Four-Stage Split-Step 2D FDTD Method with Error-Cancellation Features

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Abstract **─** We develop a methodology that enables the proper introduction of high-order spatial operators in an unconditionally-stable, split-step, finite-difference time-domain scheme. The proposed approach yields spatial approximations that guarantee better balancing of space-time errors, compared to standard fourth-order expressions. The latter are not as efficient as expected, due to their unmatched order with the scheme's second-order temporal accuracy. Our technique treats the dispersion relation as an error descriptor, derives spatial formulae that change with the cell shape and time-step size, and rectifies the performance over all frequencies.

Index Terms **─** Finite-difference time-domain (FDTD) methods, numerical-dispersion relation, split-step approaches, unconditionally-stable methods.

I. INTRODUCTION

Among the diverse advances of Yee's finite-difference time-domain (FDTD) method [1,2], approaches featuring unconditional stability [3] belong to the most significant contributions. Numerical schemes such as the alternating-direction implicit [4] and the locally one-dimensional FDTD techniques [5] are free from constraints governing their temporal sampling density, which is an advantageous property in many electromagnetic simulations. Other solutions based on split-step procedures [6-8] also exhibit similar behavior, and have been the subject of various studies [9,10].

In the context of the aforementioned implicit methods, the improvement of temporal accuracy can be a computationally expensive task, as it commonly requires the increase of the intermediate stages for the successive update of field components. On the other hand, direct incorporation of high-order spatial operators is a simpler and more straightforward approach towards performance upgrade, although it too augments the algorithm's complexity. Since the combination of accurate spatial approximations with low (first or second) temporal order usually impedes the full exploitation of high-order operators' potential, amending techniques may be applied for further error mitigation. The implementation of constant-valued correctional coefficients, calculated in diverse ways, is a popular practice in this category of useful concepts [11,12].

This paper's purpose is to efficiently incorporate four-point spatial approximations into a two-dimensional (2D) four-stage split-step FDTD (SS-FDTD) method, aiming at a balanced treatment of space-time errors. Our approach exploits the scheme's dispersion relation to represent the inherent discretization errors. By using the estimator's Taylor polynomial, improvement over all frequencies is facilitated, while its trigonometric expansion leads to accuracy correction irrespective of propagation direction. The resulting unconditionally-stable algorithm performs better than its counterpart with standard high-order operators, verifying the optimal use of computational resources.

II. MODIFIED 4-STAGE SS-FDTD METHOD

The considered SS-FDTD scheme has second-order temporal accuracy, and the time-stepping is performed according to the following splitting approach:

$$\begin{aligned}
\left([\mathbf{I}]-\tfrac{\Delta t}{4}[\mathbf{A}]\right)[\mathbf{u}]^{n+1/4} &= \left([\mathbf{I}]+\tfrac{\Delta t}{4}[\mathbf{A}]\right)[\mathbf{u}]^{n} \\
\left([\mathbf{I}]-\tfrac{\Delta t}{4}[\mathbf{B}]\right)[\mathbf{u}]^{n+1/2} &= \left([\mathbf{I}]+\tfrac{\Delta t}{4}[\mathbf{B}]\right)[\mathbf{u}]^{n+1/4} \\
\left([\mathbf{I}]-\tfrac{\Delta t}{4}[\mathbf{B}]\right)[\mathbf{u}]^{n+3/4} &= \left([\mathbf{I}]+\tfrac{\Delta t}{4}[\mathbf{B}]\right)[\mathbf{u}]^{n+1/2}, \\
\left([\mathbf{I}]-\tfrac{\Delta t}{4}[\mathbf{A}]\right)[\mathbf{u}]^{n+1} &= \left([\mathbf{I}]+\tfrac{\Delta t}{4}[\mathbf{A}]\right)[\mathbf{u}]^{n+3/4}
\end{aligned} \qquad (1)$$

where $[\mathbf{I}]$ is the 3×3 unitary matrix, $[\mathbf{u}] = [E_x\ E_y\ H_z]^{\mathrm{T}}$ is the vector with the three field components in 2D, Δt is the time increment, and $[\mathbf{A}]$,$[\mathbf{B}]$ are derivative matrices:

$$[\mathbf{A}] = \begin{bmatrix} 0 & 0 & \frac{1}{\varepsilon}D_y \\ 0 & 0 & 0 \\ \frac{1}{\mu}D_y & 0 & 0 \end{bmatrix}, \ [\mathbf{B}] = -\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\varepsilon}D_x \\ 0 & \frac{1}{\mu}D_x & 0 \end{bmatrix}. \quad (2)$$

In its conventional form [8], the methodology relies on

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standard second-order approximations of the derivatives. Here, we adopt four-point symmetric expressions,

$$D_x u\big|_{i,j}^{n} = \frac{1}{\Delta x}\sum_{m=1}^{2} C_m^x \left(u\big|_{i+\frac{2m-1}{2},j}^{n} - u\big|_{i-\frac{2m-1}{2},j}^{n} \right), \quad (3)$$

$$D_y u\big|_{i,j}^{n} = \frac{1}{\Delta y}\sum_{m=1}^{2} C_m^y \left(u\big|_{i,j+\frac{2m-1}{2}}^{n} - u\big|_{i,j-\frac{2m-1}{2}}^{n} \right), \quad (4)$$

whose final form is determined via an analytical procedure that aims at suitable error cancellation.

The basic element of the proposed optimization approach is the scheme's numerical dispersion relation, and its utilization as a means to express the inherent dispersion errors. The dispersion relation is obtained after introducing plane-wave forms in (1),

$$[\mathbf{u}] = [\mathbf{u}_0] e^{\mathrm{j}(\omega t - \tilde{k}_x x - \tilde{k}_y y)}, \quad (5)$$

and requiring the existence of non-trivial solutions for the resulting system ($\tilde{k}_x = \tilde{k}\cos\theta$, $\tilde{k}_y = \tilde{k}\sin\theta$, $\tilde{k}$ is the numerical wavenumber). In essence, the condition,

$$\det\left(e^{\mathrm{j}\omega\Delta t}[\mathbf{I}] - [\mathbf{L}_{\mathcal{A}}][\mathbf{L}_{\mathcal{B}}]^2[\mathbf{L}_{\mathcal{A}}] \right) = 0, \quad (6)$$

is obtained, where

$$[\mathbf{L}_{\mathbf{U}}] = \left([\mathbf{I}] - \tfrac{\Delta t}{4}[\mathbf{U}]\right)^{-1}\left([\mathbf{I}] + \tfrac{\Delta t}{4}[\mathbf{U}]\right), \quad (7)$$

and matrices $[\mathcal{A}]$, $[\mathcal{B}]$ are derived from $[\mathbf{A}]$, $[\mathbf{B}]$, respectively, after replacing the D_x, D_y operators with:

$$X = -\frac{2\mathrm{j}}{\Delta x}\sum_{m=1}^{2} C_m^x \sin\left(\tfrac{2m-1}{2}\tilde{k}_x \Delta x\right), \quad (8)$$

$$Y = -\frac{2\mathrm{j}}{\Delta y}\sum_{m=1}^{2} C_m^y \sin\left(\tfrac{2m-1}{2}\tilde{k}_y \Delta y\right). \quad (9)$$

The resulting dispersion equation has the form:

$$\cos(\omega\Delta t) = \frac{\alpha_{\mathrm{num}}(\tilde{k},\omega,\theta)}{\alpha_{\mathrm{den}}(\tilde{k},\omega,\theta)}, \quad (10)$$

where

$$\begin{aligned}\alpha_{\mathrm{num}} &= \left(16 + c_0^2\Delta t^2 X^2\right)^2\left(16 + c_0^2\Delta t^2 Y^2\right)^2 \\ &\quad + 64 c_0^2 \Delta t^2 \left(X^2 + Y^2\right)\left(256 + c_0^4 \Delta t^2 X^2 Y^2\right), \end{aligned} \quad (11)$$

$$\alpha_{\mathrm{den}} = \left(16 - c_0^2\Delta t^2 X^2\right)^2\left(16 - c_0^2\Delta t^2 Y^2\right)^2. \quad (12)$$

Of crucial importance is the definition of the error formula that is used to represent the discretization flaws. As we are interested in combating the inaccuracies pertinent to the phase velocity, we define,

$$\Lambda(\omega,\theta) = \cos(\omega\Delta t) - \frac{\alpha_{\mathrm{num}}(k,\omega,\theta)}{\alpha_{\mathrm{den}}(k,\omega,\theta)}, \quad (13)$$

which practically describes the deviation from the numerical dispersion relation, once the numerical wave-vector has been replaced by its exact value $k = \omega/c_0$. Now, the determination of the optimum spatial operators is reduced to the following problem: find suitable coefficients C_1^x, C_2^x, C_1^y, C_2^y, so that the magnitude of $\Lambda(\omega,\theta)$ is rendered as close to zero as possible, for all frequencies ω and propagation angles θ.

In order to satisfy – to the best possible degree – the aforementioned requirements, the Taylor-series of (13) with respect to the spatial increment is exploited. Specifically, we are working on the expression:

$$\Lambda(\omega,\theta) = \delta^{(2)}(\theta)(k\Delta x)^2 + \delta^{(4)}(\theta)(k\Delta x)^4 + \ldots. \quad (14)$$

This expansion effectively isolates the dependences on frequency and propagation direction, which significantly facilitates their separate treatment. Specifically, accuracy improvement irrespective of frequency is now possible, by cancelling the corresponding δ coefficients, which do not depend on ω. If it was possible to accomplish $\delta^{(2)} = \delta^{(4)} = \ldots = 0$, a totally error-free FDTD scheme would be devised. Apparently, this is an observation of merely theoretical interest, since the discretization error can be controlled only to a certain degree in practice. In our case, we are proceeding with the manipulation of the $\delta^{(2)}$ and $\delta^{(4)}$ coefficients.

Starting from the second-order term, we find that:

$$\delta^{(2)} = \frac{Q^2R^2}{2\left(1+R^2\right)}\left[\left(C_1^x + 3C_2^x\right)^2\tau_x^2 + \left(C_1^y + 3C_2^y\right)^2\tau_y^2 - 1\right], \quad (15)$$

where $R = \Delta y/\Delta x$, $\tau_x = \cos\theta$, $\tau_y = \sin\theta$, and Q determines the time-step size, via:

$$\Delta t = \frac{QR\Delta x}{c_0\sqrt{1+R^2}}. \quad (16)$$

In (16), $Q = 1$ yields the well-known Yee's stability criterion. Clearly, the second-order term vanishes if:

$$C_1^u + 3C_2^u = 1, \; u = x,y, \quad (17)$$

In essence, (17) guarantees that the spatial operators are at least second-order accurate, which is necessary so that their error matches the corresponding temporal one.

The treatment of the $\delta^{(4)}$ term is more involved, as it is expressed according to:

$$\begin{aligned}\delta^{(4)}(\theta) &= \frac{(QR)^4}{24\left(1+R^2\right)^2} - \frac{(QR)^2}{3072\left(1+R^2\right)^2}\Big[\\ &\quad 128\left(C_1^x + 27C_2^x\right)\tau_x^4 + 128R^4\left(C_1^y + 27C_2^y\right)\tau_y^4 \\ &\quad + 128R^2\left(C_1^x + 27C_2^x\right)\tau_x^4 + 128R^2\left(C_1^y + 27C_2^y\right)\tau_y^4 \\ &\quad + 3Q^2R^2\left(64\tau_x^4 + \tau_x^3\tau_y + 128\tau_x^2\tau_y^2 + \tau_x\tau_y^3 + 64\tau_y^4\right)\Big], \end{aligned} \quad (18)$$

where (17) has already been partially substituted for simplicity. It is clear that $\delta^{(4)}$ cannot be eliminated, as the corresponding SS-FDTD scheme cannot accomplish fourth-order space-time accuracy. A more realistic goal is to render $\delta^{(4)}$ as small as possible, so that better overall performance is attained, compared to standard fourth-order spatial approximations. For this reason, (18) is rearranged, using the identities:

$$\tau_x^4 = \frac{3}{8} + \frac{1}{2}\cos(2\theta) + \frac{1}{8}\cos(4\theta), \quad (19)$$

$$\tau_y^4 = \frac{3}{8} - \frac{1}{2}\cos(2\theta) + \frac{1}{8}\cos(4\theta), \tag{20}$$

$$\tau_x^3 \tau_y = \frac{1}{4}\sin(2\theta) + \frac{1}{8}\sin(4\theta), \tag{21}$$

$$\tau_x^2 \tau_y^2 = \frac{1}{8} - \frac{1}{8}\cos(4\theta), \tag{22}$$

$$\tau_x \tau_y^3 = \frac{1}{4}\sin(2\theta) - \frac{1}{8}\sin(4\theta). \tag{23}$$

Taking (19)-(23) into account, $\delta^{(4)}$ is expressed as a finite trigonometric series, and two additional constraints can be derived from the vanishing of an equal number of terms. If the series' constant term is set equal to zero, the following equation is obtained:

$$C_1^x + 27C_2^x + R^2\left(C_1^y + 27C_2^y\right) = -\frac{4(QR)^2}{3(1+R^2)}. \tag{24}$$

The last equation is extracted from the coefficient of the $\cos(2\theta)$ term, resulting in:

$$C_1^x + 27C_2^x - R^2\left(C_1^y + 27C_2^y\right) = 0. \tag{25}$$

The solution of the system comprising (17), (24), and (25) yields the optimum spatial operators, whose final form takes into account the cell shape and the time-step size, as the resulting coefficient expressions are:

$$C_1^x = \frac{9}{8} + \frac{Q^2}{12}\frac{R^2}{1+R^2},\ C_2^x = -\frac{1}{24} - \frac{Q^2}{36}\frac{R^2}{1+R^2}, \tag{26}$$

$$C_1^y = \frac{9}{8} + \frac{Q^2}{12}\frac{1}{1+R^2},\ C_2^x = -\frac{1}{24} - \frac{Q^2}{36}\frac{1}{1+R^2}. \tag{27}$$

Consequently, the procedure followed herein concludes that the standard fourth-order operators are the most suitable choice, only if a very small time step (i.e., $Q \to 0$) is selected. This, however, is not the case in unconditionally-stable FDTD methods, and modified approximations that do not necessarily preserve the maximum order of accuracy can guarantee lower dispersion flaws.

III. ASSESSMENT OF METHODOLOGY

The stability of the numerical scheme is revealed by obtaining the eigenvalues of its amplification matrix. The latter is equal to $[\mathbf{L}_{\mathcal{A}}][\mathbf{L}_{\mathcal{B}}]^2[\mathbf{L}_{\mathcal{A}}]$, as defined in (6), (7), and its eigenvalues are: $\lambda_1 = 1$, and,

$$\lambda_{2,3} = \frac{w - 64v \pm \mathrm{j}16\sqrt{wv}}{r}, \tag{28}$$

where

$$w = \left(16 + c_0^2\Delta t^2 X^2\right)^2\left(16 + c_0^2\Delta t^2 Y^2\right)^2, \tag{29}$$

$$v = -64c_0^2\Delta t^2\left(X^2 + Y^2\right)\left(c_0^4\Delta t^4 X^2 Y^2 + 256\right), \tag{30}$$

$$r = -c_0^2\Delta t^2\left(16 + c_0^2\Delta t^2 X^2\right)^2\left(16 + c_0^2\Delta t^2 Y^2\right)^2 \times\left(X^2 + Y^2\right)\left(c_0^4\Delta t^4 X^2 Y^2 + 256\right). \tag{31}$$

It can be shown that the magnitude of $\lambda_{1,2,3}$ is 1, regardless of the time-step size. Hence, the specific SS-FDTD updates are unconditionally stable. An exemplary plot of the eigenvalues on the complex plane is given in Fig. 1 when R = 1, the spatial density is 40 cells per wavelength, and $Q \leq 50$. As expected, all values lie on the circumference of the unit circle.

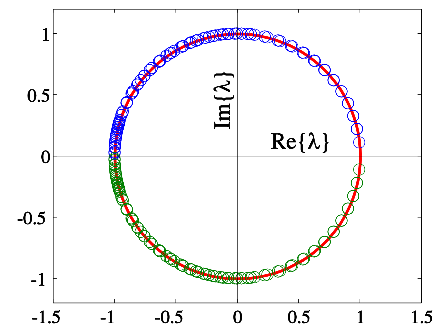

Fig. 1. Eigenvalues of the amplification matrix on the complex plane for various Δt.

Next, the algorithm's accuracy is assessed in terms of the dispersive error affecting the phase velocity, whose value $\tilde{c} = \omega / \tilde{k}$ is extracted from the dispersion relation (10), and the overall error is estimated from:

$$e_{\mathrm{t}} = \frac{1}{2\pi c_0}\int_0^{2\pi}\left|c_0 - \tilde{c}\right| d\theta. \tag{32}$$

The positive impact of the modified operators on the scheme's accuracy is illustrated in Fig. 2, where the SS-FDTD method that applies standard fourth-order approximations is also depicted (time-steps five and ten times larger than Yee's stability limit are considered). The plotted curves reveal a significant error reduction that is not confined within specific frequency bands. In fact, the evidence show that a specific accuracy level can be now accomplished with twice as large a time-step, thanks to the sophisticated design of the algorithm, ensuring better utilization of computational resources.

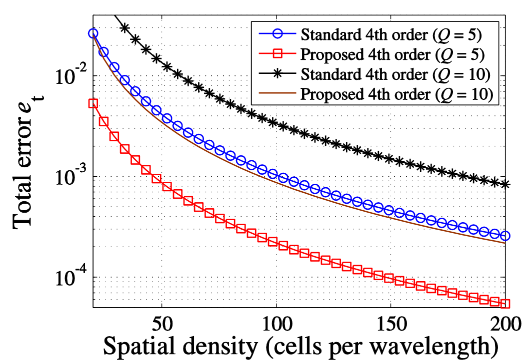

Fig. 2. Error e_{t} versus mesh density for different Δt.

IV. NUMERICAL RESULTS

The performance of the modified SS-FDTD algorithm is evaluated considering an 8 cm × 6 cm cavity, bounded by perfectly conducting walls. First, we perform two sets of simulations, one for the TE_{11} mode at 3.123 GHz and one for the TE_{21} mode at 4.504 GHz. The computational space comprises 200 × 150 cells and tests are conducted for different time-step magnitudes. In essence, the maximum L_2 error of H_z is recorded for a time period equivalent to 2000 iterations when $Q = 2$. The results are displayed in Table 1, where the standard fourth-order operators and the proposed ones are compared. It is verified that significant error cancellation is accomplished regardless of the time-step size. Specifically, accuracy is improved by 3.5 times in the first case, and by 4.2 times in the second case, verifying the potential of the new derivative approximation.

Using the same configuration as previously, the second test pertains to the detection of the structure's first 24 resonant frequencies. Now, an 80 × 60 grid is used, and simulations for 32768 time-steps with $Q = 5$ are performed. Figure 3 displays the absolute errors in the frequencies of the detected modes, and the superior spectral properties of the proposed SS-FDTD method are clearly illustrated. Specifically, the average error of the standard scheme is 55.07 MHz, which is suppressed to only 7.31 MHz by the modified operators.

Table 1: Maximum L_2 errors for different time-step sizes, in the cavity problems with single-mode support

	TE_{11} Mode		TE_{21} Mode	
Q	Standard	Proposed	Standard	Proposed
2	$1.05\cdot10^{-3}$	$2.94\cdot10^{-4}$	$3.11\cdot10^{-3}$	$7.31\cdot10^{-4}$
4	$4.19\cdot10^{-3}$	$1.18\cdot10^{-3}$	$1.24\cdot10^{-2}$	$2.92\cdot10^{-3}$
6	$9.42\cdot10^{-3}$	$2.65\cdot10^{-3}$	$2.80\cdot10^{-2}$	$6.59\cdot10^{-3}$
8	$1.67\cdot10^{-2}$	$4.72\cdot10^{-3}$	$4.95\cdot10^{-2}$	$1.17\cdot10^{-2}$
10	$2.61\cdot10^{-2}$	$7.38\cdot10^{-3}$	$7.71\cdot10^{-2}$	$1.84\cdot10^{-2}$

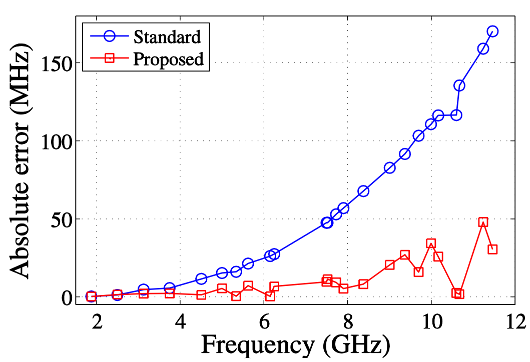

Fig. 3. Absolute error in detecting the resonant frequencies of a rectangular cavity.

V. CONCLUSION

We have successfully remedied the accuracy of an unconditionally stable SS-FDTD method, by deriving modified spatial operators with three-cell stencils. The form of these approximations is determined via a design procedure that balances space-time errors over all frequencies better than standard formulae. The modified scheme outperforms its conventional counterpart, as it guarantees similar error levels with larger time-steps.

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