The Unconditionally Stable Pseudospectral Time-Domain (PSTD) Method

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***Abstract*—This letter presents a new time-domain method for Maxwell's equations, in which the unconditionally stable techniques, the alternating direction implicit (ADI) and the split-step (SS) schemes, are developed for the pseudospectral time-domain (PSTD) algorithm to maintain stability while achieving higher accuracy and efficiency over the FDTD method. The multidomain strategy is employed to allow for a flexible treatment of internal inhomogeneities. Numerical results demonstrate the unconditional stability and the second-order accuracy for both ADI- and SS-PSTD algorithms.**

***Index Terms*—Alternating direction implicit (ADI) technique, FDTD, PSTD, split-step scheme.**

I. INTRODUCTION

IT IS WELL KNOWN that the traditional FDTD method is subject to the CFL stability condition due to the use of an explicit central-difference scheme. This condition becomes particularly restrictive in most RF circuit applications where the electrical length of the target geometry is much smaller than the wavelength. To overcome this restriction, the Alternating Direction Implicit (ADI) [1], [2] and Split-Step (SS) [3] FDTD methods have been proposed, and the unconditional stability has been demonstrated both theoretically and numerically.

Meanwhile, extensive research activities have been devoted to the improvement of efficiency and accuracy of the FDTD method. Among such efforts, the Pseudospectral Time-Domain (PSTD) method, with its low sampling density and higher order accuracy [4], [5], has been demonstrated to greatly outperform the FDTD method. With a multidomain scheme that divides the whole computational domain into a series of subdomains naturally conformal to the problem geometry, the Chebyshev PSTD method can deal with curved objects and strongly inhomogeneous media with a great flexibility. Nevertheless, it also suffers from the CFL stability condition because of the explicit time-integration scheme. This limits the PSTD method from further applications to RF circuit problems.

In this work, based on the concepts of ADI- and SS-FDTD methods as well as our previously developed 3-D PSTD methods [4], [6], we derive the unconditionally stable PSTD algorithm for single and multiple domains. We demonstrate that the implicit time-integration scheme can be applied to the PSTD method and make it free of the CFL stability condition.

Manuscript received February 20, 2003; revised July 13, 2003. This work was supported by the National Science Foundation through Grants CCR-00-98140 and IIS-0086075. The review of this letter was arranged by Associate Editor Dr. Arvind Sharma.

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Digital Object Identifier 10.1109/LMWC.2003.819372

II. THEORY

According to Lee and Fornberg [7], the ADI- and SS-FDTD methods can be generalized into a single mathematical form. The 3-D Maxwell's equations are written as

$$\frac{\partial}{\partial t}\begin{bmatrix} H_x \\ H_y \\ H_z \\ E_x \\ E_y \\ Ez \end{bmatrix} = \begin{bmatrix} \frac{1}{\mu}\frac{\partial E_y}{\partial z} \\ \frac{1}{\mu}\frac{\partial E_z}{\partial x} \\ \frac{1}{\mu}\frac{\partial E_x}{\partial y} \\ \frac{1}{\epsilon}\frac{\partial H_z}{\partial y} \\ \frac{1}{\epsilon}\frac{\partial H_x}{\partial z} \\ \frac{1}{\epsilon}\frac{\partial H_y}{\partial x} \end{bmatrix} + \begin{bmatrix} -\frac{1}{\mu}\frac{\partial E_z}{\partial y} \\ -\frac{1}{\mu}\frac{\partial E_x}{\partial z} \\ -\frac{1}{\mu}\frac{\partial E_y}{\partial x} \\ -\frac{1}{\epsilon}\frac{\partial H_y}{\partial z} \\ -\frac{1}{\epsilon}\frac{\partial H_z}{\partial x} \\ -\frac{1}{\epsilon}\frac{\partial H_x}{\partial y} \end{bmatrix} \tag{1}$$

or more compactly

$$\frac{\partial \mathbf{u}}{\partial t} = A\mathbf{u} + B\mathbf{u}. \tag{2}$$

Using the standard Crank-Nicolson approximation, (2) can be solved as

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}(Au^{n+1} + Au^n) + \frac{1}{2}(Bu^{n+1} + Bu^n) + O(\Delta t^2). \tag{3}$$

Following Lee and Fornberg [7], this can be reduced to

$$\left(1 - \frac{\Delta t}{2}A\right)\left(1 - \frac{\Delta t}{2}B\right)u^{n+1} = \left(1 + \frac{\Delta t}{2}A\right)\left(1 + \frac{\Delta t}{2}B\right)u^n + O(\Delta t^3). \tag{4}$$

A. Alternating-Direction Implicit (ADI) Method

Equation (4) suggests that Maxwell's equations in (2) can be solved by two separate stages. For example [7]

$$\begin{aligned} &1. \quad \left(1 - \frac{\Delta t}{2}A\right)u^{n+\frac{1}{2}} = \left(1 + \frac{\Delta t}{2}B\right)u^n; \\ &2. \quad \left(1 - \frac{\Delta t}{2}B\right)u^{n+1} = \left(1 + \frac{\Delta t}{2}A\right)u^{n+\frac{1}{2}} \end{aligned} \tag{5}$$

or equivalently

$$\begin{aligned} \frac{u^{n+\frac{1}{2}} - u^n}{\Delta t/2} &= Au^{n+\frac{1}{2}} + Bu^n \\ \frac{u^{n+1} - u^{n+\frac{1}{2}}}{\Delta t/2} &= Au^{n+\frac{1}{2}} + Bu^{n+1}. \end{aligned} \tag{6}$$

Using central differencing to evaluate the spatial derivatives, one finds that (6) is exactly equivalent to the ADI-FDTD scheme [2].

Another important property of the ADI-FDTD method is that it maintains the second-order accuracy as demonstrated in (4). To verify this, one can multiply the first equation of (5) by $(1+(\Delta t/2)A)$ and the second one by $(1-(\Delta t/2)A)$, and then (4) can be derived.

B. Split-Step (SS) Method

Equation (4) can also be split into two stages

$$\begin{aligned} &1.\quad \left(1-\frac{\Delta t}{2}A\right)u^{n+\frac{1}{2}} = \left(1+\frac{\Delta t}{2}A\right)u^{n};\\ &2.\quad \left(1-\frac{\Delta t}{2}B\right)u^{n+1} = \left(1+\frac{\Delta t}{2}B\right)u^{n+\frac{1}{2}} \end{aligned} \tag{7}$$

which becomes the first-order split-step method [3], [7]. The advantage of this scheme is that the original (2) can be divided into two independent subproblems: $(\partial \mathbf{u}/\partial t) = 2A\mathbf{u}$ and $(\partial \mathbf{u}/\partial t) = 2B\mathbf{u}$. The first-order SS scheme solves one subproblem at each half step.

If one multiplies the first equation of (7) by $(1+(\Delta t/2)B)$ and the second one by $(1-(\Delta t/2)A)$, the resulting equation is

$$\begin{aligned} &\left(1-\frac{\Delta t}{2}A\right)\left(1-\frac{\Delta t}{2}B\right)u^{n+1}\\ &\quad=\left(1+\frac{\Delta t}{2}A\right)\left(1+\frac{\Delta t}{2}B\right)u^{n}\\ &\qquad+\frac{\Delta t^2}{4}(BA-AB)(u^n+u^{n+\frac{1}{2}})+O(\Delta t)^3. \end{aligned}$$

Therefore, only in case that $AB = BA$, the SS1 scheme in (7) can achieve the second-order accuracy. In general, it is a first-order time-stepping strategy. Higher order accuracy can be achieved by repeatedly advancing $(\partial \mathbf{u}/\partial t) = 2A\mathbf{u}$ and $(\partial \mathbf{u}/\partial t) = 2B\mathbf{u}$ by more time divisions within a single step. For example, the second-order SS method splits one step Δt into three stages with time increments $\{\Delta t/4, \Delta t/2, \Delta t/4\}$.

Note that due to the inherent symmetry of Maxwell's equations in (1), each subproblem $(\partial \mathbf{u}/\partial t) = 2A\mathbf{u}$ and $(\partial \mathbf{u}/\partial t) = 2B\mathbf{u}$ can be further written into three pairs of mutually uncoupled 1-D equations

$$\left\{\begin{array}{l}\left\{\begin{array}{l}\frac{\partial E_x}{\partial t}=\frac{2}{\epsilon}\frac{\partial H_z}{\partial y}\\ \frac{\partial H_z}{\partial t}=\frac{2}{\mu}\frac{\partial E_x}{\partial y}\end{array}\right\}\\ \left\{\begin{array}{l}\frac{\partial E_y}{\partial t}=\frac{2}{\epsilon}\frac{\partial H_x}{\partial z}\\ \frac{\partial H_x}{\partial t}=\frac{2}{\mu}\frac{\partial E_y}{\partial z}\end{array}\right\}\\ \left\{\begin{array}{l}\frac{\partial E_z}{\partial t}=\frac{2}{\epsilon}\frac{\partial H_y}{\partial x}\\ \frac{\partial H_y}{\partial t}=\frac{2}{\mu}\frac{\partial E_z}{\partial x}\end{array}\right\}\end{array}\right\},\ \left\{\begin{array}{l}\left\{\begin{array}{l}\frac{\partial E_x}{\partial t}=-\frac{2}{\epsilon}\frac{\partial H_y}{\partial z}\\ \frac{\partial H_y}{\partial t}=-\frac{2}{\mu}\frac{\partial E_x}{\partial z}\end{array}\right\}\\ \left\{\begin{array}{l}\frac{\partial E_y}{\partial t}=-\frac{2}{\epsilon}\frac{\partial H_z}{\partial x}\\ \frac{\partial H_z}{\partial t}=-\frac{2}{\mu}\frac{\partial E_y}{\partial x}\end{array}\right\}\\ \left\{\begin{array}{l}\frac{\partial E_z}{\partial t}=-\frac{2}{\epsilon}\frac{\partial H_x}{\partial y}\\ \frac{\partial H_x}{\partial t}=-\frac{2}{\mu}\frac{\partial E_z}{\partial y}\end{array}\right\}\end{array}\right\}. \tag{8}$$

Equation (8) demonstrates that the 3-D electromagnetic problem can be greatly simplified by solving three pairs of 1-D equations at each stage [3].

C. CFL-Free Pseudospectral Time-Domain Method

Since the split-step method splits the 3-D equation (1) into three pairs of 1-D equations at each stage, the development of SS-PSTD algorithm only needs to focus on the evaluation of spatial derivatives for one single direction, for example, the x coordinate. Then, the same algorithm can be applied to the other two directions to solve the true 3-D problem.

For PSTD methods [4], [6] the approximation of spatial derivatives can be generalized as

$$\frac{\partial f(x)}{\partial x}|_{x=x_i} = \sum_{j=1}^{N} D(i,j)f(x_j) \quad i=1,2,\ldots,N \tag{9}$$

or in a matrix form

$$\frac{\partial \mathbf{f}}{\partial x} = D\mathbf{f} \tag{10}$$

where the matrix D is of size $N\times N$, and N is the number of sampling cells in the x direction. The D matrix is determined by the distribution of sampling points. The Fourier PSTD method uses uniformly distributed sampling cells; while the Chebyshev PSTD algorithm is based on the Chebyshev-Gauss-Lobatto collocation points.

1) Implicit Time-Integration Scheme: A pair of 1-D equations $\{(\partial E_z/\partial t) = (1/\epsilon)(\partial H_y/\partial x); (\partial H_y/\partial t) = (1/\mu)(\partial E_z/\partial x)\}$ can be normalized as $\{(\partial E_z/\partial t) = v(\partial H_y/\partial x); (\partial H_y/\partial t) = v(\partial E_z/\partial x)\}$, where v is the wave speed and H is normalized by multiplying with $\sqrt{\mu/\epsilon}$. Thus, the implicit scheme can be applied to this 1-D equation for one half step

$$\begin{aligned} &\frac{\mathbf{E_z}^{n+\frac{1}{2}}-\mathbf{E_z}^{n}}{\Delta t/2} = \frac{vD}{2}\left(\mathbf{H_y}^{n+\frac{1}{2}}+\mathbf{H_y}^{n}\right)\\ &\frac{\mathbf{H_y}^{n+\frac{1}{2}}-\mathbf{H_y}^{n}}{\Delta t/2} = \frac{vD}{2}\left(\mathbf{E_z}^{n+\frac{1}{2}}+\mathbf{E_z}^{n}\right)\\ &\Rightarrow \begin{bmatrix} I_N & -\frac{v\Delta t}{4}D\\ -\frac{v\Delta t}{4}D & I_N\end{bmatrix}\begin{bmatrix}\mathbf{H_y}^{n+\frac{1}{2}}\\ \mathbf{E_z}^{n+\frac{1}{2}}\end{bmatrix}\\ &= \begin{bmatrix} I_N & \frac{v\Delta t}{4}D\\ \frac{v\Delta t}{4}D & I_N\end{bmatrix}\begin{bmatrix}\mathbf{H_y}^{n}\\ \mathbf{E_z}^{n}\end{bmatrix}. \end{aligned} \tag{11}$$

For the ADI method, although it involves both operators A and B at each stage, only one matrix operates at the current step and the other operates at the previous step (5). For example, at the first half step, the ADI scheme solves for

$$\frac{u^{n+\frac{1}{2}}-u^n}{\Delta t/2} = Au^{n+\frac{1}{2}}+Bu^n.$$

Obviously, one can evaluate Bu^n first, and then the rest can still be divided into three pairs of 1-D equations like (8). Therefore, a similar implicit strategy as (11) can be applied to solving each pair of 1-D equations independently with a pseudospectral method.

2) Multidomain ADI- and SS-PSTD Method: For the multidomain scheme, a special step called subdomain patching is needed to exchange information between the individual subdomains to match the boundary conditions at their interfaces. In the previous work [6], this step is achieved explicitly by forcing the tangential field components to be continuous after the time-integration, which may result in a degradation of accuracy. In this work, we introduce an implicit subdomain-patching technique proposed by Liu [8], which implements the boundary conditions as part of the system matrix, and thereby maintains the unconditional stability as well as the high accuracy of pseudospectral method.

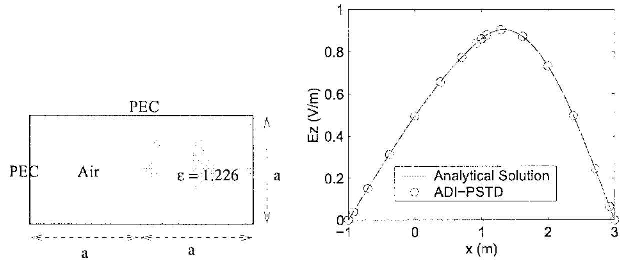

Fig. 1. Two-region problem with inhomogeneous medium, and field distribution at $y = 0$ ($a = 2$ m, $\lambda_1 = 3.798$ m, $\lambda_2 = 3.43$ m).

Consider two adjacent 1-D regions subject to their individual system equations:

$$P_{(1)}\mathbf{v}_{(1)}^{n+\frac{1}{2}} = Q_{(1)}\mathbf{v}_{(1)}^{n}; \quad P_{(2)}\mathbf{v}_{(2)}^{n+\frac{1}{2}} = Q_{(2)}\mathbf{v}_{(2)}^{n}$$

where P and Q are $2N \times 2N$ matrices given in (11), $\mathbf{v} = [\mathbf{H_y}, \mathbf{E_z}]^T$ and the subscripts denote the corresponding subdomains. If one combines the two systems as a whole

$$Ca = b$$

where

$$C = \begin{bmatrix} P_{(1)} & 0 \\ 0 & P_{(2)} \end{bmatrix}, \quad a = \begin{bmatrix} \mathbf{v}_{(1)}^{n+((1/2))} \\ \mathbf{v}_{(2)}^{n+((1/2))} \end{bmatrix} \quad \text{and}$$

$$b = \begin{bmatrix} Q_{(1)}\mathbf{v}_{(1)}^{n} \\ Q_{(2)}\mathbf{v}_{(2)}^{n} \end{bmatrix}$$

the boundary condition can be implemented through the modification of the matrix C and vector b.

For example, if $b(2N)$ and $b(3N+1)$ are the tangential electrical field components at the interface belonging to region 1 and 2, respectively, we can modify the $2N$th row of C as follows:

$$C(2N, i) = \begin{cases} 1, & i = 2N; \\ -1, & i = 3N + 1; \\ 0, & \text{otherwise.} \end{cases}$$

On the right hand side, correspondingly, $b(2N)$ is set to be zero. Obviously, this represents the boundary condition that the tangential components of electrical fields are continuous. The same strategy is also applicable to field components at the PEC or PMC interfaces.

III. Numerical Results

Our first example presents a 2-D TM$_z$ problem with two square regions with $a = 2$ m bounded with perfect conductors and filled with air and a medium with $\epsilon_r = 1.226$, as shown in Fig. 1. The coordinate system is set as x from -1 to 3 m, and y from -1 to 1 m. The multidomain ADI-PSTD method is implemented to calculate the distribution of fields and the results are compared to the analytical solutions as shown in Fig. 1. Fig. 2 demonstrates the simulation error as a function of the size of time step, and clearly indicates that the ADI-PSTD algorithm is CFL-free and of the second-order accuracy.

In addition, we have implemented the 3-D SS-PSTD algorithm for a single computational domain. Fig. 3 plots the simulation error of the 3-D first-order SS-PSTD algorithm for a periodical cube structure with size length of π m. It is worth noting that the second-order accuracy is observed for the first-order SS-PSTD scheme because the system matrices A and B are commutable.

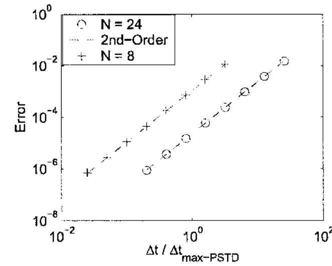

Fig. 2. Second-order accuracy of the 2-D multidomain ADI-PSTD method for ($N = 24$) and ($N = 8$), where $\Delta t_{\max-\mathrm{PSTD}}$ is the maximal allowed time step of the explicit scheme.

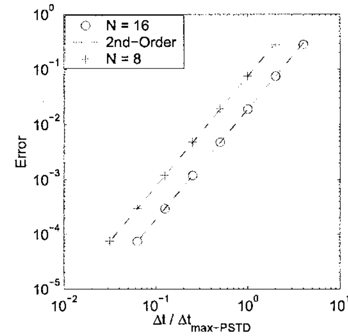

Fig. 3. Accuracy of the 3-D SS-PSTD algorithm for a periodic cube structure ($a = \pi$ m, $\lambda = 1.814$ m) with $N = 16$ and $N = 8$ cells in each direction.

IV. Conclusion

In this work, the multidomain Alternating Direction Implicit and Split-Step PSTD algorithms are proposed and developed for inhomogeneous media and perfect conductors. The unconditional stability of the algorithms has been numerically demonstrated. The simulation results are validated by analytical solutions, and confirm the second-order accuracy in time integration.

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