ADE-FDTD Scattered-Field Formulation for Dispersive Materials

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***Abstract*—This letter presents a scattered-field formulation for modeling dispersive media using the finite-difference time-domain (FDTD) method. Specifically, the auxiliary differential equation method is applied to Drude and Lorentz media for a scattered field FDTD model. The present technique can also be applied in a straightforward manner to Debye media. Excellent agreement is achieved between the FDTD-calculated and exact theoretical results for the reflection coefficient in half-space problems.**

***Index Terms*—Auxillary differential equation (ADE) method, dispersive media, finite-difference time-domain (FDTD) method, scattered-field.**

I. Introduction

ELECTROMAGNETIC scattering is an important aspect of phased arrays, microwave imaging, composite materials, fiber optics, atmospheric optics, light diffusion in tissues, etc., [1]. The finite-difference time-domain (FDTD) method has been applied to a wide variety of applications of electromagnetic scattering problems [2]. The application of the FDTD scattered-field formulation to lossy dielectric structures was reported in [3], and the total-field/scattered-field formulation was presented in [4] and [5].

To model frequency-dependent dielectric media, the recursive convolution (RC) method [6], which was later improved to the piecewise linear recursive convolution (PLRC) method [7], was developed for the total-field FDTD approach. In addition, the Z-transform method [8] and the auxiliary differential equation (ADE) method [2], [9], [10] were developed for modeling frequency-dependent media using total-field FDTD. Comparative merits and demerits of these techniques were described in [7] and [11].

For the scattered-field FDTD approach, the RC and PLRC methods were proposed [12], [13] for modeling dispersive media. In [14], a direct relation between the electric field and the electric field flux density was used to derive the scattered-field formulation, but only a Debye model was described.

Total-field FDTD codes propagate the incident wave through the grid, and therefore progressively accumulate errors of the incident wave due to numerical dispersion and anisotropy. On the other hand, scattered-field codes accurately generate the incident wave via an exact analytical function at each field vector location. Also, scattered-field FDTD codes eliminate the nonphysical leakage into the scattered-field region that is an artifact of total-field codes. If the scattered fields are weak compared to the incident field, as for an important class of low-observable radar cross section (RCS) problems, the total-field approach thereby suffers from reduced dynamic range.

In this letter, we report a scattered-field FDTD formulation for modeling Drude media (unmagnetized plasmas, especially metals at visible wavelengths) and Lorentz media using the ADE technique. Our technique can be applied to problems of recent interest involving optical plasmons where visible light interacts with metal nanostructures. Furthermore, our technique can be applied to RCS problems where scattering reduction is achieved by coating a structure with lossy materials. Example calculations of reflection from Drude and Lorentz media are reported for 1-D half-space problems and compared to the exact theoretical results. For the formulations in this letter, the electric field is related to the polarization current density. We note that the technique presented in Section II can also be applied to model Debye media in a straightforward manner.

II. Formulation

The electric and magnetic field components are decomposed into incident and scattered terms so that $\boldsymbol{E}_{\text{total}} = \boldsymbol{E}_{\text{inc}} + \boldsymbol{E}_{\text{scat}}$ and $\boldsymbol{H}_{\text{total}} = \boldsymbol{H}_{\text{inc}} + \boldsymbol{H}_{\text{scat}}$ [3]. For an incident field in free space, Ampere's Law is given by

$$\varepsilon_0 \frac{\partial \boldsymbol{E}_{\text{inc}}}{\partial t} = \nabla \times \boldsymbol{H}_{\text{inc}}. \tag{1}$$

For a medium with dispersive permittivity, the above equation is expressed for the total field as follows [11]:

$$\nabla \times \boldsymbol{H}_{\text{total}} = \varepsilon_0 \varepsilon_\infty \frac{\partial}{\partial t} \boldsymbol{E}_{\text{total}} + \sum_{p=1}^{P} \boldsymbol{J}_{p,\text{total}} \tag{2}$$

where p denotes each Debye or Drude pole or Lorentz pole-pair.

First, the update equations are derived for Drude media. Here, instead of relating the electric field and the electric field flux density [14], the electric field and the polarization current density (which is associated with the polarization vector) are re-

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lated. Thus, the following relation is used for the polarization current density in (2) for the Drude case [2]

$$\frac{\partial \boldsymbol{J}_{p,\text{total}}}{\partial t} + \gamma_p \boldsymbol{J}_{p,\text{total}} = \varepsilon_0 \omega_p^2 \boldsymbol{E}_{\text{total}} \tag{3}$$

where ω_p is the angular plasma frequency and γ_p is the collision frequency for each Drude pole p. The polarization current density term is expressed in a discretized form as

$$\boldsymbol{J}_{\text{total}}^{n+1} = k\boldsymbol{J}_{\text{total}}^{n} + \beta\left(\boldsymbol{E}_{\text{scat}}^{n+1} + \boldsymbol{E}_{\text{scat}}^{n} + \boldsymbol{E}_{\text{inc}}^{n+1} + \boldsymbol{E}_{\text{inc}}^{n}\right) \tag{4}$$

where

$$k = \frac{1-\gamma\,\Delta t/2}{1+\gamma\,\Delta t/2}; \quad \beta = \frac{\omega_p^2 \varepsilon_0 \Delta t/2}{1+\gamma \Delta t/2}. \tag{5}$$

Subtracting (1) from (2) yields the scattered-field expression for wave propagation in a dispersive medium described by zero conductivity and a single pole, which is the case for most practical problems. The scattered electric field and total current density for the Drude case are

$$\begin{aligned}\nabla \times &\boldsymbol{H}_{\text{scat}}^{n+1/2}\\ &= \frac{\varepsilon_o\varepsilon_\infty}{\Delta t}\left(\boldsymbol{E}_{\text{inc}}^{n+1} + \boldsymbol{E}_{\text{scat}}^{n+1} - \boldsymbol{E}_{\text{inc}}^{n} - \boldsymbol{E}_{\text{scat}}^{n}\right)\\ &\quad - \frac{\varepsilon_o\varepsilon_\infty}{\Delta t}\left(\boldsymbol{E}_{\text{inc}}^{n+1} - \boldsymbol{E}_{\text{inc}}^{n}\right) + 0.5\left\{(1+k)\boldsymbol{J}_{\text{total}}^{n}\right.\\ &\quad \left. + \beta\left(\boldsymbol{E}_{\text{inc}}^{n+1} + \boldsymbol{E}_{\text{scat}}^{n+1} + \boldsymbol{E}_{\text{inc}}^{n} + \boldsymbol{E}_{\text{scat}}^{n}\right)\right\}.\end{aligned} \tag{6}$$

Solving for the scattered electric field, we obtain

$$\begin{aligned}\boldsymbol{E}_{\text{scat}}^{n+1} = \frac{1}{\left(\frac{\varepsilon_0}{\Delta t} + \frac{\beta}{2}\right)} \cdot &\left\{\left(\frac{\varepsilon_0}{\Delta t} - \frac{\beta}{2}\right)\right.\\ &\times \boldsymbol{E}_{\text{scat}}^{n} - \frac{\beta}{2}\left(\boldsymbol{E}_{\text{inc}}^{n+1} + \boldsymbol{E}_{\text{inc}}^{n}\right)\\ &\left. - \left(\frac{1+k}{2}\right)\boldsymbol{J}_{\text{total}}^{n} + \nabla \times \mathbf{H}_{\text{scat}}^{n+1/2}\right\}.\end{aligned} \tag{7}$$

The scattered $\mathbf{H}$ at each grid point is obtained in the usual manner from the Yee realization of Faraday's Law for scattered field [2]. Assuming that the required $\mathbf{E}_{\text{inc}}$ components have been pre-calculated for every FDTD grid cell and time-step and stored in a look-up table, we implement (7) to obtain $\boldsymbol{E}_{\text{scat}}^{n+1}$. Then, we implement (4) to obtain $\boldsymbol{J}_{\text{total}}^{n+1}$.

The update equations for Lorentz media can be formulated in a similar fashion as for the above Drude model. For the Lorentz case, the following relation is used for the polarization current density term in (2) [2]:

$$\begin{aligned}\omega_0^2 \boldsymbol{J}_{p,\text{total}} &+ 2\delta_p \frac{\partial \boldsymbol{J}_{p,\text{total}}}{\partial t}\\ &+ \frac{\partial^2 \boldsymbol{J}_{p,\text{total}}}{\partial t^2} = \varepsilon_0\left(\varepsilon_s - \varepsilon_\infty\right)\omega_0^2 \frac{\partial \mathbf{E}_{\text{total}}}{\partial t}\end{aligned} \tag{8}$$

where ω_0 is the angular resonant frequency, ε_s is the static permittivity, ε_∞ is the permittivity at infinite frequency, and δ_p is the damping factor for each Lorentz pole-pair p.

Assuming a dispersive medium of a single Lorentz pole-pair, the resulting scattered electric field and total current density for the Lorentz model is given by

$$\begin{aligned}\mathbf{E}_{\text{scat}}^{n+1} = \frac{1}{\left(\varepsilon_0\varepsilon_\infty + \frac{\gamma}{4}\right)} \cdot &\left\{\varepsilon_0\varepsilon_\infty \mathbf{E}_{\text{scat}}^{n} + \frac{\gamma}{4}\mathbf{E}_{\text{scat}}^{n-1}\right.\\ &- \left(\varepsilon_0\varepsilon_\infty + \frac{\gamma}{4} - \varepsilon_0\right)\mathbf{E}_{\text{inc}}^{n+1}\\ &+ \varepsilon_0(\varepsilon_\infty - 1)\mathbf{E}_{\text{inc}}^{n} + \frac{\gamma}{4}\mathbf{E}_{\text{inc}}^{n-1}\\ &- \frac{(1+\alpha)\Delta t}{2}\boldsymbol{J}_{\text{total}}^{n} - \frac{\xi \Delta t}{2}\boldsymbol{J}_{\text{total}}^{n-1}\\ &\left. + \Delta t \cdot \nabla \times \boldsymbol{H}_{\text{scat}}^{n+1/2}\right\}\end{aligned} \tag{9}$$

$$\begin{aligned}\boldsymbol{J}_{\text{total}}^{n+1} = \alpha \boldsymbol{J}_{\text{total}}^{n} &+ \xi \boldsymbol{J}_{\text{total}}^{n-1} + \frac{\gamma}{2\Delta t}\\ &\times \left(\boldsymbol{E}_{\text{scat}}^{n+1} + \boldsymbol{E}_{\text{inc}}^{n+1} - \boldsymbol{E}_{\text{scat}}^{n-1} - \boldsymbol{E}_{\text{inc}}^{n-1}\right)\end{aligned} \tag{10}$$

where

$$\alpha = \frac{2-\omega_0^2 \Delta t^2}{1+\delta \Delta t} \tag{11}$$

$$\xi = \frac{\delta \Delta t - 1}{\delta \Delta t + 1} \tag{12}$$

$$\gamma = \frac{\varepsilon_0\left(\varepsilon_s - \varepsilon_\infty\right)\omega_0^2 \Delta t^2}{1+\delta \Delta t}. \tag{13}$$

The formulation for the Debye model is omitted in this letter because of space limitations. However, note that the Debye model is simpler in form than the Lorentz model and can be derived in a straightforward manner using the same procedure as for the Drude and Lorentz cases.

III. Numerical Results

We now present numerical examples and validations for the formulations of Section II. Specifically, we calculate the reflection coefficient of a plane wave normally incident from vacuum onto either a Drude half-space or a single pole-pair Lorentz half-space. These 1-D examples are shown to permit comparisons of the FDTD and exact theoretical solutions. We note, however, that this work can be extended to two and three dimensions in a straightforward manner.

We assume a $+x$-directed impulsive (Gaussian) incident wave having significant spectral energy up to 100 GHz. The FDTD algorithm computes E_z, H_y, and J_z components on a uniform grid having $\Delta x = 250\mu$ m and Δt set to the maximum value for numerical stability. The parameters for the Drude half-space are $\gamma = 2 \times 10^{10}$ and $\omega_p = 2\pi\times$ 28.7 GHz, whereas the Lorentz half space is characterized by $\varepsilon_s = 3.0, \varepsilon_\infty = 1.5, \omega_0 = 2\pi\times$ 25 GHz, and $\delta = 0.1\omega_0$.

Fig. 1 shows the FDTD-calculated time waveforms for the scattered (reflected) electric fields in the free-space region for both the Drude and Lorentz half-spaces. The observation point is 10 grid cells from the surface of the dispersive half-space.

Fig. 2 compares the FDTD-calculated and exact analytical results for the magnitude of the reflection coefficient up to

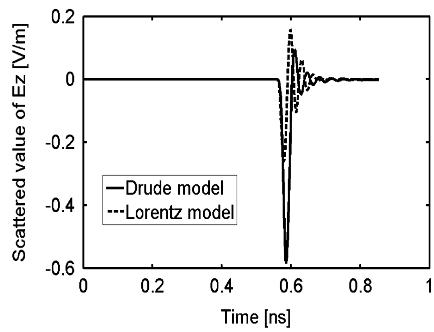

Fig. 1. FDTD-calculated time-waveforms of the scattered (reflected) electric field for both the Drude and Lorentz half-space examples. The maximum Gaussian incident value is set to 1 V/m.

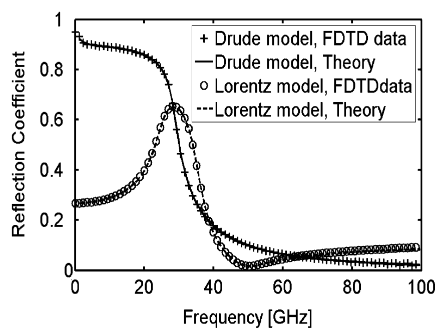

Fig. 2. Comparison of FDTD and exact theoretical results from dc to 100 GHz for the magnitude of the reflection coefficient for both the Drude and Lorentz half-space examples.

100 GHz for both the Drude and Lorentz examples. For the FDTD results, the reflection coefficients are obtained by taking the ratio of the discrete Fourier transforms of the reflected and incident field time-waveforms. For the exact analytical data, the reflection coefficients are obtained in the phasor domain from the complex-valued wave impedance of each half-space. From Fig. 2, we see that the FDTD results and the exact analytical solution are in excellent agreement for both the Drude and Lorentz cases.

IV. Conclusion

In this letter, a scattered-field FDTD formulation based on the auxiliary differential equation method was presented for both Drude and Lorentz dispersive media. Excellent agreement was obtained between the FDTD models and exact theoretical calculations. Although 1-D examples were provided here, the proposed algorithms can be applied to multidimensional problems in a straightforward manner.

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