3D Crank-Nicolson finite difference time domain method for dispersive media

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

The unconditionally stable Crank-Nicolson finite difference time domain (CN-FDTD) method is extended to incorporate frequency-dependent media in three dimensions. A Gaussian-elimination-based direct sparse solver is used to deal with the large sparse matrix system arising from the formulation. Numerical results validate and confirm that the scheme is unconditionally stable for time steps over the Courant-Friedrich-Lewy limit of classical FDTD.

Introduction: Finite difference time domain (FDTD) methods produce a time domain analysis in various kinds of media using a minimal set of assumptions compared to other techniques. They are said to be the most straightforward, robust and widely applicable electromagnetic modelling techniques. Many current and emerging technological applications involve electromagnetic wave interactions with materials having frequency-dispersive dielectric properties [1] necessitating modification of the classical Yee-FDTD scheme [2]. Frequency dependency has been incorporated in FDTD using several approaches: the auxiliary differential equation method, the z-transform method and the discrete convolution method.

The main drawback of the conventional FDTD method is the reduced computational efficiency resulting from the upper limit on the time step that needs to satisfy the Courant-Friedrich-Lewy (CFL) stability condition [1]. An alternative to the explicit FDTD is provided by the Crank-Nicolson FDTD (CN-FDTD) method [3], which presents unconditional stability beyond the CFL limit. Both methods share the discretisation of time and space derivatives by second-order centred differences, with the only difference being that the fields affected by the curl operator are averaged in time by the CN-FDTD method, whereas in Yee-FDTD they are not. The resulting scheme is a fully implicit marching-on-in-time algorithm with the same potential of the classical FDTD. However, despite its accuracy and low anisotropy [4] it has not been widely used in time domain electromagnetics as it involves the inversion of huge sparse matrices. Instead, there have been many works attempting to simplify or approximate its implementation. To some extent such approximations suffer numerical errors, which may become severe for some practical applications [5]. With the massive advancement of the technology of memory and computational resources, handling huge sparse matrices is no longer a bottleneck. This, together with the extensive research carried out during the last two decades, that resulted in highly sophisticated, robust, efficient and economical sparse solvers, makes CN-FDTD a promising affordable alternative to the classical FDTD.

In this Letter we propose a new three-dimensional frequency dependent CN-FDTD method (FD-CN-FDTD). We incorporate the frequency dependence of single-pole Debye materials into CN-FDTD by means of an auxiliary differential formulation [6]. The scheme results in a sparse system of linear equations involving the three components of the electric field. A sparse direct algorithm is used next to perform the coefficient matrix decomposition, finally leading to an marching-on-in-time unconditionally stable advancing algorithm. The scheme is validated by simple numerical experiments.

Fundamentals of FD-CN-FDTD: Maxwell's curl equations in material independent form are:

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \tag{1}$$

$$\nabla \times \boldsymbol{H} = -\frac{\partial \boldsymbol{D}}{\partial t} \tag{2}$$

where $\boldsymbol{E}$, $\boldsymbol{H}$, $\boldsymbol{D}$ and $\boldsymbol{B}$ are electric field, magnetic field, electric flux density and magnetic flux density, respectively. The constitutive relationships for isotropic, linear, non-magnetic, single-pole Debye electrically-dispersive media, are in the frequency domain:

$$\boldsymbol{B} = \mu_0 \boldsymbol{H} \tag{3}$$

$$\boldsymbol{D} = \varepsilon_0\left(\varepsilon_\infty + \frac{\varepsilon_S - \varepsilon_\infty}{1 + \jmath\omega\tau_D} - \jmath\frac{\sigma}{\omega\varepsilon_0}\right)\boldsymbol{E} \tag{4}$$

where ε_0 and μ_0 are the free-space permittivity and permeability, ε_S is the static permittivity, ε_∞ is the optical permittivity, τ_D is the relaxation time and σ is the conductivity. Equation (4) can be rewritten as:

$$(\jmath\omega)^2\tau_D\boldsymbol{D} + \jmath\omega\boldsymbol{D} = (\jmath\omega)^2\varepsilon_0\varepsilon_\infty\tau_D\boldsymbol{E} + \jmath\omega(\varepsilon_0\varepsilon_S + \sigma\tau_D)\boldsymbol{E} + \sigma\boldsymbol{E} \tag{5}$$

By mapping $(\jmath\omega)^m$, in the frequency domain, into $\partial^m/\partial t^m$, in time domain, (5) can be written as

$$\tau_D\frac{\partial^2\boldsymbol{D}}{\partial t^2} + \frac{\partial\boldsymbol{D}}{\partial t} = \varepsilon_0\varepsilon_\infty\tau_D\frac{\partial^2\boldsymbol{E}}{\partial t^2} + (\varepsilon_0\varepsilon_S + \sigma\tau_D)\frac{\partial\boldsymbol{E}}{\partial t} + \sigma\boldsymbol{E} \tag{6}$$

Application of the Crank-Nicolson method to (1–3, 6) and manipulation of the resultant discretised equations yield an equation with only electric field $E^{m+1}(i,j,k)$ terms:

$$\begin{aligned}
&E_x^{n+1} - \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_x^{n+1}}{\partial y^2} + \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_y^{n+1}}{\partial x\partial y} \\
&+ \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_z^{n+1}}{\partial z\partial x} - \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_x^{n+1}}{\partial z^2} \\
&= \frac{\xi_1}{\xi_4}D_x^n + \frac{\xi_1}{\xi_4}\frac{\Delta t^2}{2}\frac{\partial H_z^n}{\partial y} + \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_x^n}{\partial y^2} \\
&- \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_y^n}{\partial x\partial y} - \frac{\xi_1}{\xi_4}\frac{\Delta t}{2}\frac{\partial H_y^n}{\partial z} \\
&- \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_z^n}{\partial z\partial x} + \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{1}{\mu}\frac{\partial^2E_x^n}{\partial z^2} \\
&+ \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{\partial H_z^n}{\partial y} - \frac{\xi_1}{\xi_4}\left(\frac{\Delta t}{2}\right)^2\frac{\partial H_y^n}{\partial z} \\
&+ \frac{\xi_2}{\xi_4}D_x^n + \frac{\xi_3}{\xi_4}D_x^{n-1} - \frac{\xi_5}{\xi_4}E_x^n - \frac{\xi_6}{\xi_4}E_x^{n-1}
\end{aligned} \tag{7}$$

where $\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6$ are space dependent and defined as $\xi_1 = \tau_D/(\Delta t)^2 + 1/\Delta t$, $\xi_2 = -2\tau_D/(\Delta t)^2 - 1/\Delta t$, $\xi_3 = \tau_D/(\Delta t)^2$, $\xi_4 = \varepsilon_0\xi_\infty\tau_D/(\Delta t)^2 + \varepsilon_0\varepsilon_S + \sigma\tau_D/\Delta t + \sigma/2$, $\xi_5 = -2\varepsilon_0\xi_\infty\tau_D/(\Delta t)^2 - \varepsilon_0\varepsilon_S + \sigma\tau_D/\Delta t + \sigma/2$, $\xi_6 = \varepsilon_0\xi_\infty\tau_D/(\Delta t)^2$.

Permutation of x, y and z in (7) yields the remaining two E-field equations. By applying them to each Yee-grid position, a system of linear equations of $\boldsymbol{AN} = \boldsymbol{C}$ is found, with $\boldsymbol{A}$ being an extremely large and highly sparse coefficient matrix. The size of $\boldsymbol{A}$ is $(3(N_x-1)(N_y-1)(Nz-1))(3(N_x-1)(N_y-1)(Nz-1))$ where N_x, N_y, N_z are the size of the FDTD space in x, y and z directions, respectively ($i = i_{\min}, j = j_{\min}$ and $k = k_{\min}$ are excluded because at these points boundary conditions will be used). $\boldsymbol{N}$ represents a vector with the electric field components to be solved, and $\boldsymbol{C}$ is the excitation vector. The solution of the system of equations to find the electric field is the core of the scheme. All the remaining field quantities are found in an explicit manner from the electric field. In order to provide a convenient and straightforward algorithm, Mur first-order boundary conditions were employed into FD-CN-FDTD.

Solution of sparse system: The sparse system $\boldsymbol{AN} = \boldsymbol{C}$ can be solved by direct or iterative methods. Despite their intrinsic appeal for very large linear systems, iterative solvers are not robust compared to direct solvers [7] and often require preconditioning to improve their efficiency and robustness. As the purpose of this Letter is to verify the validity of the proposed FD-CN-FDTD, not to improve the way to solve $\boldsymbol{AN} = \boldsymbol{C}$, a direct solver approach was used. Direct solvers are robust, reliable and their latest implementations are quite memory efficient, and have efficient reordering techniques, which improve the performance to a great extent. In this work we used a version of sparse Gaussian elimination to solve FD-CN-FDTD. This method chooses a pivot sequence to decompose $\boldsymbol{A}$ into LU factors, in such a way that the sparsity is preserved in them. A full Markowitz search technique is used to find the best pivot and reduce the fill-ins (i.e. not to waste memory). After the factorisation, forward and backward triangular sweeps are executed to obtain $\boldsymbol{N}$. At each time step of the FD-CN-FDTD algorithm, a new $\boldsymbol{C}$ is calculated, while $\boldsymbol{A}$ is required to be factorised only once (which dominates the computational time) before the beginning of the time-stepping. Once factorised, the same factors are repeatedly used at each time step to obtain $\boldsymbol{N}$. For this reason, this method may become more computationally efficient than the iterative methods when a large number of iterations are needed, since at each time step only forward and backward solutions are required.

Numerical results: To validate FD-CN-FDTD numerically, a computational region of size (30 × 30 × 30) cells was considered. Half of it was filled with medium one ($\varepsilon_S = 71.66$, $\varepsilon_\infty = 34.58$, $\sigma = 0.49$ S/m and $\tau_D = 5.65$ ps) and the other half with medium two ($\varepsilon_S = 87.34$, $\varepsilon_\infty = 49.13$, $\sigma = 0.69$ S/m and $\tau_D = 26.89$ ps) as shown in Fig. 1. A z-directed dipole was placed at (10, 15, 15) in medium one, with a time evolution of a modulated Gaussian pulse centred at 3 GHz. Signals were recorded 10 cells away at (20, 15, 15) in medium two. A uniform spatial sampling was taken ($\Delta_x = \Delta_y = \Delta_z = 10^{-3}$m).

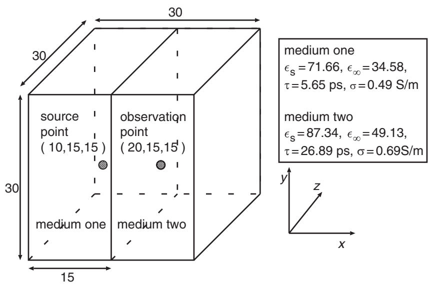

Fig. 1 *FDTD problem space for simulation with FD-CN-FDTD*

As a reference, an identical setup was taken for the standard explicit frequency dependent (FD)-FDTD. The first 600 time steps of the E_z field component at the observation point are shown in Fig. 2, computed both with FD-FDTD with CFLN $\equiv \Delta t/\Delta t_{CFL} = 1$, and with FD-CN-FDTD with CFLN $= 1, 3, 5$, where Δt_{CFL} denotes the maximum time step allowed by the CFL stability condition. Good agreement between the signals from the proposed scheme and explicit FD-FDTD was observed. The scheme is seen to be unconditionally stable beyond the CFL limit (CFLN $= 1$), although numerical errors increasingly appear with higher CFLN. Thus Δt is no longer restricted by the CFL limit but by numerical errors, a characteristic possessed by other implicit schemes like ADI-FDTD [8]. Crank-Nicolson schemes lead to finite spurious oscillations not connected with the roundoff, this problem was also recognised by Crank and Nicolson [3] and reported in the standard texts like [9, 10]. The reason behind the small discrepancy at higher CFLN and trailing oscillations, that is seen when FD-CN-FDTD is run with even higher CFLN (around 10 or more), is such characteristics are inherent to the CN scheme.

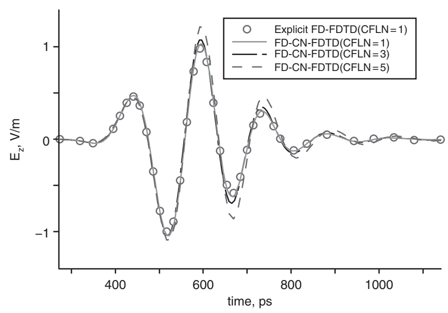

Fig. 2 *Observations from both explicit scheme and FD-CN-FDTD scheme*

For the problem described in Fig. 1 when computational space was (30 × 30 × 30) cells, CPU time required for LU decomposition was 633 min and average CPU time per iteration was 6.489 s when CFLN = 1 on the dual AMD Opteron 280 with 8 GB of memory. When the FDTD space was filled with homogeneous material of media one or when CFLN > 1 there were no significant differences in these values.

Conclusion: A method to incorporate frequency-dependent Debye-dispersive media into the unconditionally stable Crank-Nicolson FDTD method has been presented. The proposed scheme uses a direct sparse solver, which performs the LU factorisation only once (before the time-stepping begins). The major amount of computation time is employed at this stage, keeping computational times during time-marching similar to those of FDTD. The application of iterative methods to solve the sparse system is currently under investigation.

6 July 2009
doi: 10.1049/el.2009.1940

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