Approximation of Grünwald-Letnikov Fractional Derivative for FDTD Modeling of Cole-Cole Media

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***Abstract*—A finite-difference time-domain (FDTD) method for modeling wave propagation in dispersive Cole-Cole media is proposed. The main difficulty in time-domain modeling of a Cole-Cole medium is that the polarization relation that describes the medium behavior is a differential equation of fractional order. In this case, the memory demands of the FDTD would be high because the computation of the fractional derivative requires all the previous values of the polarization field. However, by an appropriate approximation of the Grünwald-Letnikov fractional derivative, we can implement an FDTD scheme with reasonable memory demands. The proposed scheme has been applied successfully to the simulation of the excitation of a Cole-Cole media by a wideband gaussian electromagnetic pulse.**

***Index Terms*—Biological materials, computational electromagnetics, finite difference methods, fractional calculus.**

I. Introduction

The finite-difference time-domain (FDTD) method is an efficient tool for simulating wave propagation in dispersive media [1]. In the FDTD schemes, the polarization relation is formulated by means of either a time-domain convolution integral or an auxiliary differential equation (ADE). In the first approach, the time representation of the permittivity is requited whereas, in the second one, the ADE is derived by appropriately transforming the frequency representation of the permittivity into a set of time-domain differential operators. Both approaches can be implemented in a quite straightforward way for Drude, Debye, and Lorentz dispersive media [1]–[3]. In the case of Cole-Cole dispersive media, which are important for describing the electromagnetic properties of biological tissues [4], the application of the FDTD meets significant difficulties because the polarization relation involves fractional time derivatives [5]. However, several FDTD schemes have been proposed for the simulation of wave propagation inside Cole-Cole media. For instance, in [6], the proposed FDTD scheme was based on the approximation of the Riemann-Liouville fractional derivative whereas, in [7], an approximate ADE of integer order was derived using Padé approximants.

In this study, a new FDTD scheme for simulating wideband electromagnetic pulses propagating in Cole-Cole media is presented. The scheme utilizes an approximation of the Grünwald-Letnikov (GL) fractional derivative by means of a truncated exponential expansion. Hence, an accurate FDTD scheme with reasonable memory requirements is derived. In the numerical results, the proposed FDTD scheme simulates the incidence of a gaussian pulse on a Cole-Cole medium. Comparisons between analytical and numerical computations of the reflection coefficient on the medium boundary and of the transfer function inside the medium illustrate the efficiency of the proposed scheme.

II. FDTD Scheme for Cole-Cole Media

The relative permittivity of a dispersive Cole-Cole medium in the frequency domain is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \Delta\varepsilon[1 + (j\omega\tau)^\alpha]^{-1} \quad (\Delta\varepsilon = \varepsilon_s - \varepsilon_\infty) \qquad (1)$$

where ε_∞ and ε_s are the optical and the static permittivities, respectively, τ is the relaxation time, and α $(0 < \alpha < 1)$ is a measure of the dispersion broadening. The Ampere's law in this medium is written as

$$\nabla \times H = \varepsilon_0\varepsilon_\infty\partial_t E + \partial_t P \qquad (2)$$

where the polarization field P satisfies the polarization relation

$$\tau^\alpha\partial_t^\alpha P + P = \varepsilon_0\Delta\varepsilon E, \qquad (3)$$

which is a fractional differential equation. In (3), $\partial_t^\alpha P$ is the αth-order fractional derivative of P, which, according to the Grünwald-Letnikov definition [5], is given by

$$\partial_t^\alpha P(t) = \lim_{n\to\infty}\left\{(t/n)^{-\alpha}\sum_{k=0}^{n-1} w_k^{(\alpha)} P(t - kt/n)\right\} \qquad (4)$$

where $w_0^{(\alpha)} = 1$ and $w_k^{(\alpha)} = (1 - (1+\alpha)/k)w_{k-1}^{(\alpha)}$. The discretized form of (4) at the time instant $t = n\Delta t$ is written as

$$\partial_t^\alpha P^n = \Delta t^{-\alpha}\sum_{k=0}^{n-1} w_k^{(\alpha)} P^{n-k} \qquad (5)$$

From both (4) and (5), it is evident that the fractional derivative is not a local operator but involves the whole "history" of the function. Furthermore, in a direct implementation of (5), as the time instant increases, more memory is required for storing the previous values of P. However, it is possible to circumvent this difficulty and develop a feasible FDTD scheme (in terms of storage requirements) by finding a recurrent relation to evaluate the fractional derivative. In particular, since $w_k^{(\alpha)} < w_{k+1}^{(\alpha)} < 0$ for $k \geq 1$, the term $w_k^{(\alpha)}$ can be approximated by a sum of M exponentials, i.e.,

$$w_k^{(a)} \approx \sum_{j=1}^{M} a_j e^{-b_j(k-1)} \quad (k \geq 1) \qquad (6)$$

where $a_j < 0$ and $b_j > 0$. By substituting (6) into (5) the discretized formula of the polarization relation (3) takes the form

$$P^n = \frac{\varepsilon_0 \Delta\varepsilon}{1+q} E^n - \frac{q}{1+q} \sum_{j=1}^{M} v_j^n \tag{7}$$

where $q = (\tau/\Delta t)^\alpha$ and $v_j^n = a_j \sum_{k=1}^{n-1} e^{-b_j(k-1)} P^{n-k}$. Using (7) and the discretized form of the Ampere's law, we derive the formula for updating the electric field, i.e.,

$$E^n = A\left(\varepsilon_0\varepsilon_\infty E^{n-1} + P^{n-1} + \frac{q}{1+q}\sum_{j=1}^{M} v_j^n + \Delta t \nabla \times H^{n-1/2}\right) \tag{8}$$

where $A = (\varepsilon_0\varepsilon_\infty + \varepsilon_0\Delta\varepsilon/(1+q))^{-1}$. Then, the updated polarization field is given by (7), while the updated magnetic field is given by

$$H^{n+1/2} = H^{n-1/2} - \mu^{-1}\Delta t \nabla \times E^n. \tag{9}$$

In the next time step $(n+1)$, the auxiliary vectors v_j^{n+1} have to be evaluated. Because of the exponential expansion (6), we can derive the recurrent formula for updating v_j given by

$$v_j^{n+1} = a_j P^n + e^{-b_j} v_j^n \qquad (1 \le j \le M). \tag{10}$$

To this end, compared to the usual FDTD for nondispersive media, the proposed scheme requires the additional storage of the M auxiliary vectors; M typically ranges from 6 to 8.

III. Numerical Results

We consider a Cole-Cole medium ($\varepsilon_\infty = 2$, $\varepsilon_s = 50$, $\tau = 153$ ps, and $a = 0.75$) occupying half space ($z \ge 0$) whereas the rest space is air. A plane wave, which propagates along the positive z direction with the electric field polarized in the x axis, excites the Cole-Cole medium. The incident wave is a modulated gaussian pulse with central frequency 6 GHz and bandwidth 5 GHz. In the FDTD implementation, the time step and the grid spacing are $\Delta t = 1.768 \times 10^{-12}$ sec and $\Delta z = 1.1$ mm, respectively, while $M = 8$.

By postprocessing the simulated electric field, we derive the numerical estimate of the magnitude of the reflection coefficient at the air-medium interface, $|\mathcal{R}(\omega)|$. Fig. 1 presents the analytical magnitude of the reflection coefficient and the one derived by the proposed FDTD scheme. Furthermore, if the electric field is recorded at two positions inside the Cole-Cole medium, $z+d$ and z, then the ratio of the corresponding fourier transforms, $\mathbf{E}(z+d,\omega)$ and $\mathbf{E}(z,\omega)$, gives an estimate of the transfer function $\mathbf{T}(d,\omega) = \mathbf{E}(z+d,\omega)/\mathbf{E}(z,\omega)$. For recordings separation distance $d = 40\Delta z$, the analytical and the estimated transfer function are presented in Fig. 2. Both Figs. 1 and 2 illustrate the accuracy of the proposed scheme over a wide frequency range.

IV. Conclusion

A new FDTD scheme for modeling wave propagation inside Cole-Cole media has been proposed. The scheme is based on the approximation of the Grünwald-Letnikov fractional derivative by means of exponential expansion, which results in limited memory storage requirements. Numerical results have shown the accuracy of the proposed FDTD method.

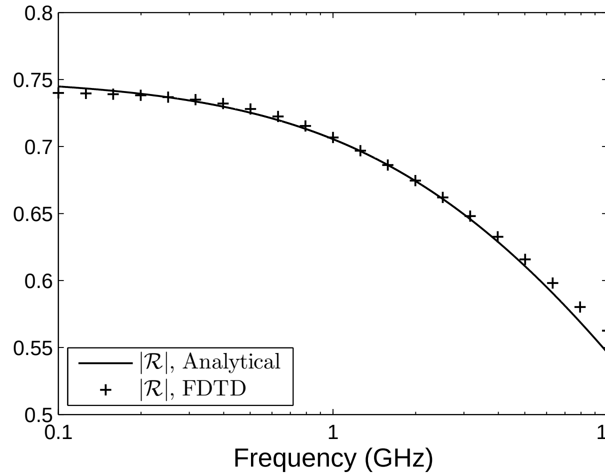

Figure 1: Magnitude of the reflection coefficient on the Cole-Cole medium.

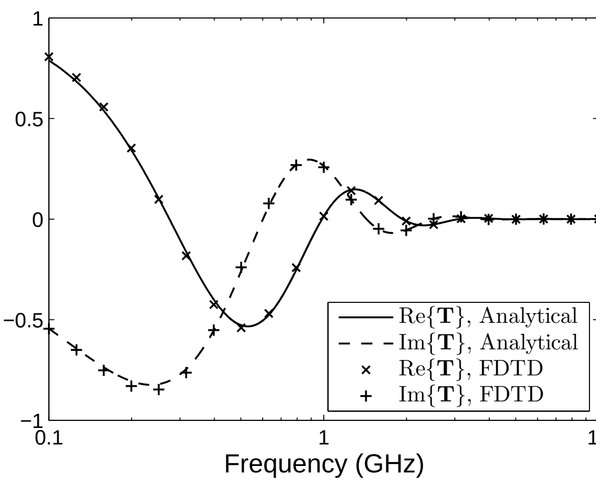

Figure 2: Transfer function inside the Cole-Cole medium for $d = 40\Delta z$.

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