convolution [1]–[6]; differential equation based methods [7]–[11] and Z-transform methods [12]–[13]. The recursive convolution (RC) approaches convolve the electric susceptibility with the electric field in the time-domain to model the dispersive polarization term which results in a very efficient implementation. The differential equation method augments the conventional FDTD method with an auxiliary differential equation (ADE) in the time-domain relating the electric displacement vector, $\vec{D}$, and the electric field intensity vector, $\vec{E}$. This method requires a bit more memory than the RC method, but usually results in improved accuracy. The Z-transform (ZT) method is a combination of the RC and ADE methods; implementing an update equation relating $\vec{D}$ to $\vec{E}$ and other recursive accumulator variables.

In recent work by Hulse and Knoesen [14], digital signal processing techniques were used to design, analyze and implement discrete models of dispersion in the FDTD method. In that paper, the electric polarization was considered to be a filter or system function, and this was used to design a corresponding digital system function. Different design approaches and implementations were considered and were rigorously analyzed for truncation errors, memory and CPU requirements. The recursive convolution, differential equation and Z-transform based methods were unified under the frequency-approximation (FA) design methodology and were similarly analyzed to compare with the frequency approximation methods. The frequency approximation methodology is an extension of the Z-transform approach by examining other digital filter design options. This class of Z-transform approaches for modeling dispersive media in FDTD is very intuitive and appealing because the FDTD method generates and operates on discrete time-domain data sequences. Therefore, frequency approximation methods provide a very natural mechanism for enhancement of the FDTD method in a variety of ways. Although various time-domain equations were presented in [14], a comparison of numerical time-domain results was not illustrated. The present work involves demonstrating two of the different frequency-

1054-4887

approximation design approaches presented in [14] for both Debye and Lorentz dispersion on one-dimensional problems involving reflection from a dispersive dielectric half-space. The intent with the present work is to present the FDTD update equations for these techniques and to validate the frequency approximation methods by illustrating how the numerical results compare with previous FDTD models of material dispersion.

2 Theory

The theory behind the frequency approximation design methods is straightforward. Previous FDTD models of material dispersion have transformed the frequency-dependent electric polarization term from the frequency domain to the time domain. In the time domain, methods were developed to discretize either the convolution integral or the auxiliary differential equation. The frequency approximation methods avoid this transformation initially by providing a discrete approximation to the analog system (or filter) function and then formulating the discrete time-domain update equations. The basic idea is to provide an approximation to the $j\omega$ terms in the frequency domain as a rational polynomial in z. This approximation is then substituted into the analog system function to transform it into the Z-domain. This approach discretizes each power of $j\omega$ identically, whereas the ADE methods will typically discretize each power of $j\omega$ (i.e. each $\partial/\partial t$ term in the time-domain) differently. A strong motivation for investigating the FA methods is because they separate the error in the FA design from other errors inherent with the FDTD method such as grid dispersion and outer boundary errors. The theoretical development in this section is adapted from [14]. A similar model was recently developed and implemented for the surface impedance boundary condition [15].

2.1 Debye Dispersion

Materials exhibiting first-order Debye dispersion can be characterized by an electric permittivity of the form

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega\tau} \tag{1}$$

where ϵ_s is the static permittivity and ϵ_∞ is the infinite frequency permittivity. For linear, dispersive and isotropic media, the electric displacement vector, $\vec{D}$, is related to the electric field intensity vector by the expression

$$\vec{D} = \epsilon(\omega)\vec{E} \tag{2}$$

The frequency approximation methods design a digital system function for the electric permittivity by expressing the $j\omega$ terms using a rational polynomial in z. The two approaches validated in this paper are the Backward Difference (BD) method and the Bilinear Transformation (BLT) method. For the BD method, $j\omega$ is approximated as [14]

$$j\omega \approx \frac{1 - z^{-1}}{T} \tag{3}$$

where T is the sampling interval. Substituting (3) into equation (1) gives the digital system permittivity function

$$\epsilon(z) = \frac{\epsilon_\infty + \epsilon_s T/\tau - \epsilon_\infty z^{-1}}{1 + T/\tau - z^{-1}} \tag{4}$$

The Z-domain analog of (2) can be rewritten as

$$\vec{E}(z) = \frac{\vec{D}(z)}{\epsilon(z)} \tag{5}$$

and substituting (4) into equation (5) yields

$$\begin{aligned} \vec{E}(z) &= \frac{1}{\epsilon_\infty\tau + \epsilon_s T}\Big\{(\tau + T)\,\vec{D}(z) - z^{-1}T\vec{D}(z) \\ &\quad + \epsilon_\infty\tau z^{-1}\vec{E}(z)\Big\} \end{aligned} \tag{6}$$

Note the z^{-1} terms are delay operators in the time domain, and the corresponding FDTD update equation for (6) is given by

$$\vec{E}^n = \frac{1}{\epsilon_\infty\tau + \epsilon_s T}\Big\{(\tau + T)\,\vec{D}^n - T\vec{D}^{n-1} + \epsilon_\infty\tau\vec{E}^{n-1}\Big\} \tag{7}$$

The bilinear transformation (BLT) method approximates $j\omega$ by

$$j\omega \approx \frac{2}{T}\frac{1 - z^{-1}}{1 + z^{-1}} \tag{8}$$

Substituting (8) in (1) gives

$$\epsilon(z) = \frac{(2\epsilon_\infty + \epsilon_s T/\tau) - (2\epsilon_\infty - \epsilon_s T/\tau)\,z^{-1}}{(2 + T/\tau) - (2 - T/\tau)\,z^{-1}} \tag{9}$$

for the digital system permittivity and the corresponding time-domain update equation is given by

$$\begin{aligned} \vec{E}^n &= \frac{1}{2\tau\epsilon_\infty + \epsilon_s T}\Big\{(2\tau + T)\,\vec{D}^n + (T - 2\tau)\,\vec{D}^{n-1} \\ &\quad + (2\tau\epsilon_\infty - \epsilon_s T)\,\vec{E}^{n-1}\Big\} \end{aligned} \tag{10}$$

2.2 Lorentz Dispersion

For materials exhibiting Lorentz dispersion, the frequency-dependent permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)\,\omega_0^2}{\omega_0^2 + j\omega\delta - \omega^2} \tag{11}$$

where ω_0 is the resonant frequency and δ is the damping coefficient. For the BD method, the digital system permittivity function is given by

$$\epsilon(z) = \left\{\left[\epsilon_\infty (1+\delta T) + \epsilon_s (\omega_0 T)^2\right] - \epsilon_\infty (2+\delta T) z^{-1} + \epsilon_\infty z^{-2}\right\} / \left\{\left[1+\delta T + (\omega_0 T)^2\right] - (2+\delta T) z^{-1} + z^{-2}\right\} \quad (12)$$

and the corresponding time-domain update equation is

$$\vec{E}^n = \left\{\left[1+\delta T + (\omega_0 T)^2\right] \vec{D}^n - (2+\delta T) \vec{D}^{n-1} + \vec{D}^{n-2} + \epsilon_\infty (2+\delta T) \vec{E}^{n-1} - \epsilon_\infty \vec{E}^{n-2}\right\} / \left[\epsilon_\infty (1+\delta T) + \epsilon_s (\omega_0 T)^2\right] \quad (13)$$

For the BLT method, the digital system permittivity function is given by

$$\epsilon(z) = \left\{\left[\epsilon_\infty (4+2\delta T) + \epsilon_s (\omega_0 T)^2\right] - \left[8\epsilon_\infty - 2\epsilon_s (\omega_0 T)^2\right] z^{-1} + \left[\epsilon_\infty (4-2\delta T) + \epsilon_s (\omega_0 T)^2\right] z^{-2}\right\} / \left\{\left[4+2\delta T + (\omega_0 T)^2\right] - \left[8 - 2(\omega_0 T)^2\right] z^{-1} + \left[4 - 2\delta T + (\omega_0 T)^2\right] z^{-2}\right\} \quad (14)$$

and the corresponding time-domain update equation is

$$\vec{E}^n = \left\{\left[4+2\delta T + (\omega_0 T)^2\right] \vec{D}^n - \left[8 - 2(\omega_0 T)^2\right] \vec{D}^{n-1} + \left[4 - 2\delta T + (\omega_0 T)^2\right] \vec{D}^{n-2} + \left[8\epsilon_\infty - 2\epsilon_s (\omega_0 T)^2\right] \vec{E}^{n-1} - \left[\epsilon_\infty (4-2\delta T) + \epsilon_s (\omega_0 T)^2\right] \vec{E}^{n-2}\right\} / \left\{\epsilon_\infty (4+2\delta T) + \epsilon_s (\omega_0 T)^2\right\} \quad (15)$$

It is interesting to note that the update equations (7), (10), (13) and (16) are very similar to the auxiliary differential equation (ADE) method [7].

3 Demonstration

The demonstrations in this section involve calculation of reflection coefficients from one-dimensional dispersive dielectric half-spaces. The numerical results using the BD and BLT frequency-approximation methods are compared with other popular FDTD models of dispersive media, which are: auxiliary differential equation (ADE) method [7], recursive convolution (RC) [1], piecewise-linear recursive convolution (PLRC) [6], and Z-transform (ZT) [12] methods.

3.1 Debye Dispersion

For the Debye dispersion demonstration, computation of wide-band reflections at an air-water interface was performed. The one-dimensional problem space had 1000 cells with 500 cells simulating the water half-space and 500 cells of free-space. The cell size was 37.5 μm and the time step was 0.0625 ps. The water parameters used were $\epsilon_s = 81\epsilon_0$, $\epsilon_\infty = 1.8\epsilon_0$ and $\tau = 9.4$ ps and Figure 1 shows the frequency dependent permittivity. The incident

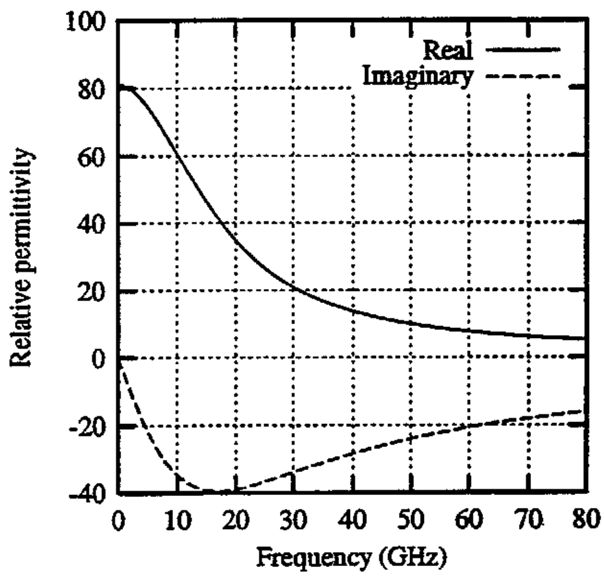

Figure 1: Relative permittivity, ϵ_r, versus frequency for Debye dispersive material.

pulse was a Gaussian pulse of the form

$$e_x^i(t) = e^{-((t-t_0)/\tau_0)^2} u(t) \quad (16)$$

where $t_0 = 25$ ps and $\tau_0 = 7.37$ ps. The pulse was truncated in time at -100 dB which resulted in a spatial pulse width of 400 cells and it contained significant energy to 145 GHz. The FDTD reflection coefficient was obtained by dividing the frequency response of the scattered field at the air-water interface by the frequency response of the incident field. The incident field was obtained by recording the electric field at the air-water interface location without the water half-space (i.e. free space only in the entire problem space). The time-domain scattered field is obtained by recording the time-domain total field at the air-water interface and subtracting the time-domain incident field. The other popular FDTD material dispersion implementations were used with equations taken directly from the appropriate articles in the literature. Figure 2 shows very good agreement between the reflection coefficient results for the BD and BLT methods and the exact solution. Figure 3 shows the percentage error of the BD

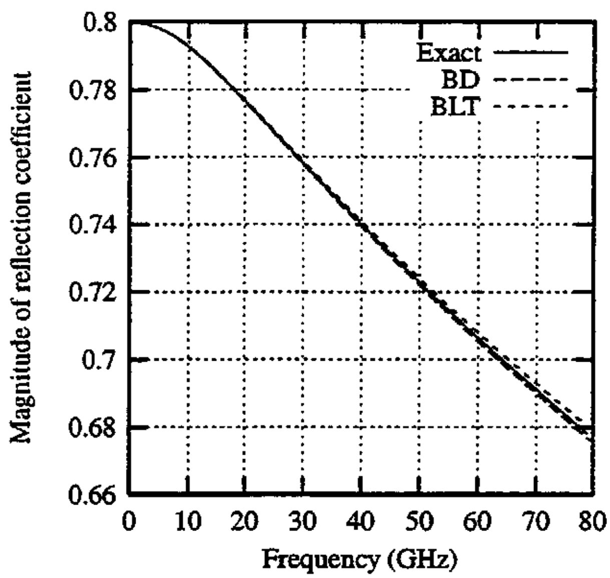

Figure 2: Reflection coefficient magnitude versus frequency for reflection from a Debye dispersive half-space.

and BLT methods compared to the other FDTD models of Debye dispersion. Note the percentage error in Figure 3 for the ADE, BLT and PLRC methods are almost identical and is increasing with frequency. The percentage error for the ZT method (which is an impulse-invariant design) is almost constant with frequency. Although these results include other inherent FDTD error sources, the general trend confirms the error analysis of the FA design methods presented in Figure 2 of [14] for Debye dispersion. The phase of the reflection coefficients for each method exhibited similar trends and levels of agreement.

3.2 Lorentz Dispersion

For the Lorentz dispersion demonstration, computation of wide-band reflections at an air-material interface were performed using two different dispersive media. The material and FDTD calculation parameters are given in Table 1. Figure 4 shows the frequency-dependent permittivity for material 1 only, since the permittivity for material 2 is very similar in frequency behavior. The same procedure was used to obtain an FDTD reflection coefficient as in the Debye dispersion example. The incident pulse was the Gaussian pulse of (16) with pulse

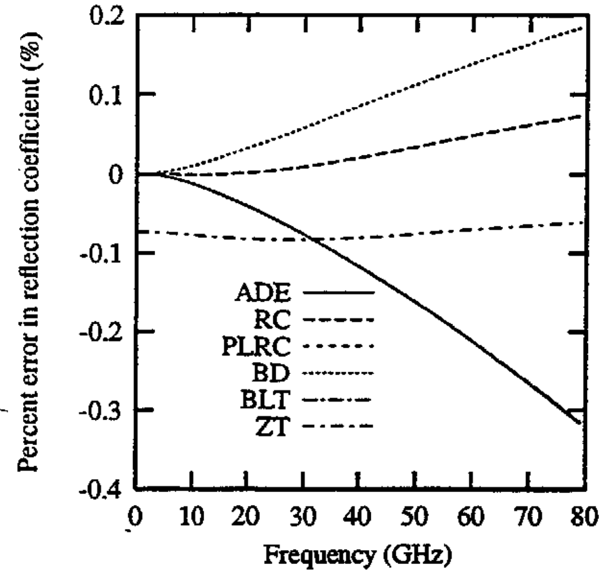

Figure 3: Percent error in reflection coefficient magnitude versus frequency for reflection from a Debye dispersive half-space.

Table 1: FDTD PARAMETERS FOR LORENTZ DISPERSION MATERIALS.

Parameter	Material 1	Material 2
Total # of cells	8000	1000
Dispersive cells	4000	500
Cell size	0.6 Å	250 μm
δt	0.2 as	0.833 ps
ϵ_s	$2.25\epsilon_0$	$3\epsilon_0$
ϵ_∞	ϵ_0	$1.5\epsilon_0$
ω_0	4×10^{16} rad/s	$40\pi \times 10^9$ rad/s
δ	0.56×10^{16} s^{-1}	$4\pi \times 10^9$ s^{-1}
t_0	42.4 as	21.5 ps
τ_0	12.5 as	6.35 ps
Pulse freq. cutoff	85 PHz	175 GHz
Pulse ampl. cutoff	-100 dB	-100 dB
Total pulse width	84.8 as	43 ps
Time steps	11,000	2,048

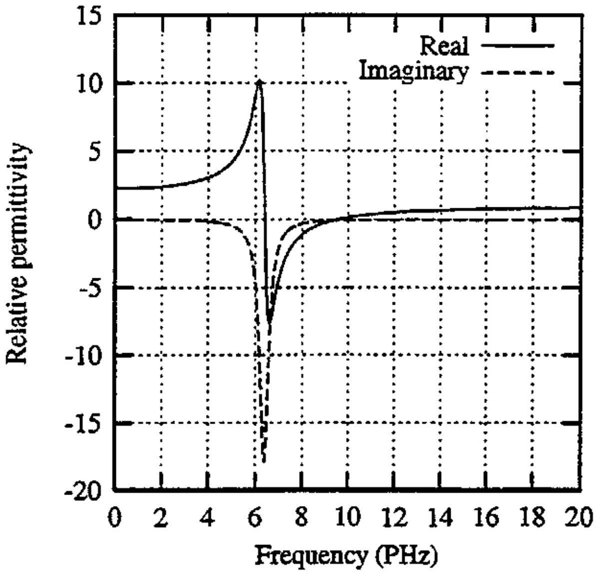

Figure 4: Relative permittivity for material 1 with Lorentz dispersion. The material properties are given in Table 1.

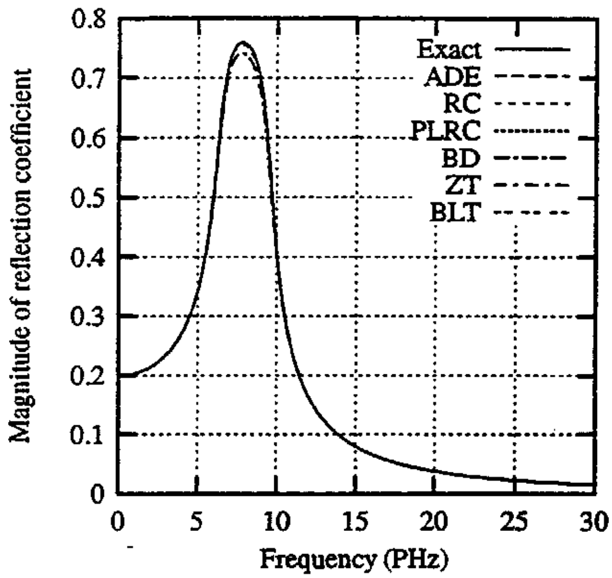

Figure 5: Reflection coefficient magnitude versus frequency (Petahertz, i.e. 10^{15} Hz) for material 1 with Lorentz dispersion.

parameters also given in Table 1. For material 1, Figure 5 shows the reflection coefficient results for the BD and BLT methods and Figure 6 shows the percentage error in the reflection coefficient using several methods. In Figure 5, the BLT method clearly has better agreement, especially in the resonance region. Figure 6 shows that the ADE and BLT methods have approximately the same level of error throughout the entire frequency band and are more accurate than the RC method (the step-invariant method) in the resonance region. Although the PLRC and ZT methods were unstable for this material and the given simulation parameters, a stabilized version was used to provide results for comparison. It was shown in [14] that the ZT method (impulse-invariant design) can be unstable for certain Lorentz materials. The cause of the instability with the PLRC is yet undetermined, but independent calculations using the same methods and parameters were made by Kelley [16] verified this instability.

Figures 7 and 8 show similar results as Figures 5 and 6, but for the second dispersive material. The FDTD simulation parameters are provided in Table 1. The BD method exhibits more error in Figure 7 for this material which is most likely due to aliasing in the digital system frequency response. The resonance region in material 2 is lower in frequency and therefore the sampling interval, T, is larger than material 1; which will result in a less accurate filter. Note in Figure 8 above the resonance region that the ADE method has the largest amount of error, followed by the BLT method and the ZT method (the impulse-invariant design). Although other error

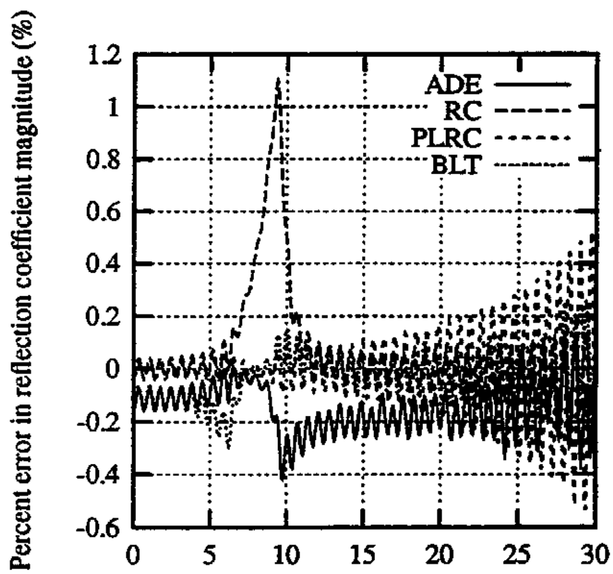

Figure 6: Percent error (%) in reflection coefficient magnitude versus frequency (Petahertz, i.e. 10^{15} Hz) for material 1 with Lorentz dispersion.

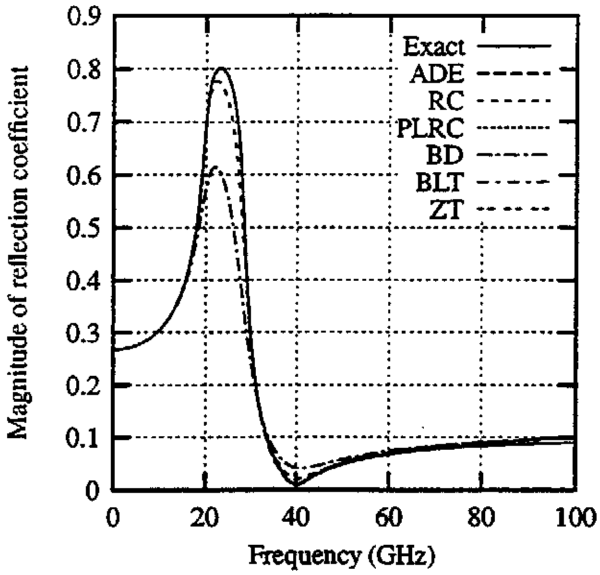

Figure 7: Reflection coefficient magnitude versus frequency for material 2 with Lorentz dispersion.

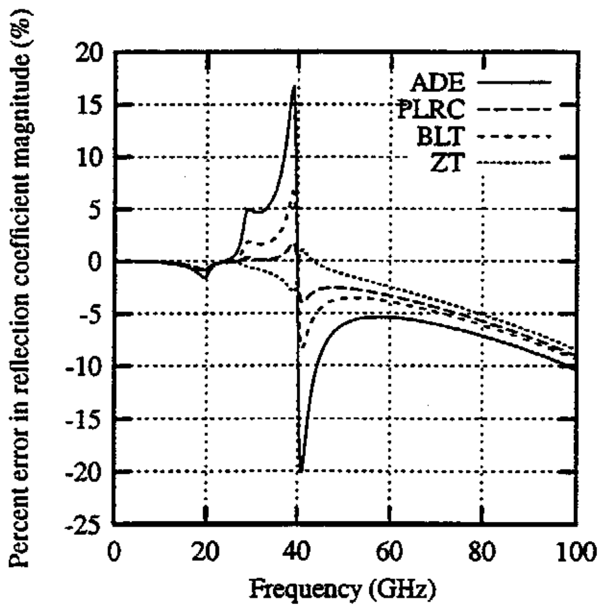

Figure 8: Percent error (%) in reflection coefficient magnitude versus frequency for material 1 with Lorentz dispersion.

sources inherent with the FDTD method are present, these general trends in the reflection coefficient results for both the Debye and Lorentz problems confirm observations in the frequency-approximation error analysis from [14]. It is clear that the BLT method is the preferred choice in the FA design methodology. Although results were not presented for the second Lorentz dispersion example, the original RC method remained stable and reasonably accurate for both problems. The RC method is a step-invariant design and is obviously a stable design for both Debye and Lorentz media.

The computational requirements of the BD and BLT methods are identical with the ADE method, which is not surprising, considering the time-domain update equations are almost identical. It can be shown that through careful programming and using optimal storage implementations, the memory requirements of the FA approaches can be made almost the same as the convolution methods, and they have better accuracy and stability behavior.

4 Conclusion

This paper has successfully demonstrated and validated frequency-approximation design models for FDTD treatment of dispersive materials exhibiting both Debye and Lorentz dispersion. FDTD update equations were provided for modeling materials with both types of dispersion. Wide-band one-dimensional reflection coefficient calculations were performed and excellent agreement with the exact solution was obtained. General trends in the FA error analyses presented in [14] were observed in the reflection coefficient results which provided further validation for the design models. It was also illustrated that the BLT method was the FA method of choice for both Debye and Lorentz dispersion to provide the best accuracy. The FA results exhibited similar levels of accuracy when compared with other FDTD implementations for dispersive media. Based upon accuracy and stability considerations, the BLT and ADE methods are the methods of choice for treatment of dispersive media using FDTD. The memory and floating point operational requirements for the FA methods are very similar (and in some cases, identical) to other FDTD dispersive media implementations. With optimal storage implementations, the BD and BLT FA methods can have almost the same memory requirements as the convolution approaches. Although this paper only considered a single Debye or Lorentz relaxation, extension of the BD or BLT methods to multiple relaxations is straightforward.

References

[1] R. J. Luebbers, F. Hunsberger, K. S. Kunz, R. B. Standler, and M. Schneider, "A frequency-dependent finite-difference time-domain formulation for dispersive materials", *IEEE Trans. Electromagn. Compat.*, vol. 32, no. 3, pp. 222–227, 1990.

[2] R. Luebbers, F. Hunsberger, and K. Kunz, "Finite difference time domain recursive convolution for second order dispersive materials", in *IEEE Antennas and Propagat. Soc. Int. Symp.*, Chicago, IL, July 1992, vol. 4, pp. 1972–1975.

[3] R. J. Luebbers and F. Hunsberger, "FDTD for Nth-order dispersive media", *IEEE Trans. Antennas Propagat.*, vol. 40, no. 11, pp. 1297–1301, 1992.

[4] R. Siushansian and J. LoVetri, "A comparison of numerical techniques for modeling electromagnetic dispersive media", *IEEE Microwave Guided Wave Lett.*, vol. 5, no. 12, pp. 426–428, 1995.

[5] D. F. Kelley and R. J. Luebbers, "The piecewise linear recursive convolution method for incorporating dispersive media into FDTD", in *11th Annual Review of Progress in Applied Computational Electromagnetics*, Monterey, CA, Mar. 1995, vol. 1, pp. 526–533.

[6] D. F. Kelley and R. J. Luebbers, "Piecewise linear recursive convolution for dispersive media using FDTD", *IEEE Trans. Antennas Propagat.*, vol. 44, no. 6, pp. 792–797, 1996.

[7] R. M. Joseph, S. C. Hagness, and A. Taflove, "Direct time integration of Maxwell's equations in linear dispersive media with absorption for scattering and propagation of femtosecond electromagnetic pulses", *Optics Lett.*, vol. 16, no. 18, pp. 1412–1414, 1991.

[8] O. P. Gandhi, B. Q. Gao, and J. Y. Chen, "A frequency-dependent finite-difference time-domain formulation for general dispersive media", *IEEE Trans. Microwave Theory Tech.*, vol. 41, no. 4, pp. 658–665, 1993.

[9] P. M. Goorjian and A. Taflove, "Direct time integration of Maxwell's equations in nonlinear dispersive media for propagation and scattering of femtosecond electromagnetic solitons", *Optics Lett.*, vol. 17, no. 3, pp. 180–182, 1992.

[10] P. M. Goorjian, A. Taflove, R. M. Joseph, and S. C. Hagness, "Computational modeling of femtosecond optical solitons from Maxwell's equations", *IEEE J. Quantum Electron.*, vol. 28, no. 10, pp. 2416–2422, 1992.

[11] O. P. Gandhi, "Reply to comments on "A frequency-dependent finite-difference time-domain formulation for general dispersive media"", *IEEE Trans. Microwave Theory Tech.*, vol. 42, no. 2, pp. 359, 1994.

[12] D. M. Sullivan, "Frequency-dependent FDTD methods using Z transforms", *IEEE Trans. Antennas Propagat.*, vol. 40, no. 10, pp. 1223–1230, 1992.

[13] D. Sullivan, "The use of Z transform theory for numerical simulation of dispersive and non-linear material with the FDTD method", in *IEEE Antennas and Propagat. Soc. Int. Symp.*, Seattle, WA, June 1994, vol. 3, pp. 1450–1453.

[14] C. Hulse and A. Knoesen, "Dispersive models for the finite-difference time-domain method: Design, analysis, and implementation", *J. Opt. Soc. Am., A Optics Image Sci. Vision*, vol. 11, no. 6, pp. 1802–1811, 1994.

[15] J. H. Beggs, "A FDTD surface impedance boundary condition using Z-transforms", *Appl. Comput. Electromagn. Soc. J.*, vol. 13, no. 1, pp. 14–24, Mar. 1998.

[16] D. F. Kelley, ", private communication.