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A General ADE-FDTD Algorithm for the Simulation of Different Dispersive Materials

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Abstract— A FDTD general algorithm, based on the auxiliary differential equation technique, for the analysis of dispersive media is presented. The algorithm is suited for cases where materials having different types of dispersion are modeled together. While having the same level of accuracy, the proposed algorithm finds its strength in unifying the formulation of different dispersion models into one form. Consequently, savings in both memory and computational requirements, compared to other ADE-based methods that model each material separately, are attained.

1. INTRODUCTION

A number of FDTD-based algorithms for the analysis of dispersive materials have been already proposed [1–5]. When the problem space involves materials having different types of dispersion with or without multi-poles, the solution algorithms become complicated. The existing algorithms require a separate formulation for each dispersion type. For example, a dispersion model like the Lorentz-Drude with six poles will require long derivations and many values to be stored in memory. In this work, a general algorithm, based on the auxiliary differential equation (ADE) technique, is proposed that will remove this complication; only one algorithm can be used for all dispersion types.

2. FORMULATIONS

Starting with the most general form of dispersion, the Lorentzian form, the polarization field in the frequency domain can be written as

$$P(\omega) = \frac{a}{b + jc\omega - d\omega^2} E(\omega) \quad (1)$$

Shifting to the time domain through inverse Fourier transform gives

$$bP(t) + cP'(t) + dP''(t) = aE(t) \quad (2)$$

The key step towards the formulation of a consistent and general FDTD algorithm is approximating the time derivatives in Equation (2) at time instant $n - 1$. Thus, using central differencing with, one obtains the following update equation.

$$bP^{n-1} + c \frac{P^n - P^{n-2}}{2\Delta t} + d \frac{P^n - 2P^{n-1} + P^{n-2}}{\Delta t^2} = aE^{n-1} \quad (3)$$

Or,

$$P^n = \frac{4d - 2b\Delta t^2}{2d + c\Delta t} P^{n-1} + \frac{-2d + c\Delta t}{2d + c\Delta t} P^{n-2} + \frac{2a\Delta t^2}{2d + c\Delta t} E^{n-1} \quad (4)$$

which can be written in the form

$$P^n = C_1 P^{n-1} + C_2 P^{n-2} + C_3 E^{n-1} \quad (5)$$

The constants C_1 , C_2 and C_3 can be found for any form of dispersion relation (see Table 1 below). In the case of multi-pole dispersion, the same relation is written for each pole with appropriate constants. The update equation for the electric field intensity is given by

$$E^n = \frac{D^n - \sum_i^N P_i^n}{\varepsilon_o \varepsilon_\infty} \quad (6)$$

where N is the number of poles and the updated value of the flux density D^n is obtained using the standard Yee's algorithm. The order in which the computations are performed in the general algorithm is shown in the flowchart of Figure 1.

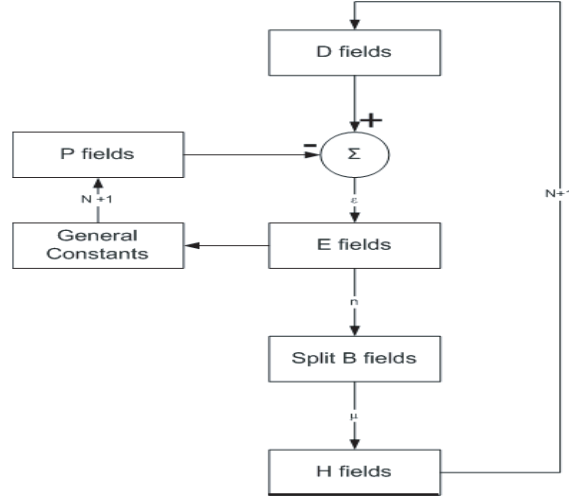


Figure 1: Order of computations in the General Algorithm. The PML is done on the D - B level and the dispersion on the D - E level.

Table 1: Dispersion types and the corresponding coefficients.

Dispersion term in frequency domain	C_1	C_2	C_3
Lorentz Pole $P(\omega) = \frac{a}{b+jc\omega-d\omega^2}E(\omega)$	$\frac{4d-2b\Delta t^2}{2d+c\Delta t}$	$\frac{-2d+c\Delta t}{2d+c\Delta t}$	$\frac{2a\Delta t^2}{2d+c\Delta t}$
Drude Pole $P(\omega) = \frac{a}{jc\omega-d\omega^2}E(\omega)$	$\frac{4d}{2d+c\Delta t}$	$\frac{-2d+c\Delta t}{2d+c\Delta t}$	$\frac{2a\Delta t^2}{2d+c\Delta t}$
Debye term $P(\omega) = \frac{a}{b+jc\omega}E(\omega)$	$\frac{-2b\Delta t}{c}$	1	$\frac{2a\Delta t}{c}$

3. NUMERICAL RESULTS

Two examples are considered for the validation of the proposed algorithm. In both cases, the numerical results are compared to analytical calculations. First, a wideband pulse is incident from air onto a dispersive half-space [5]. The permittivity of the dispersive medium is given by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_o^2}{\omega_o + j2\delta\omega - \omega^2} \quad (7)$$

where $\varepsilon_s = 2.25$, $\varepsilon_\infty = 1$, $\omega_o = 4 \times 10^{16}$ rad/sec and $\delta = 0.28 \times 10^{16}$ s⁻¹. Calculations of the reflection coefficient at the boundary of the two media using the proposed general algorithm show excellent agreement with the analytical results, as shown in Figure 2. Next, a case that involves a multi-term dispersion is considered. This case was also simulated in [6]. The permittivity of the dispersive medium is given by

$$\varepsilon(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_{p=1}^2 \frac{G_p \omega_p^2}{\omega_p^2 + j2\delta_p \omega - \omega^2} \quad (8)$$

where $\varepsilon_s = 3$, $\varepsilon_\infty = 1.5$, $\omega_1 = 20 \times 10^9$ Hz, $G_1 = 0.4$, $\delta_1 = 0.1\omega_1$, $\omega_2 = 50 \times 10^9$ Hz, $G_2 = 0.6$ and $\delta_2 = 0.1\omega_2$. Figure 3 shows the excellent agreement between the proposed algorithm and the exact calculations of the reflection coefficient at the interface. If the previous example was to be solved using the classical ADE algorithm [5], the solution routine would involve higher order derivatives and requires the use of matrix inversion. For two complex pole pairs of Lorentz model for example, derivatives of the fourth order result. The update equations in this case contain several future quantities that are yet to be evaluated. So, the problem is transformed into a mixed explicit-implicit scheme that can be solved by matrix inversion. On the other hand, the ADE algorithm

reported in [3] would result in a similar level of computational requirements as the general algorithm proposed in this paper. However, if multiple dispersive materials are involved, the ADE algorithm in [3] would require more constants to be evaluated and stored in memory.

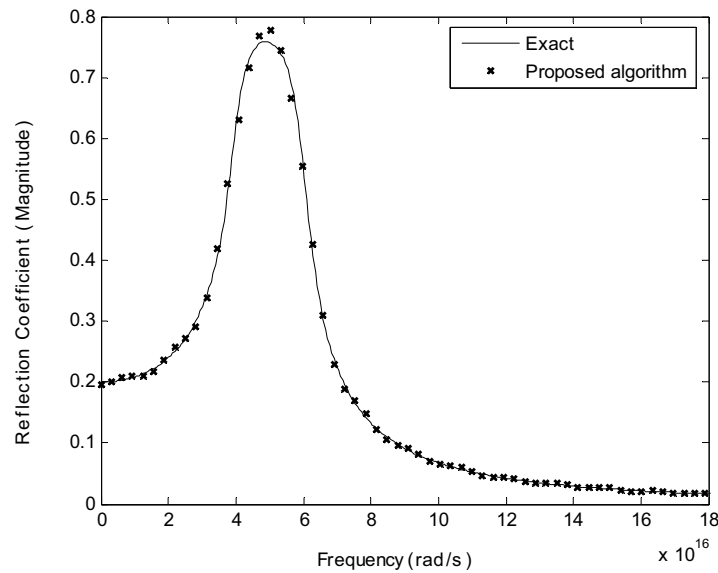


Figure 2: Reflection coefficient as calculated by the proposed algorithm and compared to exact solution for a single Lorentzian dispersion case.

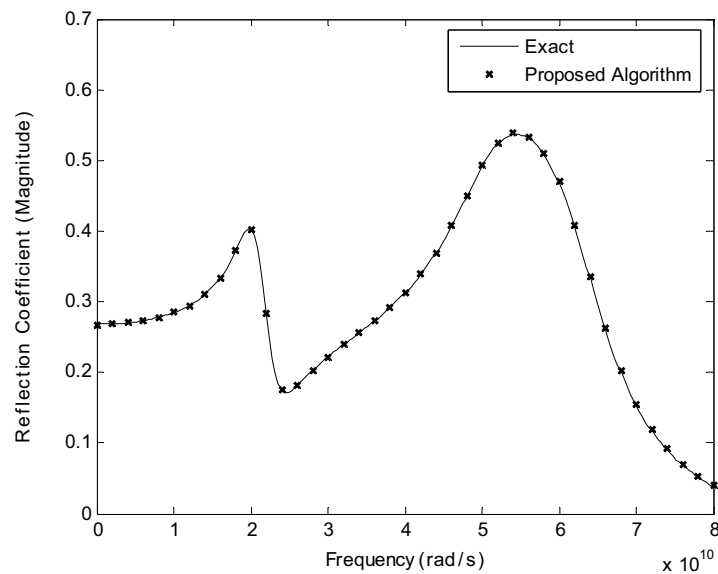


Figure 3: Reflection coefficient as calculated by the proposed algorithm and compared to exact solution for a multi-pole dispersion case.

4. CONCLUSIONS

An ADE-FDTD general algorithm for the analysis of dispersive media is presented. The algorithm is suited for cases where materials having different types of dispersion are modeled together. In these situations, the same algorithm is used to fit all dispersion types. While having the same level of accuracy and because the proposed ADE-FDTD algorithm unifies all dispersion forms into one form with three constants, it provides savings in both memory and computational requirements compared to other ADE-based algorithms.

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