Simple Treatment of Multi-Term Dispersion in FDTD

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***Abstract*—Three new simple and efficient algorithms are proposed for the numerical treatment of the multi-term Debye or Lorentz dispersion in the FDTD method. The formulation is based on the auxiliary differential equation, but requires much fewer operations than the published schemes. The approach is equivalent to the best higher order recursive schemes in terms of memory and computational expense, but without the linearity assumptions.**

***Index Terms*—Dispersive dielectrics, FDTD.**

I. Introduction

In recent years, several techniques have emerged for modeling dispersive phenomena in media described by multi-pole Debye or Lorentz models. In the recursive convolution (RC) approach (e.g., [1]–[3]), the exponential form of the time-domain susceptibility function is used to replace the convolution integral. The second-order accuracy in time is obtained in the piecewise linear recursive convolution (PLRC) [2] and the trapezoidal rule recursive convolution (TRC) [3]. The recursive convolution (RC) techniques are difficult to derive, require complex arithmetic, and assume that the medium is linear. The second category of methods for higher order dispersion utilizes auxiliary differential equations (ADE) linking the polarization vector and the electric flux density [4]. Since the medium does not have to be linear, the ADE method is particularly attractive for modeling nonlinear effects. The ADE method has identical accuracy and memory requirements (for Lorentz media) as the PLRC. In its published formulation [4], this method requires solution of the system of P linear equations. This implies performing a matrix multiplication at each time step, at a cost of at least $O(P^2)$ operations. A higher order dispersion potentially can also be treated using the Z-transform, but only a single-term dispersion has been described [5].

In this letter, the ADE method is reformulated so that the solution of the system of linear equations is no longer necessary. Three second-order algorithms for Debye and Lorentz dispersion with $O(P)$ numerical complexity are obtained. These algorithms require fewer or equal number of unknowns than the corresponding PLRC and TRC schemes.

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II. Formulation and Discretization

For both Debye or Lorentz media the relative permittivity can be expressed as

$$\epsilon(\omega) = \epsilon_\infty + \sum_p^P \frac{N_{D,L}^p}{M_{D,L}^p(\omega)} \tag{1}$$

For Debye media $N_D = \Delta\epsilon A_p$; $M_D(\omega) = 1 + j\omega\tau_p$ and for Lorentz media $N_L = \Delta\epsilon A_p \omega_p^2$; $M_L(\omega) = \omega_p^2 + 2j\omega\delta_p - \omega^2$ where $\Delta\epsilon = \epsilon_s - \epsilon_\infty$, ϵ_s is the static permittivity, ϵ_∞ is the permittivity at infinite frequency, A_p is the pole amplitude, τ_p is the relaxation time, ω_p is the pole location, and δ_p is the dumping factor.

For either medium, the Ampere's equation in the time domain becomes

$$\begin{aligned}\nabla \times \mathbf{H}(t) &= \epsilon_0\epsilon_\infty \frac{d}{dt}\mathbf{E}(t) + \sigma\mathbf{E}(t) + \\ &\quad \epsilon_0 \sum_p^P \mathcal{F}^{-1}\left\{ j\omega \frac{N_{D,L}^p}{M_{D,L}^p(\omega)} \mathbf{E}(\omega) \right\} \\ &= \epsilon_0\epsilon_\infty \frac{d}{dt}\mathbf{E}(t) + \sigma\mathbf{E}(t) + \sum_p^P \mathbf{J}_p(t)\end{aligned} \tag{2}$$

where $\mathbf{J}_p(t)$ are the polarization currents. To find the relation between the $\mathbf{J}_p(t)$ and $\mathbf{E}_p(t)$ the inverse Fourier transform is taken of the equations:

$$M_{D,L}^p(\omega)\mathbf{J}_p(\omega) = j\omega\epsilon_0 N_{D,L}^p\,\mathbf{E}(\omega) \tag{3}$$

This results in (for Debye and Lorentz respectively):

$$\frac{d}{dt}\mathbf{J}_p = \epsilon_0\Delta\epsilon\frac{A_p}{\tau_p}\frac{d}{dt}\mathbf{E} - \frac{1}{\tau_p}\mathbf{J}_p \tag{4}$$

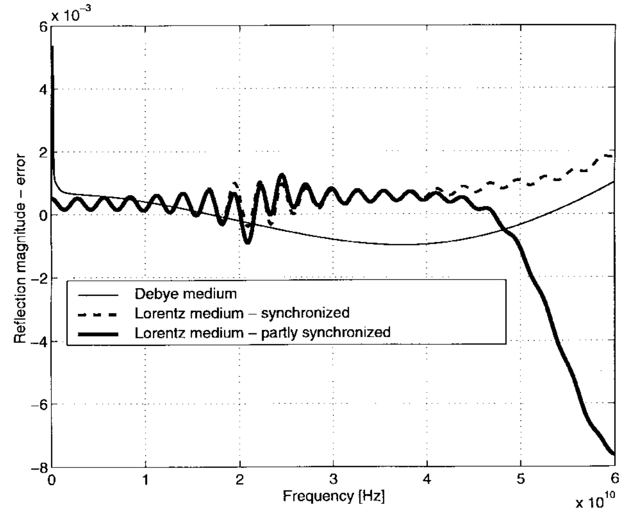
$$\frac{d^2}{dt^2}\mathbf{J}_p = \epsilon_0\Delta\epsilon\omega_p^2 A_p\frac{d}{dt}\mathbf{E} - \omega_p^2\mathbf{J}_p - 2\delta_p\frac{d}{dt}\mathbf{J}_p. \tag{5}$$

An equation similar to (4) was previously given in [7], but the coefficients were likely in error, as the dimensions were not correct.

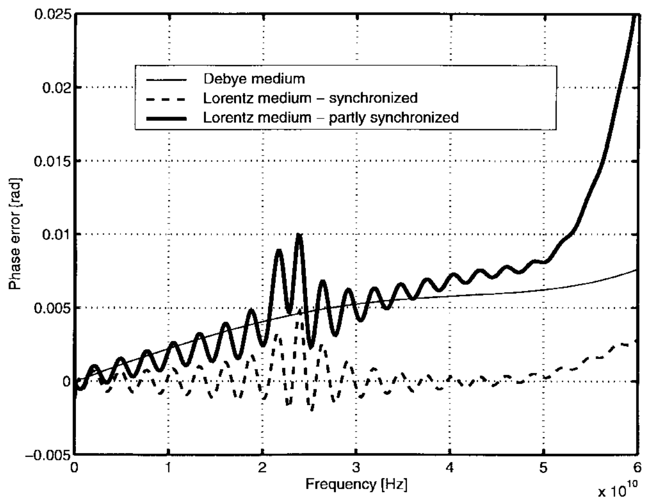
Implementation in FDTD requires discretization of (2), (4), and (5). All relevant quantities should be expressed in the same instant of time:

$$\nabla\times\mathbf{H}^{n+1/2} = \epsilon_0\epsilon_\infty\frac{d}{dt}\mathbf{E}^{n+1/2} + \sigma\mathbf{E}^{n+1/2} + \sum_p^P \mathbf{J}_p^{n+1/2}. \tag{6}$$

For synchronism, the semi-implicit scheme is adopted, where yet-to-be computed field E^{n+1} is used to create an update



(a)



(b)

Fig. 1. Absolute errors in the reflection coefficient for all three algorithms presented in the paper. (a) magnitude and (b) phase. The Debye medium was represented by 3-pole muscle [6] with $\epsilon_s = 2046.4$, $\epsilon_\infty = 4.3$, $\Delta\epsilon = \epsilon_s - \epsilon_\infty$, $\tau_1 = (5.2\pi)^{-1}\mu s$, $\tau_2 = (680\pi)^{-1}\mu s$, $\tau_3 = (46\pi)^{-1} ns$, $A_1\Delta\epsilon = 1970$, $A_2\Delta\epsilon = 30.8$, $A_3\Delta\epsilon = 41.3$ and $\sigma = 0.106S$. Lorentz medium was assumed as $P = 2$, $\epsilon_s = 3$, $\epsilon_\infty = 1.5$, $\omega_1 = 40\pi$ Grad/s, $\omega_2 = 100\pi$ Grad/s , $\delta_1 = 0.1\omega_1$, $\delta_2 = 0.1\omega_2$, $A_1 = 0.4$, $A_2 = 0.6$. Spatial resolution $\Delta z = 37.5\mu$m

formula for current J_p^{n+1}. For a Debye medium, this results in

$$J_p^{n+1} = \frac{\beta_p}{\Delta t}(E^{n+1} - E^n) + k_p J_p^n \tag{7}$$

where $k_p = (1 - \frac{\Delta t}{2\tau_p})/(1 + \frac{\Delta t}{2\tau_p})$ and $\beta_p = \epsilon_0 \Delta\epsilon A_p \frac{\Delta t}{\tau_p}/(1 + \frac{\Delta t}{2\tau_p})$. For Lorentz media, the semi-implicit approach gives

$$J_p^{n+1} = \alpha_p J_p^n + \xi_p J_p^{n-1} + \gamma_p \left(\frac{dE}{dt}\right)^n \tag{8}$$

where $\alpha_p = \frac{2-\Delta t^2\omega_p^2}{1+\delta_p\Delta t}$, $\xi_p = \frac{\delta_p\Delta t - 1}{\delta_p \Delta t + 1}$ and $\gamma_p = \Delta t^2 \epsilon_0 \Delta\epsilon A_p \omega_p^2$

Full time synchronism requires that $\left(\frac{dE}{dt}\right)^n$ is computed as $(E^{n+1} - E^{n-1})/(2\Delta t)$. This increases storage requirements, as E^{n-1} has to be back-stored. If the time synchronism is compromised and $(E^{n+1} - E^n)/\Delta t$ is used instead, the additional back-storage is not necessary.

Before currents J_p^{n+1} are computed, their update formulae are used to express $J^{n+1/2} = \frac{1}{2}(J^{n+1} + J^n)$ in (8). The resulting three schemes: 1) Debye ADE synchronized (DADES); 2) Lorentz ADE Partially Synchronized (LADEP); and 3) Lorentz ADE Synchronized (LADES) can be sketched as follows (cast into a single pseudo-code):

For each field location:
  $E_{tmp} = E^n$; $E^{n+1} = p_e E^n + p_m \nabla \times H$;
  Case (DADES)
    For $p = 1$:P; $E^{n+1} = E^{n+1} - p_m(k_p + 1)/2\, J_p^n$;
    For $p = 1$:P;
$J_p^{n+1} = \frac{\beta_p}{\Delta t}(E^{n+1} - E_{tmp}) + k_p J_p^n$;
  Case (LADEP)
    For $p = 1$:P;
      $E^{n+1} = E^{n+1} - p_m(\alpha_p + 1)/2\, J_p^n - p_m \xi_p/2\, J_p^{n-1}$;
    For $p = 1$:P;
      $J_p^{n+1} = \frac{\gamma_p}{\Delta t}(E^{n+1} - E_{tmp}) + \alpha_p J_p^n + \xi_p J_p^{n-1}$;
  Case (LADES)
    $E^{n+1} = E^{n+1} + p_m \chi E^{n-1}$
    For $p = 1$:P;
      $E^{n+1} = E^{n+1} - p_m(\alpha_p + 1)/2\, J_p^n - p_m \xi_p/2\, J_p^{n-1}$;
    For $p = 1$:P;
      $J_p^{n+1} = \frac{\gamma_p}{2\Delta t}(E^{n+1} - E^{n-1}) + \alpha_p J_p^n + \xi_p J_p^{n-1}$;
end;

where for DADES: $p_e = (1 - \frac{\Delta t\sigma}{2\chi})/\nu$, $p_m = \frac{\Delta t}{\chi}/\nu$, and $\nu = 1 + \frac{\Delta t \sigma}{2\chi}$, $\chi = \epsilon_0\epsilon_\infty + \frac{1}{2}\sum_p^P \beta_p$; LADEP: $p_e = (1 - \frac{\Delta t\sigma}{2\chi})/\nu$, $p_m = \frac{\Delta t}{\chi}/\nu$, and $\nu = 1 + \frac{\Delta t\sigma}{2\chi}$, $\chi = \epsilon_0\epsilon_\infty + \frac{1}{2}\sum_p^P \gamma_p$; LADES: $p_e = (1 - \frac{\Delta t \sigma}{2\epsilon_\infty \epsilon_0})/\nu$, $p_m = (\frac{\Delta t}{\epsilon_\infty\epsilon_0})/\nu$, and $\nu = 1 + \frac{\Delta t}{\epsilon_\infty \epsilon_0}(\sigma/2 + \chi)$, $\chi = \frac{1}{4\Delta t}\sum_p^P \gamma_p$.

The algorithms require $P, 2P{+}1$ and $2P$ additional real variables per electric field components, respectively, for DADES, LADES, and LADEP. The number of extra real additions and multiplications is, respectively, $(3P)$, $(5P)$, and $(5P + 1)$. It can be noted that in terms of memory, LADEP is equivalent to TRC (while it avoids its restrictions), and LADES to PLRC. DADES saves one variable over corresponding PLRC scheme. It also appears that our algorithms require considerably fewer floating point operations than TRC and PLRC schemes.

III. Numerical Results

Fig. 1 shows absolute errors in the magnitude and phase of the reflection coefficient of the TEM wave incident from vacuum onto a dispersive media as compared to the analytical solution. As expected, the accuracy of LADEP deteriorates as the frequency increases. As the time variation of field becomes more rapid, the lack of synchronism decreases the accuracy. On the other hand, the imperfect synchronization saves memory. The relative error norms in the three tests are $1.7 \cdot 10^{-3}$, $4.1 \cdot 10^{-4}$, $2.8 \cdot 10^{-3}$ for the magnitude and $9.6 \cdot 10^{-4}$, $2.1 \cdot 10^{-3}$, $6 \cdot 10^{-3}$ for the phase and Debye, Lorentz fully synchronized, and Lorentz partly synchronized algorithms, respectively.

IV. Conclusions

Three simple algorithms for dealing with Pth-order Debye and Lorentz dispersion were derived based on the ADE approach. The algorithms are faster than previous formulations of ADE technique. Not only do they require fewer computational resources than the recursive convolutions schemes, but also they are much simpler to derive, use only real arithmetic, and do not impose the linearity constraint.

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