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Heh, Ding Yu; Tan, Eng Leong

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Divergence-Preserving Alternating Direction Implicit Scheme for Multi-Pole Debye Dispersive Media

Ding Yu Heh, *Member, IEEE* and Eng Leong Tan, *Senior Member, IEEE*

Abstract—This letter presents the formulation of divergence-preserving alternating direction implicit (DP-ADI) scheme for multi-pole Debye dispersive media. The analytical proof of divergence-preserving property of the scheme in Debye media is provided. Numerical results of modeling human skin as Debye media further validate our proposed scheme.

Index Terms—divergence-preserving, alternating direction implicit, finite-difference time-domain, dispersive media

I. INTRODUCTION

Compared to the explicit finite-difference time-domain (FDTD) method [1], the alternating direction implicit (ADI) finite-difference time-domain method [2], [3] has the advantage of unconditional stability in which the time step is no longer bounded by the Courant-Friedrich-Lewy (CFL) stability condition. Unfortunately, unlike the explicit FDTD method which inherently preserves the divergence property of Maxwell's equations (Gauss's Law), the ADI method is found to be non divergence-preserving. Recently, a divergence-preserving ADI (DP-ADI) scheme has been introduced in [4], whereby the ADI scheme not only features unconditional stability, but also exhibits divergence-preserving property. This has opened up much room for further extensions into various media.

The extension of the conventional ADI method into Debye dispersive media has been provided in [5]. Like its non-dispersive counterpart, such extension based on conventional ADI method will also be non divergence-preserving. On the other hand, although the DP-ADI scheme for non-dispersive media is divergence-preserving, there is no guarantee that the same will hold true for dispersive media. In this letter, we shall present the formulation of DP-ADI scheme for multi-pole Debye dispersive media. Analytical proof of divergence-preserving property in Debye dispersive media will be given. Numerical results of modeling human skin as Debye dispersive media shall further validate our proposed scheme.

II. FORMULATION AND ANALYTICAL PROOF OF DIVERGENCE-PRESERVING PROPERTY

The DP-ADI scheme for non-dispersive media takes the general matrix form as [4]

$$\mathbf{v}_{DP}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right) \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right)^{-1} \times \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{A} \right) \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \mathbf{v}_{DP}^n \quad (1)$$

where the divergence-preserving field vector $\mathbf{v}_{DP}$ are defined as

$$\mathbf{v}_{DP} = [\mathbf{E}_{DP}; \mathbf{H}_{DP}] = [E_x \ E_y \ E_z \ H_x \ H_y \ H_z]^T. \quad (2)$$

The matrix operators $\mathbf{A}$, $\mathbf{B}$ are standard curl splitting operators found in [7], and ϵ and μ are permittivity and permeability respectively.

For multi-pole Debye media, the p -th pole polarization $\mathbf{P}_p$ is related to the electric field in frequency domain by

$$\sum_p \mathbf{P}_p(\omega) = \sum_p \frac{\epsilon_0 \Delta \epsilon_p}{1 + j\omega \tau_p} \mathbf{E}(\omega) \quad (3)$$

where ϵ_0 is the permittivity of free space, $\Delta \epsilon_p$ and τ_p are the p -th pole change in permittivity and relaxation time, respectively.

To incorporate Debye dispersive media into DP-ADI scheme, we use auxiliary differential equation (ADE) method and obtain

$$\mathbf{v}_{DP}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right) \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right)^{-1} \times \left[\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{A} \right) \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \mathbf{v}_{DP}^n - \frac{\Delta t}{2} \sum_p \left(\frac{\mathbf{p}_p^{n+\frac{1}{2}} - \mathbf{p}_p^n}{\Delta t/2} \right) \right] - \frac{\Delta t}{2} \sum_p \left(\frac{\mathbf{p}_p^{n+1} - \mathbf{p}_p^{n+\frac{1}{2}}}{\Delta t/2} \right) \quad (4)$$

where $\mathbf{p}_p = [\mathbf{P}_p / \epsilon_0 \epsilon_\infty; \mathbf{0}]$, ϵ_∞ is relative permittivity at infinite frequency and the conductivity is excluded.

To prove that (4) is still divergence-preserving, we adopt the identities of

$$\left(\mathbf{I} \mp \frac{\Delta t}{2} \mathbf{A} \right) \left(\mathbf{I} \pm \frac{\Delta t}{2} \mathbf{B} \right)^{-1} = \mathbf{I} \mp \frac{\Delta t}{2} (\mathbf{A} + \mathbf{B}) \left(\mathbf{I} \pm \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \quad (5)$$

to manipulate (4) and arrive at

$$\begin{aligned} \mathbf{v}_{DP}^{n+1} - \mathbf{v}_{DP}^n = & - \sum_p \left(\mathbf{p}_p^{n+1} - \mathbf{p}_p^{n+\frac{1}{2}} + \mathbf{p}_p^{n+\frac{1}{2}} - \mathbf{p}_p^n \right) \\ & + \frac{\Delta t}{2} (\mathbf{A} + \mathbf{B}) \left[\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \mathbf{v}_{DP}^n \right. \\ & \left. + \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \left(\mathbf{v}_{DP}^{n+1} + \sum_p (\mathbf{p}_p^{n+1} - \mathbf{p}_p^{n+\frac{1}{2}}) \right) \right]. \end{aligned} \quad (6)$$

Applying numerical divergence (by means of central spatial differencing), denoted by $\nabla_{FD} \cdot$ to both sides, and taking note that $\nabla_{FD} \cdot (\mathbf{A} + \mathbf{B}) \cdot \mathbf{x} = 0$ for any vector $\mathbf{x}$, one obtains

$$\nabla_{FD} \cdot (\mathbf{v}_{DP}^{n+1} - \mathbf{v}_{DP}^n) = -\nabla_{FD} \cdot \sum_p (\mathbf{p}_p^{n+1} - \mathbf{p}_p^n). \quad (7)$$

Taking only the electric field components, (7) reduces to

$$\begin{aligned} \nabla_{FD} \cdot (\epsilon_0 \epsilon_\infty \mathbf{E}_{DP}^{n+1} + \sum_p \mathbf{P}_p^{n+1}) \\ - \nabla_{FD} \cdot (\epsilon_0 \epsilon_\infty \mathbf{E}_{DP}^n + \sum_p \mathbf{P}_p^n) = 0. \end{aligned} \quad (8)$$

Substituting electric flux density $\mathbf{D} = \epsilon_0 \epsilon_\infty \mathbf{E}_{DP} + \sum_p \mathbf{P}_p$ into (8), we finally arrive at

$$\nabla_{FD} \cdot \mathbf{D}^{n+1} - \nabla_{FD} \cdot \mathbf{D}^n = 0. \quad (9)$$

From (9), one can see that if the numerical divergence of $\mathbf{D}$ is zero initially (at source-free regions), the numerical divergence of $\mathbf{D}$ will still be preserved as the algorithm marches in time. The proof is useful in showing that the DP-ADI scheme for dispersive media satisfies the Gauss's Law and may be useful in applications for stable and accurate electromagnetic particle-in-cell simulation by ensuring no charge accumulation in grids [4]. With the divergence-preserving property, it may also be possible to develop memory efficient ADI methods by utilizing Maxwell's divergence equations [6].

Having proven the divergence-preservation, (4) is to be implemented readily in two procedures as follows:

$$\mathbf{v}_{DP}^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{A} \right) \mathbf{v}^n - \sum_p \left(\mathbf{p}_p^{n+\frac{1}{2}} - \mathbf{p}_p^n \right) \quad (10a)$$

$$\mathbf{v}_{DP}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right) \mathbf{v}_{DP}^{n+\frac{1}{2}} - \sum_p \left(\mathbf{p}_p^{n+1} - \mathbf{p}_p^{n+\frac{1}{2}} \right) \quad (10b)$$

where

$$\mathbf{v}^n = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right)^{-1} \mathbf{v}_{DP}^n; \quad \mathbf{v}^{n+\frac{1}{2}} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right)^{-1} \mathbf{v}_{DP}^{n+\frac{1}{2}} \quad (11)$$

$$\mathbf{v} = [\mathbf{E}; \mathbf{H}] \quad (12)$$

and $\mathbf{P}_p$ is to be updated in the following manner:

$$\mathbf{P}_p^{n+\frac{1}{2}} = k_1 \mathbf{P}_p^n + k_2 [\mathbf{E}^{n+\frac{1}{2}} + \mathbf{E}^n] \quad (13a)$$

$$\mathbf{P}_p^{n+1} = k_1 \mathbf{P}_p^{n+\frac{1}{2}} + k_2 [\mathbf{E}^{n+1} + \mathbf{E}^{n+\frac{1}{2}}] \quad (13b)$$

with $k_1 = \left(\frac{\tau_p - \Delta t/4}{\tau_p + \Delta t/4} \right)$ and $k_2 = \left(\frac{\epsilon_0 \tau_p \Delta \epsilon_p \Delta t/4}{\tau_p + \Delta t/4} \right)$. For brevity, we shall not present the details of algorithm but it should be noted that the fundamental scheme of [7]-[10] may be adopted for its efficient implementation.

Fig. 1. Divergence of $\mathbf{D}$ (in dB) for (a) DP-ADI, (b) Yee explicit, (c) ADI and (d) LOD schemes.

III. NUMERICAL RESULTS

For numerical illustration, we first consider a homogeneous human skin of domain size $50 \times 50 \times 9$ cells having 2-pole Debye parameters: $\epsilon_\infty = 2.58$, $\Delta\epsilon_1 = 10.54$, $\Delta\epsilon_2 = 1.58$, $\tau_1 = 1.45$ ps and $\tau_2 = 0.0611$ ps [8], [11]. The computational domain is terminated by 10-cell perfectly matched layers (PML). A z -directed point current source of Terahertz (THz) modulated Gaussian pulse with centre frequency 1.1 THz and pulse width 0.8 ps is excited at the centre. To verify the divergence-preserving property of DP-ADI scheme, the divergence of electric flux density $\mathbf{D}$ is computed numerically via $\nabla_{FD} \cdot \mathbf{D} = \nabla_{FD} \cdot (\epsilon_0 \epsilon_\infty \mathbf{E}_{DP} + \sum_p \mathbf{P}_p)$. Cell size is chosen as $2 \mu\text{m}$ and time step is specified in terms of $\text{CFLN} = \Delta t / \Delta t_{\text{CFL}}$ where Δt_{CFL} is the maximum allowed time step in Yee explicit scheme. Here we choose $\text{CFLN} = 4$. Fig. 1 plots the divergence of $\mathbf{D}$ (in dB) for (a) DP-ADI, (b) Yee explicit, (c) ADI and (d) Locally One Dimensional (LOD) schemes at xy -plane across the centre of the skin. (For Yee explicit scheme, $\text{CFLN} = 1$.) It can be observed that the divergence of $\mathbf{D}$ for DP-ADI and Yee explicit schemes at the source-free region is around -250 dB, which is as low as the numerical noise level. On the contrary, the divergence of $\mathbf{D}$ for both ADI and LOD schemes shows significantly higher value (non divergence-preserving). This non divergence-preserving property is also observed in complex envelope ADI scheme [12]. Note that it may still be non divergence-free at source region as evident by higher divergence value at the centre due to presence of charges, even for Yee explicit scheme. There may also be other non divergence-free regions such as PEC edges and/or PEC/dielectric interfaces, etc [13].

We now simulate a plane wave propagation from air impinging upon a $300 \mu\text{m}$ -thick human skin sample. Cell size for air region is $5 \mu\text{m}$ while the cell size for the human skin sample and interface regions is $2.5 \mu\text{m}$. Time step is set with $\text{CFLN} = 4$. The simulation is repeated with a $300 \mu\text{m}$ -thick Basal Cell Carcinoma (BCC) sample, also modeled as 2-pole Debye media with parameters: $\epsilon_\infty = 2.65$, $\Delta\epsilon_1 = 13.37$, $\Delta\epsilon_2 = 1.58$, $\tau_1 = 1.55$ ps and $\tau_2 = 0.0614$ ps [8], [11]. Fig. 2 plots the magnitude of transmission coefficient of the healthy

Fig. 2. Transmission coefficient for healthy skin and BCC. Inset shows transmitted electric field across skin samples with and without (healthy) presence of BCC tumor.

TABLE I
NORMALIZED 2-NORM ERROR FOR VARIOUS SCHEMES AND CFLNs

Media	Scheme	CFLN			
		1	4	7	10
Lossless	Yee explicit	0.0006	N/A	N/A	N/A
	ADI	0.0007	0.0085	0.0268	0.0558
	DP-ADI	0.0008	0.0151	0.0481	0.1021
Dispersive	Yee explicit	0.0042	N/A	N/A	N/A
	ADI	0.0060	0.0243	0.0656	0.1310
	DP-ADI	0.0056	0.0187	0.0492	0.1002

skin and BCC samples computed using DP-ADI scheme. The results are compared with Yee explicit scheme and analytical solution. Good agreement is observed among all curves. Due to higher absorption of the BCC, its magnitude of transmission coefficient is lower than that of healthy skin.

We next consider an inhomogeneous skin sample whereby a BCC tumor is present inside a healthy skin sample. The human skin has a thickness of $300 \mu\text{m}$ and a surface area of $400 \times 400 \mu\text{m}^2$, while tumor is an ellipsoid having radii of 300, 200 and $400 \mu\text{m}$. Uniform cell size is chosen as $5 \mu\text{m}$ and CFLN=4. The inset shows the transmitted electric field across skin samples with and without (healthy) presence of BCC tumor. These results are also in well agreement with Yee explicit scheme, which further validate our DP-ADI scheme.

Finally, Table I shows the normalized 2-norm error $\frac{\|E_{\text{scheme}} - E_{\text{analytical}}\|_2}{\|E_{\text{analytical}}\|_2}$ for various schemes and CFLNs, where E is the magnitude of transmitted electric field in frequency domain and the 2-norm error is taken across THz frequencies. The numerical experiments are conducted for both lossless and Debye dispersive media. It is observed that the 2-norm errors of DP-ADI scheme in lossless medium are slightly larger than that of ADI scheme. This may be attributed to errors related to the approximation of the so-called steady-state equations in [4] and source excitations. However, for dispersive medium, the fields are attenuated in steady-state due to its dissipative nature and such errors may be less pronounced, which result in more comparable 2-norm errors between DP-ADI and ADI schemes.

IV. CONCLUSION

This letter has presented the formulation of divergence-preserving alternating direction implicit (DP-ADI) scheme for multi-pole Debye dispersive media. The analytical proof of divergence-preserving property of the scheme in Debye media has been provided. Numerical results of modeling human skin as Debye media have further validated our proposed scheme.

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