

An Implicit LU/AF FDTD Method

John H. Beggs* and W. Roger Briley

NASA/Langley Research Center
Electromagnetics Research Branch
Mail Stop 490
Hampton, VA 23681

I. INTRODUCTION

There has been some recent work to develop two and three-dimensional alternating direction implicit (ADI) FDTD schemes [1]–[4]. These ADI schemes are based upon the original ADI concept developed by Peaceman and Rachford [5] and Douglas and Gunn [6], which is a popular solution method in Computational Fluid Dynamics (CFD). These ADI schemes work well and they require solution of a tridiagonal system of equations. A new approach proposed in this paper applies a LU/AF approximate factorization technique from CFD to Maxwell's equations in flux conservative form for one space dimension. The result is a scheme that will retain its unconditional stability in three space dimensions, but does not require the solution of tridiagonal systems. The theory for this new algorithm is outlined in a one-dimensional context for clarity. An extension to two and three-dimensional cases is discussed in [7]. Results of Fourier analysis are discussed for both stability and dispersion/damping properties of the algorithm. Results are presented for a one-dimensional model problem, and the explicit FDTD algorithm is chosen as a convenient reference for comparison.

II. ONE-DIMENSIONAL LU/AF ALGORITHM

To develop the one-dimensional LU/AF algorithm, Maxwell's equations for the one-dimensional TE mode are written in flux conservative form to include the electric and magnetic conduction currents as

$$\frac{\partial \bar{q}}{\partial t} + \frac{\partial \bar{f}}{\partial x} = -\bar{P} \bar{q} \quad (1)$$

where \bar{P} is given by

$$\bar{P} = \begin{bmatrix} \sigma/\epsilon & 0 \\ 0 & \sigma^*/\mu \end{bmatrix} \quad (2)$$

and $\bar{q} = [E_y, H_z]^T$, $\bar{f} = [H_z/\epsilon, E_y/\mu]^T$ and T denotes transpose. To develop the upwind LU/AF algorithm, the flux conservative form of Maxwell's equations in (1) is recast in the following form

$$\frac{\partial \bar{q}}{\partial t} + \bar{A} \frac{\partial \bar{q}}{\partial x} = -\bar{P} \bar{q} \quad (3)$$

where \bar{A} is the Jacobian of $\bar{f} = \bar{A} \bar{q}$ and is given by

$$\bar{A} = \frac{\partial \bar{f}}{\partial \bar{q}} = \begin{bmatrix} 0 & 1/\epsilon \\ 1/\mu & 0 \end{bmatrix} \quad (4)$$

The matrix \bar{A} has eigenvalues $\lambda_{1,2} = \pm 1/\sqrt{\mu\epsilon}$ corresponding to right and left propagating waves with speeds $\pm c$. The eigenvalue matrix is given by

$$\bar{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \quad (5)$$

The matrix \bar{A} can be obtained from the eigenvalue matrix via a similarity transformation given by $\bar{A} = \bar{S} \bar{\Lambda} \bar{S}^{-1}$ where the matrix \bar{S} is composed of the eigenvectors of \bar{A} . The eigenvalue matrix

$\bar{\Lambda}$ can be split into two parts, one each for the right and left propagating waves and is given by $\bar{\Lambda} = \bar{\Lambda}^+ + \bar{\Lambda}^-$. Using this relation, we can split \bar{A} into two parts as $\bar{A}^\pm = \bar{S}\bar{\Lambda}^\pm\bar{S}^{-1}$. The flux vector \bar{f} is then split into two parts given by $\bar{f} = \bar{f}^+ + \bar{f}^-$ and the relation $\bar{f}^\pm = \bar{A}^\pm\bar{q}$. For more details on this development, see reference [7]. This flux-vector-splitting method is similar to that developed by Steger and Warming [8] for the Euler equations governing inviscid fluid flow. To construct the LU/AF algorithm, time and space are discretized to $t^n = n\Delta t$, $x_i = i\Delta x$ and the time derivative in (3) is approximated by a β -weighted, $O(\Delta t^2)$ difference equation given by

$$\frac{\partial \bar{q}}{\partial t} \approx \frac{(2\beta + 1)q_i^{n+1} - 4\beta q_i^n + (2\beta - 1)q_i^{n-1}}{2\Delta t} \quad (6)$$

The spatial derivative is again replaced by a β -weighted average between time level $n + 1$ and n . This can be rewritten using the operator notation as

$$\frac{\partial \bar{f}}{\partial x} \approx \beta (\Delta_{2i}^- \bar{f}_i^+ + \Delta_{2i}^+ \bar{f}_i^-)^{n+1} + (1 - \beta) (\Delta_{2i}^- \bar{f}_i^+ + \Delta_{2i}^+ \bar{f}_i^-)^n \quad (7)$$

The Δ_{2i}^\pm operators are now $O(\Delta x^2)$ difference operators to be defined shortly. The parameter β can be used to construct a series of explicit and implicit schemes. For example, if $\beta = 0$, this results in a leapfrog scheme; $\beta = 0.5$ results in a Crank-Nicolson scheme and $\beta = 1$ results in an Euler implicit scheme. Using (6) and (7), the finite-difference equation for (3) is

$$\begin{aligned} & \frac{(2\beta + 1)\Delta q_i^n - (2\beta - 1)\Delta q_i^{n-1}}{2\Delta t} + \beta (\Delta_{2i}^- \bar{f}_i^+ + \Delta_{2i}^+ \bar{f}_i^-)^{n+1} + \\ & (1 - \beta) (\Delta_{2i}^- \bar{f}_i^+ + \Delta_{2i}^+ \bar{f}_i^-)^n = -\beta \bar{P} \bar{q}_i^{n+1} - (1 - \beta) \bar{P} \bar{q}_i^n \end{aligned} \quad (8)$$

This can be rearranged as

$$[\bar{I}/(2\Delta t) + \beta\alpha\bar{P} + \beta\alpha(\Delta_{2i}^- A^+(\cdot) + \Delta_{2i}^+ A^-(\cdot))] \Delta \bar{q}_i^n = -\bar{R}_{2i}^n \quad (9)$$

where $\Delta \bar{q}_i^n \equiv \bar{q}_i^{n+1} - \bar{q}_i^n$. The residual, \bar{R}_{2i}^n , is defined by

$$\bar{R}_{2i}^n = \alpha \left\{ \bar{P} \bar{q}_i^n + \Delta_{2i}^- \bar{A}^+ \bar{q}_i^n + \Delta_{2i}^+ \bar{A}^- \bar{q}_i^n - \frac{2\beta - 1}{2\Delta t} \Delta \bar{q}_i^{n-1} \right\} \quad (10)$$

with $\alpha \equiv 1/(2\beta + 1)$. The difference operators in the residual are replaced by $O(\Delta x^2)$ backward and forward upwind difference operators on three-point one-sided stencils defined by $\Delta_{2i}^-(\cdot) \equiv (3(\cdot)_i - 4(\cdot)_{i-1} + (\cdot)_{i-2})/(2\Delta x)$ and $\Delta_{2i}^+(\cdot) \equiv (-3(\cdot)_i + 4(\cdot)_{i+1} - (\cdot)_{i+2})/(2\Delta x)$. Equation (9) is an $O(\Delta t^2, \Delta x^2)$, unfactored, upwind scheme for electromagnetics. The LU/AF scheme is defined by factoring the left side of (9) into two operators, each designed for a forward and backward grid sweep as in the first order implementation. The LU/AF scheme is then given by

$$[\bar{I}/(2\Delta t) + \beta\alpha\bar{P} + \beta\alpha\Delta_{2i}^- \bar{A}^+(\cdot)] \Delta \bar{q}_i^* = -\bar{R}_{2i}^n \quad (11)$$

$$[\bar{I}/(2\Delta t) + \beta\alpha\bar{P} + \beta\alpha\Delta_{2i}^+ \bar{A}^-(\cdot)] \Delta \bar{q}_i^n = [\bar{I}/(2\Delta t) + \beta\alpha\bar{P}] \Delta \bar{q}_i^* \quad (12)$$

III. FOURIER ANALYSIS

A Fourier analysis shows that both the first and second-order upwind LU/AF algorithms are unconditionally stable for $\beta \geq 1/2$, and that they contain both numerical dissipation (or damping) and dispersion. The dissipation is present due to even order spatial derivatives in the truncation error which are a result of the upwind approximation. The complete Fourier analysis for dispersion and damping errors showed that the LU/AF algorithm has larger dispersion errors than the explicit FDTD method for $\nu \leq 1$. This is not particularly troublesome, because for $\nu \leq 1$, explicit schemes are generally more efficient and are preferred. However, for $\nu > 1$, explicit schemes cannot be used and the LU/AF algorithm has its lowest dispersion error around $\nu = 2$. The results also showed that the lowest numerical dispersion is obtained when $\beta = 1/2$. The dispersive errors also increased with β and ν . Since the LU/AF method uses windward differencing, numerical dissipation (or damping) is present in the solution. The dissipation is very small using a second-order LU/AF algorithm, and it decreases as the grid resolution is increased or as ν is increased.

IV. BOUNDARY CONDITIONS

A. Outer Radiation Boundary Condition

The characteristic based LU/AF method requires no extraneous boundary condition such as the Liao absorbing boundary condition [9] or the PML [10]. The only additional information required is information about waves that are *entering* the domain. Waves exiting the domain are naturally handled by the interior point algorithm. Therefore, the characteristic boundary conditions are implemented as follows: at grid point $i = 0$, equation (12) is used along with a specification of the incoming, right-going flux, f_0^+ . At grid point $i = imax$, equation (11) is used along with a specification of the incoming, left-going flux, f_{imax}^- . The only additional information introduced at the boundary is nothing more than what is required by the physical system. In multidimensional problems, the local coordinates at the outer boundaries are rotated to align with the direction of wave propagation defined by $\vec{E} \times \vec{H}$. The characteristic equations are developed along this direction and are appropriately applied at the boundaries. This procedure was discussed and outlined by Shang [11].

B. Dielectric Surface Boundary Condition

Since the LU/AF scheme follows the direction of information propagation (i.e. the *characteristic*), at a material interface, the slope of the characteristic curve (i.e. the speed of light in the material) changes. Therefore, for the LU/AF method to be widely applicable, a careful treatment of material interfaces is required. With a material boundary in place, the right-going and left-going characteristics see a change in characteristic speeds, and therefore, a material interface condition needs to be implemented to correctly model the physics. This feature was recently developed and is outlined in [12].

V. RESULTS

The second-order LU/AF algorithm was tested by implementing equations (11) and (12) for interior grid points away from absorbing boundaries and a first-order scheme at grid points next to the absorbing boundaries. Characteristic-based boundary conditions were used to terminate the computational domain and the incoming flux (f_{imax}^-) at the right boundary was set to zero. The code was initialized by writing a time snapshot of a propagating pulse in the grid. A standard Gaussian pulse of the form $E_{yi} = e^{-\left(\frac{t-t_0}{\tau}\right)^2}$ was used as an excitation source. The main parameters of interest are the time resolution (i.e. number of time steps/period) and the grid resolution (i.e. number of cells/wavelength) of the highest frequency of interest in any given problem. These parameters will be designated as N_t and N_x , respectively. The highest frequency of interest, f_{max} , is calculated based upon N_x and the largest cell size, and the time step for the implicit scheme is calculated based upon f_{max} and the desired time resolution, N_t . For the FDTD method, the time step was calculated based upon the Courant stability condition using the smallest grid size.

To illustrate the use of the LU/AF scheme for EM problems, propagation on a uniform mesh and reflection from a lossy dielectric half-space were considered. The dielectric interface scheme discussed in Section IV-B was implemented and the results are compared with the explicit FDTD method. To solve the reflection problem, the problem space is a uniform grid with 2000 cells, a cell size of 1 cm, and it is filled with a lossy dielectric material from cell numbers 751-2000. The time step is 33.3 ps and $\nu = 1$. The total electric field is recorded versus time at cell number 750. The incident field is obtained by running the code with free space only and recording the field versus time at the same location. The incident field is subtracted from the total field to give the scattered field. A point source located at the left boundary of the

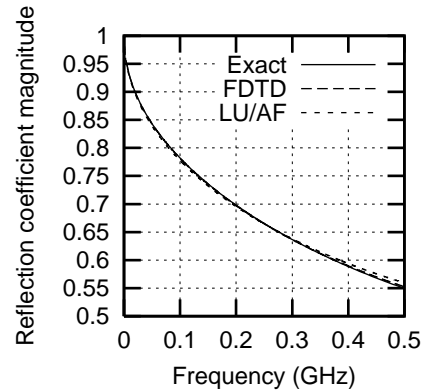


Fig. 1. Reflection coefficient magnitude versus frequency for scattering from a lossy dielectric half-space on a uniform mesh with $\beta = 1/2$ and $\nu = 1$.

grid was used as the excitation source and the dielectric half-space material parameters are $\epsilon = 4\epsilon_0$, $\mu = \mu_0$ and $\sigma = 0.2$ S/m. Figure 1 shows the reflection coefficient results and the agreement is excellent.

For the propagation problem, the pulse was allowed to propagate for approximately 50 meters and periodic boundary conditions were used along with $\nu = 2$. Figure 2 shows the error in electric field for LU/AF method. We see that the results are accurate to within about 1%.

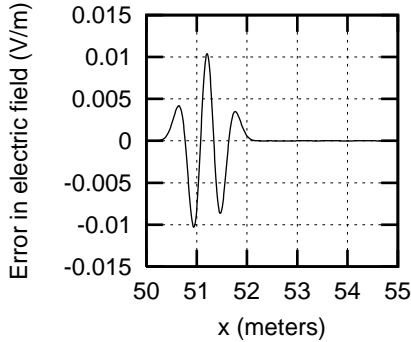


Fig. 2. Error in electric field versus distance for free space propagation on a uniform mesh with $\beta = 1/2$ and $\nu = 2$.

From additional tests, it was determined that the LU/AF method produces less accurate results for moderate conductivity values. This is due to the factorization error terms. As σ is increased, the factorization errors become larger. In principle, this factorization error can be reduced through iterative error reduction [7]. For perfect conductors, we simply set $\bar{q} = 0$.

VI. CONCLUSIONS

This paper has introduced an implicit LU/AF FDTD method for computational electromagnetics. A second-order accurate, LU/AF, characteristic based algorithm for electromagnetics has been implemented and tested on one-dimensional model problems for uniform and nonuniform grids. The one-dimensional model problem results show that accurate solutions for wave propagation can be obtained using Courant number greater than one and the method works well with lossy dielectric materials. The present results demonstrate potential advantages in a one dimensional context, and this approach appears promising for development of stable, accurate and efficient implicit LU/AF schemes for complex two and three dimensional applications. Extensions to two and three-dimensional applications have been outlined [14], but details of this work will be the subject of future reports and articles.

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