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FDTD Modeling for Dispersive Media Using Matrix Exponential Method

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Abstract— **This letter presents a finite-difference time-domain (FDTD) formulation to model electromagnetic wave propagation in dispersive media using matrix exponential method. The Maxwell's curl equations and the time domain relations between electric fields and auxiliary variables are formulated as a first order differential matrix system. The fundamental solution to such a system is derived in terms of matrix exponential and the update equations can be extracted conveniently from the solution. Numerical results show that this formulation yields higher accuracy compared to many other previous methods, without incurring additional auxiliary variable and complexity.**

Index Terms—**Matrix exponential, Dispersive media, Finite-Difference Time-Domain (FDTD)**

I. Introduction

THE conventional Yee's finite-difference time-domain (FDTD) method requires additional treatments in order to model electromagnetic wave propagation in dispersive media, due to the frequency dependent permittivity or permeability of the media. One popular method is based on the Auxiliary Differential Equation (ADE) [1],[2], which converts the frequency dependent equations into discretized time domain update equations using the central difference approximation. Other techniques include the Recursive Convolution (RC) method [3] and its improved Piecewise Linear Recursive Convolution (PLRC) method [4], which are obtained by discretizing the convolution integral between the *D* and *E* fields using a recursive accumulator. Another approach is the Z-transform method (or classical impulse invariance method) [5],[6], which converts the transfer function in frequency domain into Z domain before obtaining the actual update equations. The corrected impulse invariance method [7] offers another alternative to the classical impulse invariance method with a greater accuracy when the time domain susceptibility function of the media is discontinuous at initial time zero, such as in the Debye case.

In all the above-mentioned methods, the discretizations are applied independently to the Maxwell's curl equations and the time domain relations between *E* fields and auxiliary variables. In this letter, we present a new formulation whereby all equations and relations are cast in a first order differential matrix system. The fundamental solution to such a system is derived in terms of matrix exponential and the update equations can be extracted conveniently from the solution. The matrix exponential can be derived analytically (as shown below), or computed numerically (as in [8]).

II. Formulation For Debye Media

For simplicity, we shall consider single-pole Debye media in the sequel, although the method can be extended for multi-term, Lorentz or Drude media. The complex permittivity of a Debye model is known as

$$\varepsilon(\omega) = \varepsilon + \frac{\Delta\varepsilon}{1 + j\omega\tau} \tag{1}$$

where $\varepsilon = \varepsilon_0 \varepsilon_\infty$ $\Delta\varepsilon = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)$, ε_0 is the permittivity in free space, ε_s is the static relative permittivity, ε_∞ is the relative permittivity at infinite frequency and τ is the relaxation time.

The Maxwell's curl equations and the time domain relations between *E* fields and auxiliary variables are represented in compact matrix form as

$$\frac{\partial}{\partial t}\begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{P} \end{bmatrix} = \Lambda \cdot \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{P} \end{bmatrix} + \begin{bmatrix} 1/\varepsilon \\ 0 \end{bmatrix} \nabla \times \boldsymbol{H} \tag{2}$$

where

$$\Lambda = \begin{bmatrix} -\Delta\varepsilon/(\varepsilon\tau) & 1/(\varepsilon\tau) \\ \Delta\varepsilon/\tau & -1/\tau \end{bmatrix}$$

and $\boldsymbol{P}$ is the auxiliary polarization current.

The above formulation can be viewed as a system of first order differential equations whose solution can be expressed as

$$\begin{aligned} \begin{bmatrix} \boldsymbol{E}(t) \\ \boldsymbol{P}(t) \end{bmatrix} &= \exp\big(\Lambda(t - t_0)\big) \cdot \begin{bmatrix} \boldsymbol{E}(t_0) \\ \boldsymbol{P}(t_0) \end{bmatrix} \\ &\quad + \int_{t_0}^{t} \exp\big(\Lambda(t - t')\big) \cdot \begin{bmatrix} 1/\varepsilon \\ 0 \end{bmatrix} \nabla \times \boldsymbol{H}(t')\,dt' \end{aligned} \tag{3}$$

where t_0 is the initial time. Integrating over the interval of one time step Δt and setting $\nabla \times \boldsymbol{H}(t')$ to its value at mid-point, one can obtain

$$\begin{aligned} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{P} \end{bmatrix}^{n+1} &= \exp\big(\Lambda\Delta t\big) \cdot \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{P} \end{bmatrix}^{n} \\ &\quad + \int_{0}^{\Delta t} \exp\big(\Lambda t\big) dt \cdot \begin{bmatrix} 1/\varepsilon \\ 0 \end{bmatrix} \nabla \times \boldsymbol{H}^{n+1/2} \end{aligned} \tag{4}$$

where *n* is the time index.

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It can be shown that the matrix exponential can be expressed as

$$\exp\left(\Lambda\Delta t\right)=\begin{bmatrix}1-\Delta\varepsilon\gamma & \gamma\\ \varepsilon\Delta\varepsilon\gamma & 1-\varepsilon\gamma\end{bmatrix} \tag{5}$$

where

$$\gamma=\frac{1-\exp\left(-(\varepsilon+\Delta\varepsilon)\Delta t/(\varepsilon\tau)\right)}{(\varepsilon+\Delta\varepsilon)}$$

Integrating the matrix exponential from time zero to Δt gives the following expression

$$\int_0^{\Delta t}\exp\left(\Lambda t\right)dt=\frac{1}{(\varepsilon+\Delta\varepsilon)} \times\begin{bmatrix}\varepsilon\Delta t+\Delta\varepsilon\varepsilon\tau\gamma & \Delta t-\varepsilon\tau\gamma\\ \varepsilon\Delta\varepsilon(\Delta t-\varepsilon\tau\gamma) & \Delta\varepsilon\Delta t+\varepsilon^2\tau\gamma\end{bmatrix} \tag{6}$$

Substituting (5) and (6) into (4), one arrives at

$$\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{P}\end{bmatrix}^{n+1}=\begin{bmatrix}1-\Delta\varepsilon\gamma & \gamma\\ \varepsilon\Delta\varepsilon\gamma & 1-\varepsilon\gamma\end{bmatrix}\cdot\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{P}\end{bmatrix}^{n} +\frac{1}{(\varepsilon+\Delta\varepsilon)}\begin{bmatrix}\Delta t+\Delta\varepsilon\tau\gamma\\ \Delta\varepsilon(\Delta t-\varepsilon\tau\gamma)\end{bmatrix}\nabla\times\boldsymbol{H}^{n+1/2} \tag{7}$$

The update equations for $\boldsymbol{E}$ and $\boldsymbol{P}$ can be extracted from (7) as

$$\boldsymbol{E}^{n+1}=\left(1-\Delta\varepsilon\gamma\right)\boldsymbol{E}^{n}+\gamma\boldsymbol{P}^{n}+\frac{\Delta t+\Delta\varepsilon\tau\gamma}{(\varepsilon+\Delta\varepsilon)}\nabla\times\boldsymbol{H}^{n+1/2} \tag{8a}$$

$$\boldsymbol{P}^{n+1}=\left(1-\varepsilon\gamma\right)\boldsymbol{P}^{n}+\varepsilon\Delta\varepsilon\gamma\boldsymbol{E}^{n} +\frac{\Delta\varepsilon\Delta t-\varepsilon\Delta\varepsilon\gamma\tau}{(\varepsilon+\Delta\varepsilon)}\nabla\times\boldsymbol{H}^{n+1/2} \tag{8b}$$

To eliminate the dependency of $\boldsymbol{P}$ on $\nabla\times\boldsymbol{H}$ in the second update equation, (8a) can be substituted into (8b) and upon some manipulation, the final update equation for $\boldsymbol{P}$ reads

$$\boldsymbol{P}^{n+1}=c_1\boldsymbol{P}^{n}+c_2\boldsymbol{E}^{n+1}+c_3\boldsymbol{E}^{n} \tag{9}$$

where

$$c_1=\frac{\Delta\varepsilon\gamma\tau+(1-\varepsilon\gamma-\Delta\varepsilon\gamma)\Delta t}{\Delta\varepsilon\gamma\tau+\Delta t}$$

$$c_2=\frac{\Delta\varepsilon\Delta t-\varepsilon\Delta\varepsilon\gamma\tau}{\Delta\varepsilon\gamma\tau+\Delta t}$$

$$c_3=\frac{\varepsilon\Delta\varepsilon\gamma\tau+\Delta\varepsilon(1-\varepsilon\gamma-\Delta\varepsilon\gamma)\Delta t}{\Delta\varepsilon\gamma\tau+\Delta t}$$

The $\boldsymbol{H}$ field is updated as in the conventional Yee's FDTD scheme.

III. Dispersion Analysis And Numerical Results

For illustration, we consider a 1-D plane wave with E_x and H_y components traveling in z direction. Using Fourier analysis in conjunction with second order spatial central difference on Yee's cell, the updating procedures can be represented in matrix as

$$A\cdot e^{j\omega\Delta t}I\cdot\begin{bmatrix}E_x\\ H_y\\ P\end{bmatrix}=B\cdot\begin{bmatrix}E_x\\ H_y\\ P\end{bmatrix} \tag{10}$$

where I is the 3 by 3 identity matrix,

$$A=\begin{bmatrix}1 & 0 & 0\\ -2jW_z/\mu_0 & 1 & 0\\ -c_2 & 0 & 1\end{bmatrix},$$

$$B=\begin{bmatrix}1-\Delta\varepsilon\gamma & \frac{2jW_z}{\Delta t}\frac{\Delta t+\Delta\varepsilon\gamma}{(\varepsilon+\Delta\varepsilon)} & \gamma\\ 0 & 1 & 0\\ c_3 & 0 & c_1\end{bmatrix},$$

$W_z=\left(\Delta t/\Delta z\right)\sin\left(k\Delta z/2\right)$ and μ_0 is the permeability in free space. For nontrivial field solution, the dispersion relation can be derived by setting

$$\det\left(A\cdot e^{j\omega\Delta t}I-B\right)=0 \tag{11}$$

The complex roots of propagation constant can then be solved and compared to the analytical propagation constant with $k(\omega)=\omega\sqrt{\mu_0\varepsilon_0\varepsilon(\omega)}$. It is noted that the real part and (negative) imaginary part of k are associated with the phase constant and attenuation constant respectively. The normalized phase and attenuation error are defined as $\left|\frac{\mathrm{Re}(k_{solved})-\mathrm{Re}(k_{analytical})}{\mathrm{Re}(k_{analytical})}\right|$ and $\left|\frac{\mathrm{Im}(k_{solved})-\mathrm{Im}(k_{analytical})}{\mathrm{Im}(k_{analytical})}\right|$ respectively. Similarly, the normalized phase and attenuation constant error for other methods are obtained by performing the same procedure and comparison can then be made among them.

Figure 1a plots the normalized phase constant error and Fig. 1b the corresponding normalized attenuation constant error. The Debye medium considered is water, characterized by $\varepsilon_s=81$, $\varepsilon_\infty=1.8$, and $\tau=9.4ps$ [3]. The cell size Δz and time step Δt are set at $37.5\mu m$ and $0.125ps$ respectively. It can be seen from both figures that the RC and classical impulse invariance method have relatively high errors, which essentially put them nearly off the graphs. The ADE, PLRC and corrected impulse invariance method give relatively lower error, but it is evident that both the normalized phase and attenuation error of the exponential matrix method are the lowest throughout the whole frequency range considered. This indicates that this method indeed features the highest accuracy among all other methods.

For further illustration, we consider 1000 cells filled with water. Let the plane wave propagation be initiated by a hard source Gaussian pulse excitation at initial point. The E field in space can be traced after certain time steps and the result can be compared to the analytical solution obtained by numerically integrating the exact frequency domain solution.

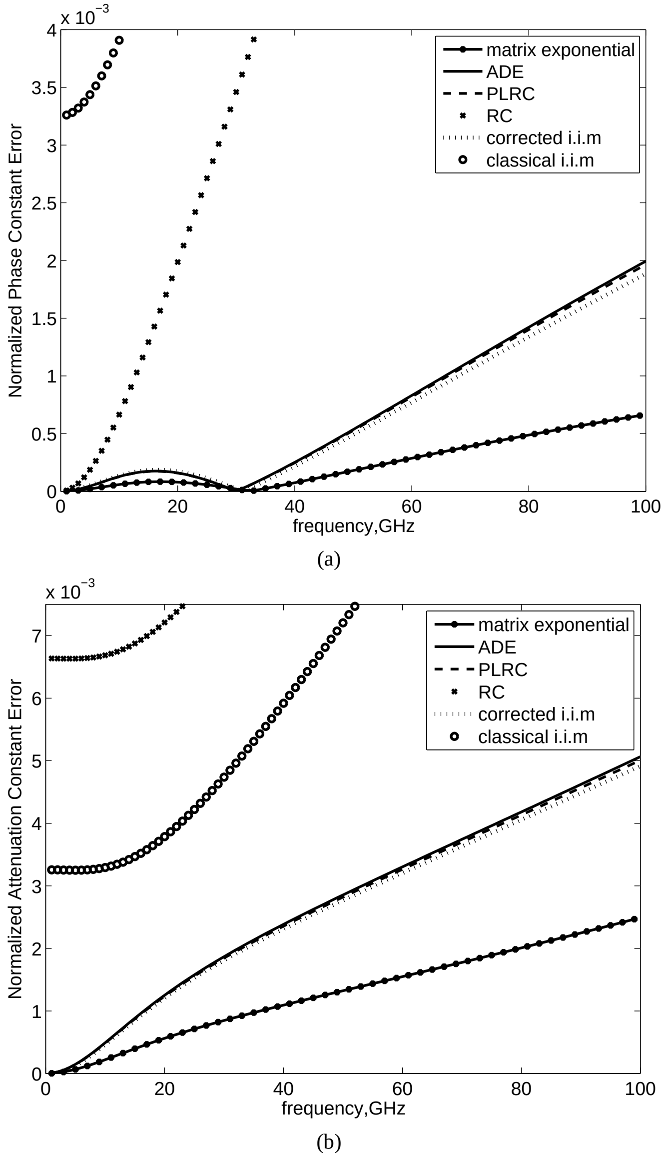

Fig 1. Normalized phase (a) and attenuation (b) error versus frequency.

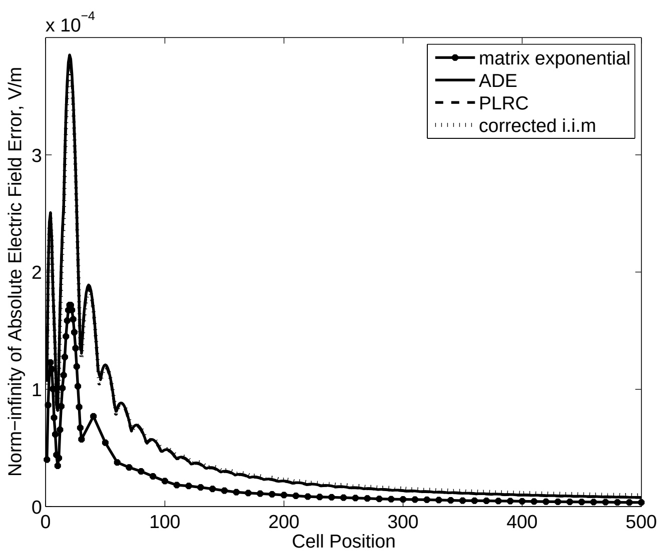

Fig 2. Norm-infinity of absolute electric field error versus cell position.

Figure 2 shows the norm-infinity of absolute electric field error versus cell position in the Debye medium. The norm is computed over 6500 time steps sampled at the interval of 100 time steps. Owing to the high phase and attenuation constant errors exhibited by the RC and classical impulse invariance method (as depicted previously from the dispersion analysis), their results are omitted herein. Comparison is made directly among the matrix exponential, ADE, PLRC and corrected impulse invariance methods. It can be seen again that the error incurred by using matrix exponential method is the lowest compared to others. This further reaffirms its higher accuracy feature, resulting from the fact that the update equations are derived directly from the fundamental solution to the system of first order differential equations. The memory storage requirement for this method is found to be less than the classical and corrected impulse invariance methods. It is the same as the ADE, RC and PLRC methods utilizing the same number of auxiliary variables, and yet retains the high accuracy feature of the matrix exponential.

IV. CONCLUSION

This letter has presented the FDTD formulation for electromagnetic wave propagation in dispersive media using matrix exponential method. Dispersion analysis for the method is performed and numerical result has been shown. Compared to other previous methods, the matrix exponential shows a promising higher accuracy without incurring additional auxiliary variable. For extension to multi-term dispersion or higher order pole such as the Lorentz media, the analytical derivation of update equations herein can be omitted by directly computing the matrix exponential and its time integral numerically. The update equations can then be derived readily without incurring much complexity.

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