Reduction of numerical errors in frequency dependent ADI-FDTD

H.K. Rouf, F. Costen and S.G. Garcia

A new method modifying the frequency dependent alternating direction implicit finite difference time domain (FD-ADI-FDTD) is presented. The method can improve the accuracy of FD-ADI-FDTD without significant increase of computational costs. The proposed method is validated by numerical tests.

Introduction: One major breakthrough in finite difference time domain (FDTD) research has been the development of alternating direction implicit (ADI)-FDTD [1], since it removes the bound on the time step of conventional FDTD imposed by the Courant Friedrich Lewy (CFL) stability condition. ADI-FDTD can be seen as a computationally affordable approximation of the Crank-Nicolson (CN)-FDTD scheme [2], found by adding a perturbation term to the latter [3]. This term permits splitting the fully implicit step advancing from n to $n+1$ in CN-FDTD, into two tridiagonally implicit substeps in ADI-FDTD going from n to $n+1/2$ and from $n+1/2$ to $n+1$. ADI-FDTD exhibits a loss of accuracy with respect to CN-FDTD that may become severe for some practical applications [3]. Thus, ADI-FDTD improves computational efficiency at the cost of accuracy. There have been efforts to improve the accuracy of ADI-FDTD. For instance, the approach of [4] is based on an iterative procedure ideally converging to CN-FDTD. An alternative solution is given by [5] employing an average approximation of some of the implicit fields. Although both of these techniques are stable in 2D, their generalisation to 3D seems to become unstable [6, 7].

In this Letter we present an extension of the approach by [5], for the frequency dependent ADI-FDTD (FD-ADI-FDTD) described in [8]. Numerical experiments show that this modified FD-ADI-FDTD scheme is more accurate than normal FD-ADI-FDTD.

Modified frequency dependent ADI-FDTD: Maxwell's 2D equations for TM polarisation are

$$\frac{\partial D_z}{\partial t}=\frac{\partial H_y}{\partial x}-\frac{\partial H_x}{\partial y}-\sigma E_z \tag{1}$$

$$\frac{\partial H_x}{\partial t}=-\frac{1}{\mu}\frac{\partial E_z}{\partial y} \tag{2}$$

$$\frac{\partial H_y}{\partial t}=\frac{1}{\mu}\frac{\partial E_z}{\partial x} \tag{3}$$

where ***E, H, D*** are, respectively, electric field, magnetic field and electric flux density, and μ and σ are the permeability and conductivity of the medium. We model the frequency dependent media by the single-pole Debye relationship $\boldsymbol{D}=\epsilon_0\epsilon_r\,.\,\boldsymbol{E}$ with $\epsilon_r=\epsilon_\infty+(\epsilon_S-\epsilon_\infty)/(1+j\omega\tau_D)$. Here ϵ_r, ϵ_0, ϵ_S, ϵ_∞, τ_D and ω are relative permittivity, free-space permittivity, static permittivity, optical permittivity, relaxation time and angular frequency, respectively. The frequency domain constitutive relationship for this medium can be translated into time domain using an auxiliary differential formulation: $\tau_D\partial D_z/\partial t-\tau_D\epsilon_0\epsilon_\infty\partial E_z/\partial t=\epsilon_0\epsilon_S E_z-D_z$.

Inserting (1) into the constitutive relationship, the time derivative of E_z is obtained:

$$\frac{\partial E_z}{\partial t}=-\left(\frac{\epsilon_S}{\tau_D\epsilon_\infty}+\frac{\sigma}{\epsilon_0\epsilon_\infty}\right)E_z+\frac{1}{\tau_D\epsilon_0\epsilon_\infty}D_z+\frac{1}{\epsilon_0\epsilon_\infty}\frac{\partial H_y}{\partial x}-\frac{1}{\epsilon_0\epsilon_\infty}\frac{\partial H_x}{\partial y} \tag{4}$$

(1), (2), (3), (4) can be written as $\partial U/\partial t=AU+BU$ where

$$A=\begin{pmatrix}0 & \dfrac{1}{\tau_D\epsilon_0\epsilon_\infty} & 0 & \dfrac{1}{\epsilon_0\epsilon_\infty}\dfrac{\partial}{\partial x}\\ 0 & 0 & 0 & \dfrac{\partial}{\partial x}\\ 0 & 0 & 0 & 0\\ \dfrac{1}{\mu}\dfrac{\partial}{\partial x} & 0 & 0 & 0\end{pmatrix} \tag{5}$$

$$B=\begin{pmatrix}-\left(\dfrac{\epsilon_S}{\tau_D\epsilon_\infty}+\dfrac{\sigma}{\epsilon_0\epsilon_\infty}\right) & 0 & -\dfrac{1}{\epsilon_0\epsilon_\infty}\dfrac{\partial}{\partial y} & 0\\ -\sigma & 0 & -\dfrac{\partial}{\partial y} & 0\\ -\dfrac{1}{\mu}\dfrac{\partial}{\partial y} & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix} \tag{6}$$

$$U=\left[E_z\quad D_z\quad H_x\quad H_y\right]^T \tag{7}$$

Now, using finite differences for the time derivative and averaging the fields over time in $\partial U/\partial t=AU+BU$, the CN-FDTD scheme is found

$$\left(I-\frac{\Delta t}{2}A-\frac{\Delta t}{2}B\right)U^{n+1}=\left(I+\frac{\Delta t}{2}A+\frac{\Delta t}{2}B\right)U^n \tag{8}$$

where I is a 4×4 identity matrix. (8) can also be written as

$$\begin{aligned}\left(I-\frac{\Delta t}{2}A\right)\left(I-\frac{\Delta t}{2}B\right)U^{n+1}&=\left(I+\frac{\Delta t}{2}A\right)\\ \times\left(I+\frac{\Delta t}{2}B\right)U^n&+\frac{\Delta t^2}{4}AB(U^{n+1}-U^n)\end{aligned} \tag{9}$$

In ADI-FDTD the last term of (9) is dropped and then solved in two steps, leading to truncation error which is a function of $(\Delta t/2)^2$ times the space derivatives of the field [3]. So the truncation error increases with larger time steps, imposing a restriction on the time step, particularly when accuracy of the problem is crucial for strong-gradient fields. Instead, we follow the strategy of [5] and write (9) in a two-step implicit form, but without dropping any term:

$$\left(I-\frac{\Delta t}{2}A\right)U^{n+1/2}=\left(I+\frac{\Delta t}{2}B\right)U^n+\frac{\Delta t^2}{8}AB(U^{n+1}-U^n) \tag{10}$$

$$\left(I-\frac{\Delta t}{2}B\right)U^{n+1}=\left(I+\frac{\Delta t}{2}A\right)U^{n+1/2}+\frac{\Delta t^2}{8}AB(U^{n+1}-U^n) \tag{11}$$

Now, from the approximations: $U^n=(U^{n+1/2}+U^{n-1/2})/2$ and $U^{n+1/2}=(U^{n+1}+U^n)/2$ [5], we obtain $U^{n+1/2}$ and U^{n+1} by extrapolation and use in (10) and (11), yielding a couple tridiagonally implicit set of equations

$$\left(I-\frac{\Delta t}{2}A\right)U^{n+1/2}=\left(I+\frac{\Delta t}{2}B\right)U^n+\frac{\Delta t^2}{4}AB(U^n-U^{n-1/2}) \tag{12}$$

$$\left(I-\frac{\Delta t}{2}B\right)U^{n+1}=\left(I+\frac{\Delta t}{2}A\right)U^{n+1/2}+\frac{\Delta t^2}{4}AB(U^{n+1/2}-U^n) \tag{13}$$

Replacing (5) and (6) into (12), we find the first substep of equations

$$\begin{aligned}E_z^{n+1/2}-\frac{\Delta t}{2\tau_D\epsilon_0\epsilon_\infty}D_z^{n+1/2}-\frac{\Delta t}{2}\frac{1}{\epsilon_0\epsilon_\infty}\frac{\partial H_y^{n+1/2}}{\partial x}&\\ =\left[1+\frac{\Delta t}{2}\left(\frac{\epsilon_S}{\tau_D\epsilon_\infty}+\frac{\sigma}{\epsilon_0\epsilon_\infty}\right)\right]E_z^n&\\ +\frac{\Delta t}{2}\frac{1}{\epsilon_0\epsilon_\infty}\frac{\partial H_x^n}{\partial y}-\left(\frac{\Delta t}{2}\right)^2\frac{\sigma}{\tau_D\epsilon_0\epsilon_\infty}(E_z^n-E_z^{n-1/2})&\\ -\left(\frac{\Delta t}{2}\right)^2\frac{1}{\tau_D\epsilon_0\epsilon_\infty}\left(\frac{\partial H_x^n}{\partial y}-\frac{\partial H_x^{n-1/2}}{\partial y}\right)&\end{aligned} \tag{14}$$

$$D_z^{n+1/2}-\frac{\Delta t}{2}\frac{\partial H_y^{n+1/2}}{\partial x}=-\frac{\Delta t}{2}\sigma E_z^n+D_z^n+\frac{\Delta t}{2}\frac{\partial H_x^n}{\partial y} \tag{15}$$

$$H_x^{n+1/2}=\frac{\Delta t}{2}\frac{1}{\mu}\frac{\partial E_z^n}{\partial y}+H_x^n \tag{16}$$

$$\begin{aligned}-\frac{\Delta t}{2}\frac{1}{\mu}\frac{\partial E_z^{n+1/2}}{\partial x}+H_y^{n+1/2}=H_y^n-\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}&\\ \times\left(\frac{\epsilon_S}{\tau_D\epsilon_\infty}+\frac{\sigma}{\epsilon_0\epsilon_\infty}\right)\left(\frac{\partial E_z^n}{\partial x}-\frac{\partial E_z^{n-1/2}}{\partial x}\right)&\\ -\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu\epsilon_0\epsilon_\infty}\left(\frac{\partial^2 H_x^n}{\partial x\partial y}-\frac{\partial^2 H_x^{n-1/2}}{\partial x\partial y}\right)&\end{aligned} \tag{17}$$

Substituting $D_z^{n+1/2}$ from (15) into (14), $E_z^{n+1/2}$ is found in terms of $H_y^{n+1/2}$, which is then used in (17) resulting in

$$\begin{aligned}
&H_y^{n+1/2} - \left[\left(\frac{\Delta t}{2}\right)^3 \frac{1}{\mu\tau_{\mathrm{D}}\epsilon_0\epsilon_\infty} + \left(\frac{\Delta t}{2}\right)^2 \frac{1}{\mu\epsilon_0\epsilon_\infty}\right]\frac{\partial^2 H_y^{n+1/2}}{\partial x^2} \\
&= \frac{\partial E_z^n}{\partial x}\left\{\frac{\Delta t}{2}\frac{1}{\mu}\left[1 + \frac{\Delta t}{2}\left(\frac{\epsilon_{\mathrm{S}}}{\tau_{\mathrm{D}}\epsilon_\infty} + \frac{\sigma}{\epsilon_0\epsilon_\infty}\right)\right] - \left(\frac{\Delta t}{2}\right)^2\frac{\sigma}{\mu}\right. \\
&\quad \left. - \left(\frac{\Delta t}{2}\right)^3 \frac{\sigma}{\mu\tau_{\mathrm{D}}\epsilon_0\epsilon_\infty} - \left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\left(\frac{\epsilon_{\mathrm{S}}}{\tau_{\mathrm{D}}\epsilon_\infty} + \frac{\sigma}{\epsilon_0\epsilon_\infty}\right)\right\} \\
&\quad + \frac{\Delta t}{2}\frac{1}{\mu}\frac{\partial D_z^n}{\partial x} + \frac{\partial^2 H_x^n}{\partial x \partial y}\left\{\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu} - \left(\frac{\Delta t}{2}\right)^3\frac{1}{\mu\tau_{\mathrm{D}}\epsilon_0\epsilon_\infty}\right\} \\
&\quad + \frac{\partial E_z^{n-1/2}}{\partial x}\left\{\left(\frac{\Delta t}{2}\right)^3\frac{\sigma}{\mu\tau_{\mathrm{D}}\epsilon_0\epsilon_\infty} + \left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\left(\frac{\epsilon_{\mathrm{S}}}{\tau_{\mathrm{D}}\epsilon_\infty} + \frac{\sigma}{\epsilon_0\epsilon_\infty}\right)\right\} \\
&\quad + \frac{\partial^2 H_x^{n-1/2}}{\partial x\partial y}\left\{\left(\frac{\Delta t}{2}\right)^3\frac{1}{\mu\tau_{\mathrm{D}}\epsilon_0\epsilon_\infty} + \left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu\epsilon_0\epsilon_\infty}\right\} + H_y^n
\end{aligned} \tag{18}$$

Eqn. (18) forms a system of linear equations of $\boldsymbol{Au} = \boldsymbol{c}$ where $\boldsymbol{A}$ is a tridiagonal matrix, $\boldsymbol{u}$ is the unknown field vector $H_y^{n+1/2}$ and $\boldsymbol{c}$ is the excitation vector. The solution of this tridiagonal system of equations provides the values of H_y at half-step. Then using them in (14)–(17), $D_z^{n+1/2}$, $E_z^{n+1/2}$, $H_x^{n+1/2}$ are explicitly found.

Similarly, for the second step, another tridiagonal system of equations is found and solved to get the values of E_z^{n+1}. Then H_x^{n+1}, H_y^{n+1} and D_z^{n+1} are solved explicitly. A close look to these equations shows that the tridiagonal matrices of the modified FD-ADI-FDTD are those of the normal FD-ADI-FDTD [8] except for additional terms which do not increase the computational burden significantly.

Numerical validation: To validate the proposed modified FD-ADI-FDTD scheme, numerical tests were conducted for a 2D computational space of 400×400 cells (in x- and y-directions) consisting of two media and truncated by Mur first-order boundary conditions. Half of the computational space ($x \le 200$) had the parameters $\epsilon_{\mathrm{S}} = 9.5$, $\epsilon_\infty = 4.2$, $\sigma = 0.0$ S/m, $\tau_{\mathrm{D}} = 77.0$ ps and the other half ($x > 200$) had $\epsilon_{\mathrm{S}} = 6.2$, $\epsilon_\infty = 3.5$, $\sigma = 0.0$ S/m, $\tau_{\mathrm{D}} = 39.0$ ps. A line source was applied at (180,200) in the first medium. The excitation waveform was a Gaussian pulse centred at 2.3 GHz. A test point, 40 cells away into the second medium, at (220,200) was taken. A uniform spatial sampling of $\Delta x = \Delta y = \Delta s = 0.3$ mm was used. The time step was variably taken at or above the CFL limit of explicit FDTD: $\Delta t = CFLN \times \Delta s/(c\sqrt{2})$ with *CFLN* referred to as the CFL number and c the free-space light-speed.

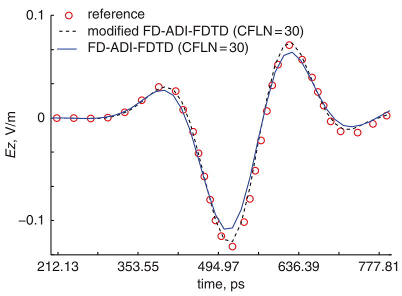

Fig. 1 *Observed signals using FD-ADI-FDTD and modified FD-ADI-FDTD for CFLN = 30*

To quantify the improvement of modified FD-ADI-FDTD, we have defined an average error $\mathcal{E}$ calculated over the whole frequency band of the transient excitation as $\mathcal{E} = \sqrt{\sum_f (\mathcal{S}_{rcd} - \mathcal{S}_{rcd}^{ref})^2 / \sum_f (\mathcal{S}_{rcd}^{ref})^2}$. Here, $\mathcal{S}_{rcd}$ is the amplitude spectrum of the field received at the test point by modified FD-ADI-FDTD and $\mathcal{S}_{rcd}^{ref}$ is that of the reference, here taken as the solution provided by FD-ADI-FDTD [8] for $CFLN = 1$. The average errors for FD-ADI-FDTD and modified FD-ADI-FDTD for three values of $CFLN > 1$ are given in Table 1. Results for the time evolution of E_z at the test point from the two methods are also shown in Fig. 1 for $CFLN = 30$. Noticeable errors are seen when FD-ADI-FDTD is used, while in the case of the modified scheme these are significantly reduced. Splitting errors resulting from the dropped last term of (9) account for these errors, which have been taken care of in the modified FD-ADI-FDTD.

Table 1: Average error of FD-ADI-FDTD and modified FD-ADI-FDTD at different *CFLN*

CFLN	FD−ADI−FDTD	Modified FD−ADI−FDTD
10	0.096932	0.052911
20	0.471145	0.091383
30	0.718453	0.124622

Conclusion: A method capable of reducing errors in FD-ADI-FDTD is shown and numerically verified. Like FD-ADI-FDTD, the scheme still requires to solve only a tridiagonal system, but can reduce the perturbations introduced in CN-FDTD to formulate ADI-FDTD.

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One or more of the Figures in this Letter are available in colour online.

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