Direct time integration of Maxwell's equations in linear dispersive media with absorption for scattering and propagation of femtosecond electromagnetic pulses

Rose M. Joseph, Susan C. Hagness, and Allen Taflove

Department of Electrical Engineering and Computer Science, McCormick School of Engineering, Northwestern University, Evanston, Illinois 60208-3118

Received May 29, 1991

We report the initial results for femtosecond pulse propagation and scattering interactions for a Lorentz medium obtained by a direct time integration of Maxwell's equations. The computational approach provides reflection coefficients accurate to better than 6 parts in 10,000 over the frequency range of dc to 3×10^{16} Hz for a single 0.2-fs Gaussian pulse incident upon a Lorentz-medium half-space. New results for Sommerfeld and Brillouin precursors are shown and compared with previous analyses. The present approach is robust and permits two-dimensional and three-dimensional electromagnetic pulse propagation directly from the full-vector Maxwell's equations.

A pulse propagating in a dispersive medium such as an optical fiber exhibits complicated behavior. It is of interest to have an accurate numerical model for this behavior as well as for other electromagnetic interactions with frequency-dependent materials.

The finite-difference time-domain (FD-TD) method is a numerical technique for direct time integration of Maxwell's equations.[1–4] It is a computationally efficient approach to modeling sinusoidal or impulsive electromagnetic interactions with arbitrary three-dimensional structures consisting of linear, possibly anisotropic, lossy dielectric and permeable media with frequency-independent parameters. It has been used for predicting electromagnetic wave scattering, penetration, and radiation for a variety of problems.[5] Recently, the range of FD-TD modeling applications has been substantially expanded to include ultra-high-speed signal lines,[6] subpicosecond electro-optic switches,[7] and linear optical directional couplers.[8]

Attempts have been made to extend FD-TD to frequency-dependent materials. Chromatic dispersion can be expressed in the time domain as a convolution integral involving the electric field and a causal susceptibility function. This convolution integral can be efficiently incorporated into the FD-TD algorithm for a first-order (Debye) dispersion.[9] In this Letter we present a more general approach that permits modeling of media having arbitrary-order dispersions. Our approach is based on a suggestion by Jackson (Ref. 10, p. 331) to relate the electric displacement $D(t)$ to the electric field $E(t)$ through an ordinary differential equation in time.

We consider a one-dimensional problem with field components E_z and H_y propagating in the x direction. If we assume first that the medium is nonpermeable, isotropic, and nondispersive, Maxwell's curl equations in one dimension are

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0}\frac{\partial E_z}{\partial x}, \tag{1a}$$

$$\frac{\partial D_z}{\partial t} = \frac{\partial H_y}{\partial x}. \tag{1b}$$

Here $D_z = \varepsilon E_z$, where the permittivity ε is independent of frequency. Using central differencing in time and space,[1] we can express the curl equations in finite-difference form as the following second-order accurate leapfrog algorithm:

$$H_y^{n+\frac{1}{2}}y(i+\tfrac{1}{2}) = H_y^{n-\frac{1}{2}}(i+\tfrac{1}{2}) + \frac{\Delta t}{\mu_0 \Delta x}[E_z^{n}(i+1) - E_z^{n}(i)], \tag{2a}$$

$$E_z^{n+1}(i) = E_z^{n}(i) + \frac{\Delta t}{\varepsilon \Delta x}[H_y^{n+\frac{1}{2}}(i+\tfrac{1}{2}) - H_y^{n+\frac{1}{2}}(i-\tfrac{1}{2})], \tag{2b}$$

where $E_z^{n}(i)$ denotes the electric field sampled at space point $x = i\Delta x$ and time point $t = n\Delta t$. (Please refer to Ref. 2 for the proper numerical stability criterion.)

For many dispersive media of interest, however, $\varepsilon = \varepsilon(\omega)$. We propose to include this frequency dependence in the FD-TD model by concurrently integrating an ordinary differential equation in time that relates $D_z(t)$ to $E_z(t)$. As suggested by Jackson, this equation is derived by taking the inverse Fourier transform of the complex permittivity expression,

$$\varepsilon(\omega) = \frac{D_z(\omega)}{E_z(\omega)}. \tag{3}$$

For an order-M dispersion, the computational model now becomes a three-step recursive process that re-

0146-9592/91/181412-03$5.00/0

tains the fully explicit nature of the original dispersionless FD-TD formulation,

$$H_y^{n+\frac{1}{2}}(i+\tfrac{1}{2}) = H_y^{n-\frac{1}{2}}(i+\tfrac{1}{2}) + \frac{\Delta t}{\mu_0 \Delta x}[E_z^n(i+1) - E_z^n(i)], \quad (4a)$$

$$D_z^{n+1}(i) = D_z^n(i) + \frac{\Delta t}{\Delta x}[H_y^{n+\frac{1}{2}}(i+\tfrac{1}{2}) - H_y^{n+\frac{1}{2}}(i-\tfrac{1}{2})], \quad (4b)$$

$$E_z^{n+1}(i) = f(D_z^{n+1}, \ldots, D_z^{n-M+1}; E_z^n, \ldots, E_z^{n-M+1}). \quad (4c)$$

At any time step n, this method requires storage of M previous values of D_z and $M-1$ previous values of E_z beyond the current field values. The approach will be made clear by the following examples:

Example 1: A first-order (Debye) dispersion can be specified by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - j\omega\tau} = \frac{D_z(\omega)}{E_z(\omega)}, \quad (5)$$

where $\varepsilon_s = \varepsilon(0)$, $\varepsilon_\infty = \varepsilon(\infty)$, and τ is the Debye relaxation time constant. If we take the inverse Fourier transform of Eq. (5) as defined by

$$f(t) = \int_{-\infty}^{+\infty} f(\omega)\exp(-j\omega t)\,\mathrm{d}\omega, \quad (6)$$

the result is a first-order differential equation in time relating D_z and E_z,

$$D_z + \tau\frac{\mathrm{d}D_z}{\mathrm{d}t} = \varepsilon_s E_z + \tau\varepsilon_\infty\frac{\mathrm{d}E_z}{\mathrm{d}t}. \quad (7)$$

This differential equation can be easily differenced to solve for E_z^{n+1} in terms of known values of E_z and D_z for insertion into Eq. (4c),

$$E_z^{n+1}(i) = \frac{\Delta t + 2\tau}{2\tau\varepsilon_\infty + \varepsilon_s\Delta t} D_z^{n+1}(i) + \frac{\Delta t - 2\tau}{2\tau\varepsilon_\infty + \varepsilon_s\Delta t} D_z^n(i) + \frac{2\tau\varepsilon_\infty - \varepsilon_s\Delta t}{2\tau\varepsilon_\infty + \varepsilon_s\Delta t} E_z^n(i). \quad (8)$$

Example 2: A second-order (Lorentz) dispersion can be specified by

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_0^2(\varepsilon_s - \varepsilon_\infty)}{\omega^2 + 2j\omega\delta - \omega_0^2} = \frac{D_z(\omega)}{E_z(\omega)}, \quad (9)$$

where $\varepsilon_s = \varepsilon(0)$, $\varepsilon_\infty = \varepsilon(\infty)$, ω_0 is the resonant frequency, and δ is the damping coefficient. Figure 1 shows the relative permittivity curve for a Lorentz medium that has the following parameters:

$$\varepsilon_s = 2.25\varepsilon_0, \quad \varepsilon_\infty = \varepsilon_0, \quad \omega_0 = 4.0 \times 10^{16}\ \text{rad/s},$$
$$\delta = 0.28 \times 10^{16}\ \text{s}^{-1}.$$

Inverse Fourier transformation of Eq. (9) results in the following second-order differential equation relating D_z and E_z:

$$\omega_0^2 D_z + 2\delta\frac{\mathrm{d}D_z}{\mathrm{d}t} + \frac{\mathrm{d}^2D_z}{\mathrm{d}t^2} = \omega_0^2\varepsilon_s E_z + 2\delta\varepsilon_\infty\frac{\mathrm{d}E_z}{\mathrm{d}t} + \varepsilon_\infty\frac{\mathrm{d}^2E_z}{\mathrm{d}t^2}. \quad (10)$$

This differential equation can be easily differenced to solve for E_z^{n+1} in terms of known values of E_z and D_z for insertion into Eq. (4c),

$$E_z^{n+1} = [(\omega_0^2\Delta t^2 + 2\delta\Delta t + 2)D_z^{n+1} - 4D_z^n + (\omega_0^2\Delta t^2 - 2\delta\Delta t + 2)D_z^{n-1} + 4\varepsilon_\infty E_z^n - (\omega_0^2\Delta t^2\varepsilon_s - 2\delta\Delta t\varepsilon_\infty + 2\varepsilon_\infty)E_z^{n-1}]/(\omega_0^2\Delta t^2\varepsilon_s + 2\delta\Delta t\varepsilon_\infty + 2\varepsilon_\infty). \quad (11)$$

We first demonstrate the accuracy of this method by computing the wideband reflection coefficient for a planar interface between vacuum and a half-space made of the Lorentz medium of Fig. 1. A single 0.2-fs duration Gaussian pulse (between the $1/e$ points) is normally incident upon the interface. This pulse has a spectrum that covers the full range from dc to 3×10^{16} Hz. Data are taken every time step ($\Delta t = 2.0 \times 10^{-19}$ s) at a fixed observation point on the vacuum side of the interface. The FD-TD computed complex-valued reflection coefficient is obtained by taking the ratio of the discrete Fourier transforms of the reflected and incident pulses. Figure 2 compares the magnitude and phase of this

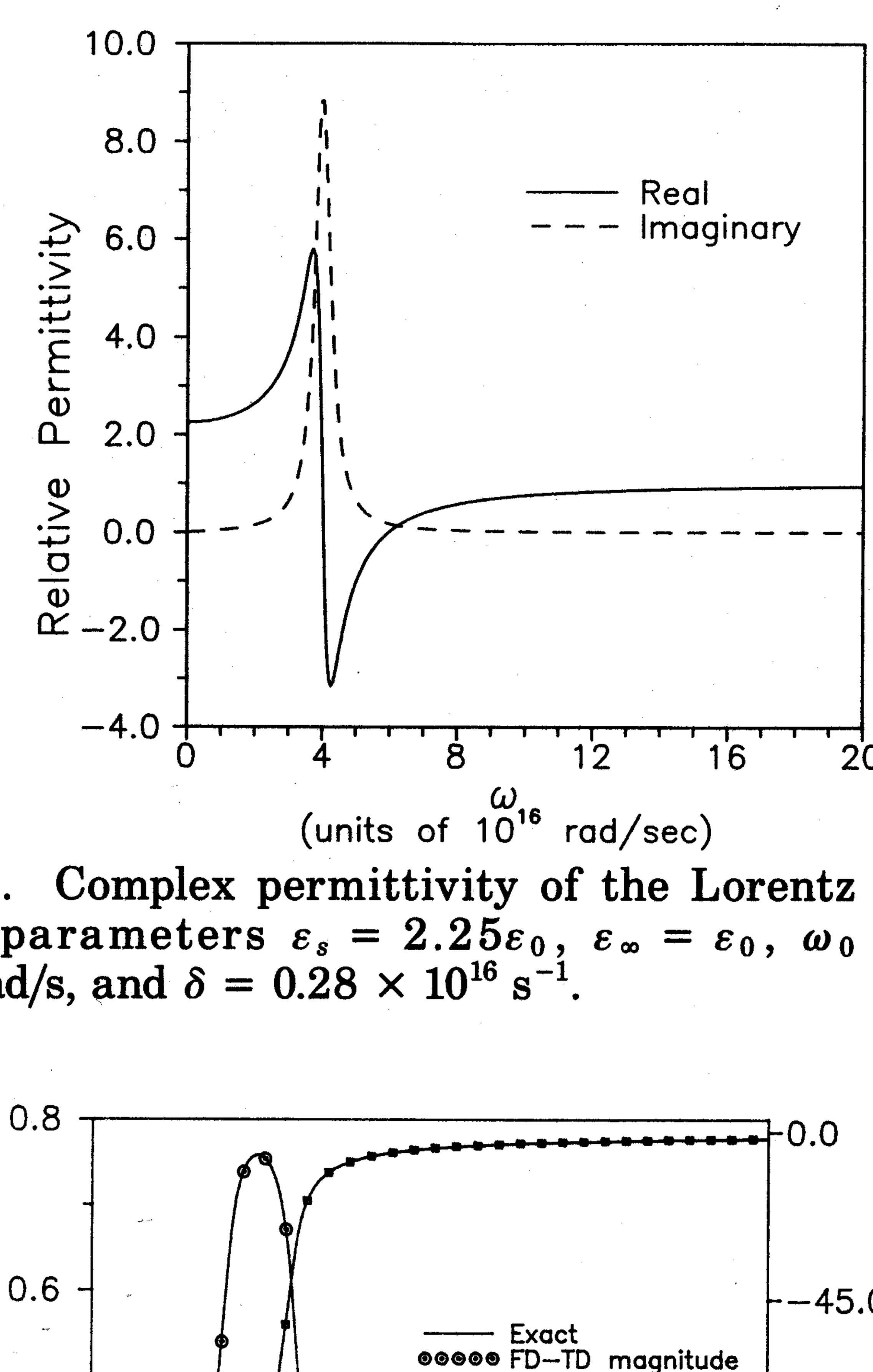

Fig. 1. Complex permittivity of the Lorentz medium with parameters $\varepsilon_s = 2.25\varepsilon_0$, $\varepsilon_\infty = \varepsilon_0$, $\omega_0 = 4.0 \times 10^{16}$ rad/s, and $\delta = 0.28 \times 10^{16}\ \text{s}^{-1}$.

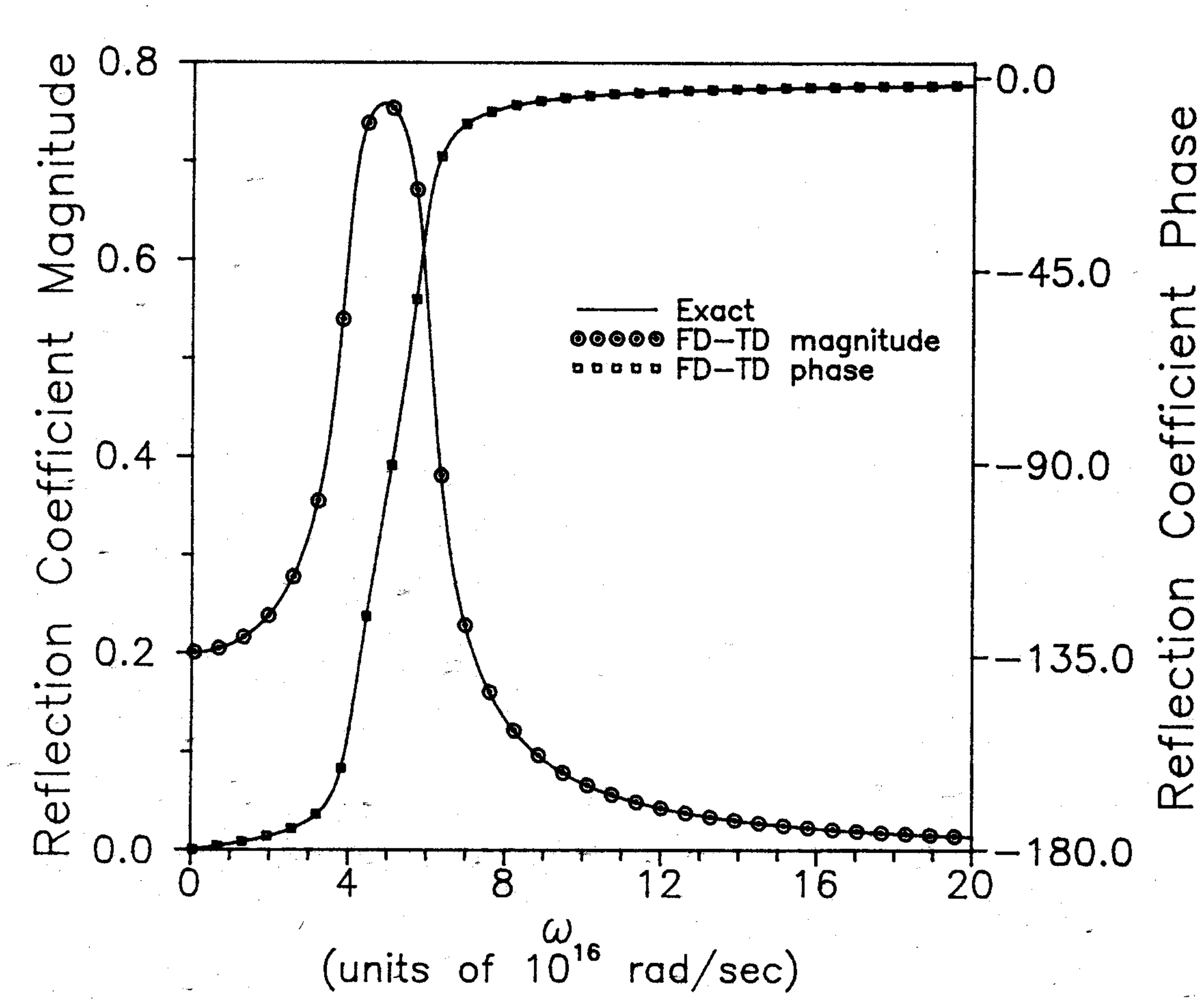

Fig. 2. Comparison of FD-TD and exact results from dc to 3×10^{16} Hz for the magnitude and phase of the reflection coefficient of a half-space made of the Lorentz medium of Fig. 1.

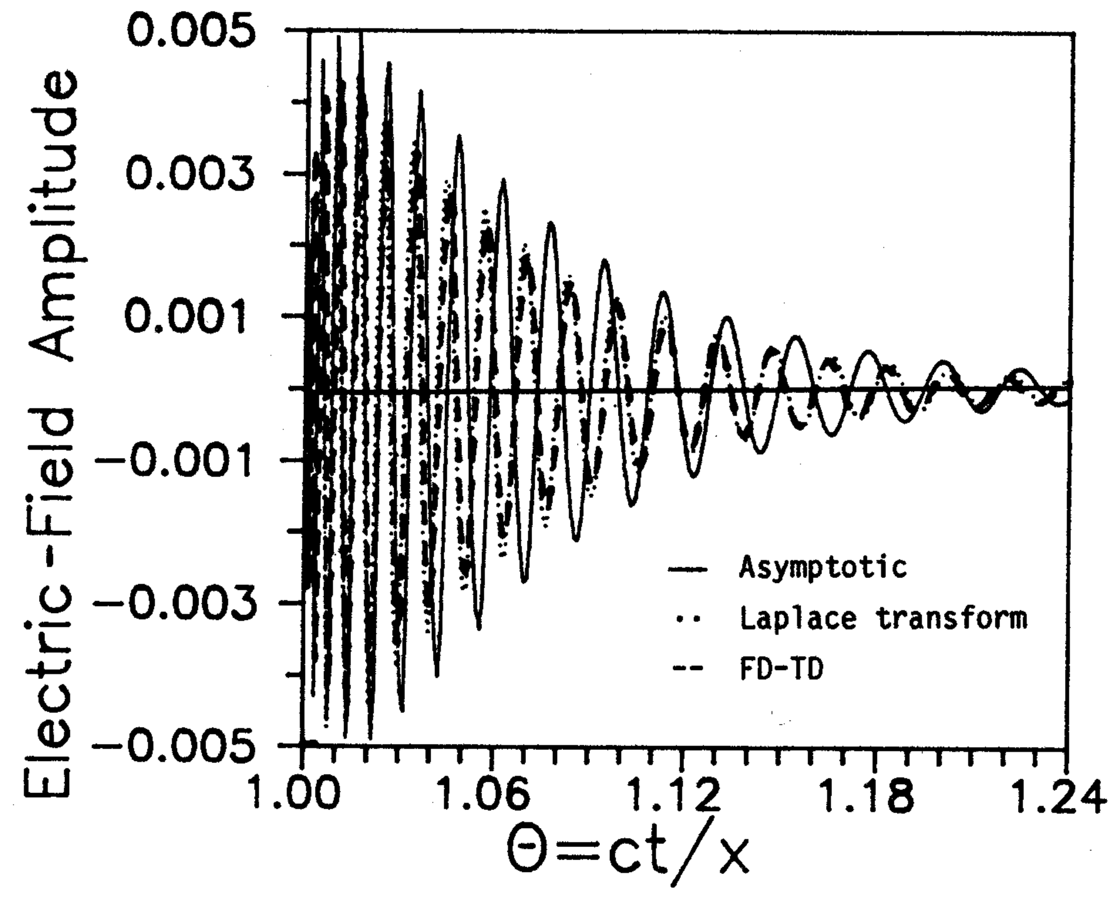

Fig. 3. Comparison of FD-TD, asymptotic,[13] and Laplace-transform[14] results for the Sommerfeld precursor observed at $x = 1\ \mu$m in the Lorentz medium of Fig. 1 for a unit-step modulated sinusoidal excitation ($\omega_c = 1.0 \times 10^{16}$ rad/s) at $x = 0$.

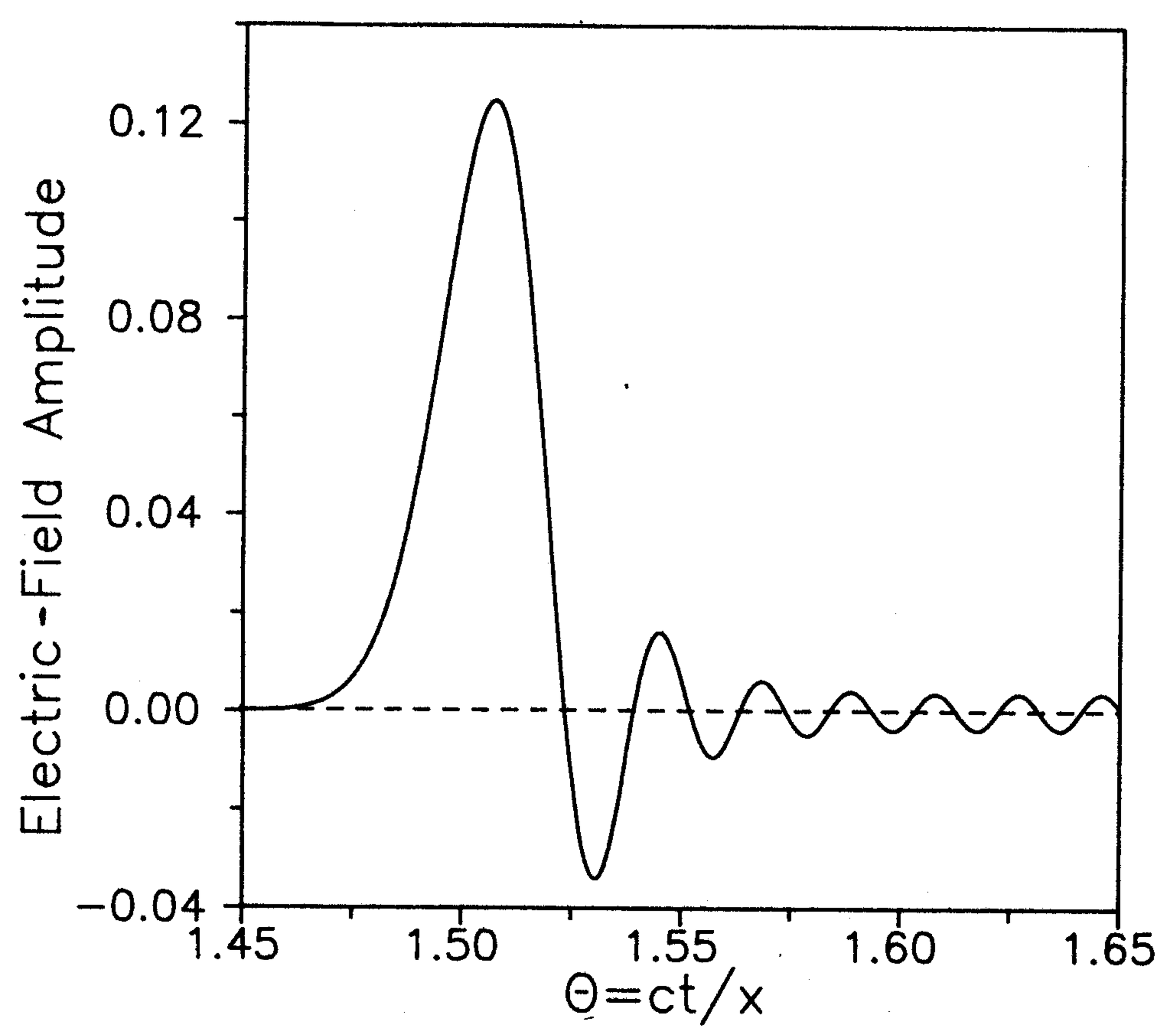

Fig. 4. FD-TD results for the total signal (including the Brillouin precursor) at $x = 10\ \mu$m in the Lorentz medium of Fig. 1 for the unit-step modulated sinusoidal excitation.

reflection coefficient as a function of frequency to the exact solution (Ref. 10, p. 282). The deviation from the exact solution over the complete range of dc to 3×10^{16} Hz is less than 6 parts in 10,000. (This 6/10,000 error occurs at the peak of the reflection magnitude curve.)

The time integration of Maxwell's equations permits the computation of a pulse propagating in a dispersive medium at any space–time point. Historically, such pulse dynamics have been obtained only by asymptotic analyses, notably by Sommerfeld[11] and Brillouin[12] in 1914. More recently, advances in uniform asymptotic analysis for such problems have been made by Oughstun and Sherman[13] and in Laplace transform analysis by Wyns *et al.*[14]

To demonstrate the integration of Maxwell's equations to obtain pulse dynamics, we now use the FD-TD method to compute the precursor fields for a unit-step modulated sinusoidal signal propagating in the Lorentz medium discussed in Figs. 1 and 2. Now the signal source is located at $x = 0$. The carrier frequency ω_c is 10^{16} rad/s. Figure 3 compares the FD-TD computed Sommerfeld precursor observed at $x = 1\ \mu$m to the asymptotic[13] and Laplace-transform[14] predictions. Much closer agreement with the Laplace-transform calculation is noted. Extensive numerical convergence studies of the FD-TD results indicate that the zero crossings of the precursor converge quickly (at relatively coarse grid resolutions), while the envelope converges more slowly to a limiting distribution. Overall, we believe that the FD-TD computed envelope distribution shown in Fig. 3 is within 3% of the limiting distribution obtained at infinitely fine grid resolution.

For completeness, Fig. 4 shows the total signal at $x = 10\ \mu$m in the Lorentz medium computed with the FD-TD method. This includes the Brillouin precursor. These results are again somewhat different from the asymptotic results reported in Ref. 13, yet the FD-TD calculations here exhibit at least the same degree of convergence as those of Fig. 3.

The method of this Letter should be directly applicable to full-vector electromagnetic pulse propagation and scattering effects for inhomogeneous dispersive media in two and three dimensions. We foresee the possibility of incorporating material nonlinearity to obtain the dynamics of soliton propagation and scattering directly from the time-dependent Maxwell's equations.

This research was supported in part by U.S. Office of Naval Research contract N00014-88-K-0475, NASA–Ames University Consortium Joint Research Interchange no. NCA2-562, and Cray Research, Inc. We thank K. E. Oughstun for providing graphical results of his precursor analyses[13,14] and P. Goorjian of NASA–Ames for suggesting the improved time-stepping scheme of Eq. (11).

References

1. K. S. Yee, IEEE Trans. Antennas Propag. **AP-14,** 302 (1966).
2. A. Taflove and M. E. Brodwin, IEEE Trans. Microwave Theory Tech. **MTT-23,** 623 (1975).
3. G. Mur, IEEE Trans. Electromagn. Compat. **EC-23,** 377 (1981).
4. K. R. Umashankar and A. Taflove, IEEE Trans. Electromagn. Compat. **EC-24,** 397 (1982).
5. A. Taflove, Wave Motion **10,** 547 (1988).
6. G. C. Liang, Y. W. Liu, and K. K. Mei, IEEE Trans. Microwave Theory Tech. **MTT-37,** 1949 (1989).
7. E. Sano and T. Shibata, IEEE J. Quantum Electron. **26,** 372 (1990).
8. S. T. Chu and S. K. Chaudhuri, IEEE J. Lightwave Technol. **7,** 2033 (1989).
9. R. Luebbers, F. P. Hunsberger, K. S. Kunz, R. B. Standler, and M. Schneider, IEEE Trans. Electromagn. Compat. **EC-32,** 222 (1990).
10. J. D. Jackson, *Classical Electrodynamics,* 2nd ed. (Wiley, New York, 1975).
11. A. Sommerfeld, Ann. Phys. **44,** 177 (1914).
12. L. Brillouin, Ann. Phys. **44,** 203 (1914).
13. K. E. Oughstun and G. C. Sherman, J. Opt. Soc. Am. A **6,** 1394 (1989).
14. P. Wyns, D. P. Foty, and K. E. Oughstun, J. Opt. Soc. Am. A **6,** 1421 (1989).