Efficient solvers for the frequency dependent Crank Nicolson FDTD method

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Abstract—The Finite Difference Time Domain (FDTD) method is a widely used numerical technique in the computational electrodynamics. But it is computationally inefficient as the size of the time-step is restricted by Courant-Friedrich-Lewy (CFL) limit. We have developed a three dimensional Crank Nicolson FDTD method for the frequency dependent media (FD-CN-FDTD). The FD-CN-FDTD method is unconditionally stable beyond the CFL limit. However, when the time step is far above the CFL limit, the coefficient matrix, that needs to be solved at each iteration of the FD-CN-FDTD method, is no longer diagonally dominant. This causes the iterative solvers increase their solution time per FD-CN-FDTD iteration. We compare two widely employed iterative solvers for sparse systems: Bi-Conjugate Gradient Stabilised (BiCGStab) and Generalised Minimum Residual (GMRES). Results from our simulations manifest that BiCGStab outperforms GMRES in terms of computational efficiency. We point out the necessity of further research for developing the pre-conditioners and efficient solvers to get the most benefit from the FD-CN-FDTD method.

Index Terms—Crank-Nicolson method, FDTD, Debye media, sparse matrix solver, iterative methods, pre-conditioners

I. INTRODUCTION

This work is on numerical techniques in electrodynamics with an aim to study the application of electromagnetic fields for the treatment of diseases. The treatment of Perkinson’s, Alzheimers etc. diseases are still in the development stage and one effective option is using the deep brain stimulation (DBS) procedure. The DBS procedure involves the placement of a medical device and thin, insulated wires called leads completely inside the body. While the device is implanted beneath the skin in the chest, the leads are implanted within the brain. Electrical stimulation is then sent directly to the targeted areas within the brain that control the movement of the body, in order to make these areas function better. However, such treatments have the problem of being invasive which requires to open up the skull. Our ultimate target in this research is to achieve the similar effect like in DBS but in a non-invasive way. However our research can also be useful for the invasive DBS procedure. By doing numerical simulation before applying invasive DBS on a patient, the medical practitioner can get the understanding of where to place the lead.

The Finite Difference Time Domain (FDTD) method is one of the most widely used numerical techniques used in computational electrodynamics. The FDTD method is straightforward, robust, versatile and widely applicable for wide-band systems. However, for many problems of interest it may become computationally inefficient, due to the upper limit for the time-step imposed by the Courant-Friedrich-Lewy (CFL) stability condition. This typically happens when a high spatial resolution is required to model fine geometries which leads to spatial sampling much shorter than the minimum wavelength of interest, enforcing an unnecessarily large FDTD iteration numbers. This is exactly the case when the interaction between EM waves with high-resolution human body is simulated. There is a growing interest in overcoming this limitation.
by employing unconditionally stable implicit FDTD methods, for which time and space steps can be independently chosen. This trend will continue because high accuracy in modelling is increasingly demanded with the massive improvement of computational resources.

An alternative to the explicit FDTD method is the Crank-Nicolson \cite{3} FDTD (CN-FDTD) method, for being unconditionally stable beyond the CFL limit. As in the classical FDTD method, the CN-FDTD method replaces the time and space derivatives by centred differences, but unlike the FDTD method, the fields affected by the curl operators are also averaged in time. The resulting method is an unconditionally stable fully implicit marching-on-in-time algorithm with high accuracy and low anisotropy \cite{4}.

There have been works attempting to simplify or approximate the CN-FDTD method but these methods suffer up to some extent of numerical errors, which may become severe for some practical applications \cite{5}. In this work we focus on the actual Crank Nicolson method applied to the FDTD method to solve the Maxwell’s equation. The tissues of the human body are frequency dependent meaning that the electrical properties of these tissues vary over the frequencies. Therefore the Crank Nicolson FDTD method need to be able to handle the frequency dependent materials. We have developed a three dimensional Crank Nicolson FDTD method for the frequency dependent media (FD-CN-FDTD). The FD-CN-FDTD method is unconditionally stable and can use time-step beyond the CFL limit. The FD-CN-FDTD method results in a system of equations giving rise to a huge sparse matrix that need to be solved at every FDTD iteration. The selection of the matrix solver is the critical part of the method to fully take the advantages of using larger time-step, since the computational costs associated with the solver must be kept as low as possible. Either direct or iterative solvers can be employed. Direct solvers are not the preferred choice for large problems of practical importance because of their enormous memory requirements \cite{6}. Iterative solvers based on Krylov subspace theory have proven to be suitable for practical problems \cite{7}, \cite{8}. However the computational efficiency of an iterative solver is application-dependent and therefore determination of the effectiveness of each method is essential.

In this paper, we present the study of different Krylov subspace based solvers to solve the sparse matrix systems of the 3D FD-CN-FDTD method. The remaining of this paper is organised as follows: Section II introduces the FD-CN-FDTD method mathematically. The techniques to solve the system and numerical results are presented in section III. Section IV presents the conclusion and discuss on open issues for future work.

II. THEORY OF THE FD-CN-FDTD METHOD

Maxwell’s curl equations in material independent form are

\[
\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1}
\]

\[
\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} \tag{2}
\]

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

\[
\mathbf{B} = \mu_0 \mathbf{H} \tag{3}
\]

\[
\mathbf{D} = \epsilon_0 (\epsilon_\infty + \frac{\epsilon_S - \epsilon_\infty}{1 + j \omega \tau_D} - j \frac{\sigma}{\omega \epsilon_0}) \mathbf{E} \tag{4}
\]

where \(\epsilon_0\) and \(\mu_0\) are the free-space permittivity and permeability, \(\epsilon_S\) is the static permittivity, \(\epsilon_\infty\) is the optical permittivity, \(\tau_D\) is the relaxation time and \(\sigma\) is the static conductivity. (4) can be re-written as

\[
(j \omega)^2 \tau_D \mathbf{D} + j \omega \mathbf{D} = \tag{5}
\]

\[
(j \omega)^2 \epsilon_0 \epsilon_\infty \tau_D \mathbf{E} + j \omega (\epsilon_0 \epsilon_S + \sigma \tau_D) \mathbf{E} + \sigma \mathbf{E}
\]

By mapping \((j \omega)^m\), in frequency domain, into \(\frac{\partial^m}{\partial t^m}\), in time domain, (5) can be written as

\[
\tau_D \frac{\partial^2 \mathbf{D}}{\partial t^2} + \frac{\partial \mathbf{D}}{\partial t} = \tag{6}
\]

\[
\epsilon_0 \epsilon_\infty \tau_D \frac{\partial^2 \mathbf{E}}{\partial t^2} + (\epsilon_0 \epsilon_S + \sigma \tau_D) \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E}
\]
The application of Crank-Nicolson method [6] to (1), (2), (3), (6), after algebraic manipulation, yields an equation only with electric field $E^{n+1}$ terms:

$$\begin{align*}
E_x^{n+1} &= \frac{\xi_1}{\xi_4} \Delta t^2 \frac{1}{\mu} \left( \frac{\partial^2 E_x^{n+1}}{\partial y^2} - \frac{\partial^2 E_y^{n+1}}{\partial x \partial y} \right) \\
+ \frac{\xi_1}{\xi_4} \Delta t^2 \frac{1}{\mu} \left( \frac{\partial^2 E_y^{n+1}}{\partial z \partial x} - \frac{\partial^2 E_z^{n+1}}{\partial x^2} \right) \\
&= \frac{\xi_1}{\xi_4} \Delta t^2 \frac{1}{\mu} \left( \frac{\partial^2 E_x^{n+1}}{\partial y^2} - \frac{\partial^2 E_y^{n+1}}{\partial x \partial y} \right) \\
&\quad + \frac{\xi_1}{\xi_4} \Delta t^2 \frac{1}{\mu} \left( \frac{\partial^2 E_y^{n+1}}{\partial z \partial x} - \frac{\partial^2 E_z^{n+1}}{\partial x^2} \right) \\
&\quad + \frac{\xi_1}{\xi_4} \Delta t^2 \frac{1}{\mu} \left( \frac{\partial^2 E_z^{n+1}}{\partial y \partial x} - \frac{\partial^2 E_x^{n+1}}{\partial y^2} \right)
\end{align*}$$

where $\xi_1$, $\xi_2$, $\xi_3$, $\xi_4$, $\xi_5$, $\xi_6$ are space dependent constants function of the Debye parameters and of $\Delta t$ [6].

Cyclic permutation of $x$, $y$ and $z$ in (7) yield the remaining two E-field equations. By applying them to each Yee-grid position, a system of linear equations of $AN = C$ is set up. $A$ is the coefficient matrix, $N$ represents a vector with the electric field components to be solved, and $C$ is the excitation vector. The system of equations $AN = C$ is solved first to find the $E$ field. $D$ and $H$ fields are calculated in an explicit manner from the $E$ field. In order to terminate the computational space simple Mur first order boundary conditions are employed in this work.

III. SOLUTION OF THE FD-CN-FDTD METHOD
A. Sparse Matrix

The coefficient matrix $A$ generated by the FD-CN-FDTD method is highly sparse. The size of $A$ is $9(N_x)^2(N_y)^2(N_z)^2$ where $N_x$, $N_y$, $N_z$ are the size of the FDTD space in $x$, $y$ and $z$ directions. When the problem space is homogeneous, the coefficient matrix is symmetric and otherwise asymmetric. Fig. 1 shows the sparsity pattern of $A$ in the case where the entire computational space is filled with Debye parameters $\epsilon_S = 6.2$, $\epsilon_\infty = 3.5$, $\sigma = 0.029$ S/m and $\tau_D = 39.0$ ps. The sparsity pattern of Fig. 1 is similar to that of three dimensional Finite Difference Frequency Domain (FDFD) method [9], and therefore the discussions in this paper could also be useful to the FDFD researchers.

In this paper, two cases are considered for study. The first one consists of an inhomogeneous medium, in a cubic space of size $80^3$ cells, with 5 different media as shown in Fig. 2. The second one involves the same cubic space of the previous case, now filled with a homogeneous medium with Debye parameters $\epsilon_S = 6.2$, $\epsilon_\infty = 3.5$, $\sigma = 0.029$ S/m and $\tau_D = 39.0$ ps. In both cases a $z$-directed dipole hard source with a time variation given by a Gaussian pulse centred at $6.9$ GHz, with $4.94$ GHz bandwidth ($-3$ dB decay), was placed at the centre of the computational space. Spatial sampling was uniform: $\Delta x = \Delta y = \Delta z = \Delta = 10^{-3}$ m. The time step is taken equal or above the CFL stability condition of the explicit FDTD method: $\Delta t = CPLF \times \Delta/\sqrt{3}$ with CPLF henceforth referred to as CFL number, and $c$ the free-space
light-speed. The level of accuracy in waveform compared with explicit frequency dependent FDTD method is the same as the one presented in Fig. 2 in [6]

![Diagram](image)

**Fig. 2.** Computational environment for numerical studies using the FD-CN-FDTD method

### B. Condition number and diagonal dominance

The ease of solution on a linear system of equations can be measured by the condition number of \( A \). [10] reports that the condition number of the coefficient matrix \( A \) for frequency independent Crank-Nicolson method increases with the CFL number, which naturally also applies to the FD-CN-FDTD method. Hence for high CFLN, the matrix becomes severely ill-conditioned, requiring high computation time to be solved by iterative methods.

Similar conclusions are found by realising that the diagonal dominance of the coefficient matrix improves when CFLN decreases, leading to matrices which are easier to solve. Fig. 3 shows how the absolute values of diagonal and the sum of absolute values of off-diagonal elements of \( A \) vary with CFLN, both for the homogeneous and inhomogeneous cases previously described. A representative row of \( A \) has been taken, corresponding to the interior computational space, which comprises nearly the whole coefficient matrix (except the rows which include the FDTD boundaries). For low CFLN all the rows of the coefficient matrix are strictly diagonally dominant except a very few which are contributed by the boundary cases, whereas high CFLN deteriorates this property. As shown in Fig. 3 the advantageous diagonal property of the coefficient matrix is lost with increased CFLN irrespective of the media parameters or homogeneity, The diagonal-dominance criterion is simpler to handle than the condition-number one, which is expensive to compute in practice. An additional advantage of the diagonal dominance criterion is that it points us a direction to research in the building of appropriate pre-conditioners to alleviate this problem.

### C. Iterative Solvers

To solve the FD-CN-FDTD method either direct or iterative solvers can be used. Although direct solvers are robust and reliable [6], they are computationally more expensive than iterative solvers, and require excessively large memory. For example, a \( 30^3 \) cells computational space solved by the direct solver in double precision using sparse Gaussian elimination requires 2.4 GB of memory whereas iterative solvers like BiCGStab (Bi-Conjugate Gradient Stabilised) and GMRES (Generalised Minimum Residual) require only 62 MB and 65 MB, respectively. Thus for practical problems iterative solvers should be used [11].

Depending on the homogeneity of the computational space the FD-CN-FDTD method yields symmetric and asymmetric matrices. Since for homogeneous problems the coefficient matrix is sym-
metric, iterative solvers like Conjugate Gradient (CG) method can be used. However practical problems are inhomogeneous, and we have to resort to iterative solvers for asymmetric matrices. Usual ones are GMRES, BiCGStab, or Conjugate Gradient Squared (CGS) (Appendix D of [12]). CGS suffers from irregular convergence, which may lead to substantial build-up of rounding errors, because it is based on squaring the residual polynomial [11] [12]. Therefore, this paper focuses only in GMRES and BiCGStab. An advantage of BiCGStab method is that its computational cost per iteration is similar to that of CGS, but it avoids the irregular convergence patterns of CGS while maintaining about the same rate of convergence. GMRES is said to be a very robust solver for non-symmetric matrices. It leads to the smallest residual for a fixed number of iteration steps. But the iteration steps become increasingly expensive and memory intensive as the increase of iteration steps. In order to limit the memory requirement to store the history of the iteration and limit CPU time per iteration step, the restarting of the iteration is necessary. In this paper GMRES(m) that restarts every $m$ iterations [13] and BiCGStab of [14] were used.

D. Performance study of BiCGStab and GMRES

The performance of BiCGStab and GMRES is compared both for the homogeneous and inhomogeneous media cases. Fig. 4 shows the convergence pattern for $CFLN = 20$, plotting the threshold of the residual error as a function of the average number of iterations required to achieve a specified accuracy (i.e., the specified threshold of the residual error). For example, to make the residual error lower than $10^{-8}$ BiCGStab requires about 45 iterations whereas GMRES requires about 97 iterations in both homogeneous and inhomogeneous cases. The convergence rate of the solvers is weakly affected by homogeneity. For $CFLN < 20$ the average iteration numbers are lower than those showed in Fig. 4 ($CFLN = 20$). Our finding of BiCGStab outperforming GMRES in computational efficiency is contrary to the findings of [10] which reports GMRES is the fastest for the frequency independent CNFDTD method presented there.

Fig. 5 shows how the average number of iterations, required by BiCGStab and GMRES to converge, increases with the $CFLN$ number. Stopping criteria in this case was $10^{-13}$ and the reason for selecting this small value of convergence tolerance is, in the FD-CN-FDTD method, unlike the frequency independent CN-FDTD method, $D = \epsilon E$ is used and therefore $D$ can have a value of such small order because of $\epsilon$ (permittivity). GMRES stagnates when convergence tolerance is below $10^{-13}$ whilst BiCGStab can work even at a lower convergence tolerance. Both solvers require more iterations to converge as the increase of $CFLN$, but the rate of increase of iteration numbers with $CFLN$ is higher for GMRES than for BiCGStab. Homogeneity does not affect significantly this rate, particularly, for BiCGStab. In the FD-CN-FDTD method, the total number of FDTD iterations required to complete the simulation decreases with $CFLN$, but the increase of computational costs per FDTD iteration with $CFLN$, as shown in Fig. 5 can undermine this positive effect, unless the solution is very efficient.

Fig. 6 shows the total CPU time required by the FD-CN-FDTD method using BiCGStab or GMRES as a function of $CFLN$. The stopping criterion of $10^{-13}$ was employed and simulation was performed to reach $1200/CFLN$ time steps on a dual AMD Opteron 280 with 8GB of memory. Observe that the CPU-time decreases with $CFLN$, for both solvers, although GMRES requires more CPU time than
BiCGStab.

Table I presents the memory required by the two solvers for three different computational space sizes. GMRES always requires more memory than BiCGStab.

From all the above, we can conclude that BiCGStab outperforms GMRES in computational efficiency. This finding is in contrary to that of the frequency independent CN-FDTD method of [10]. The work of [10] is based on [1] and [2] while the FD-CN-FDTD method additionally involves [6] which has 2nd order time derivative terms. The FD-CN-FDTD method involves nine field components in place of six for the CN-FDTD method and the sparsity pattern of the former has more bands than the latter [8]. Apart from this, the concerned problem of simulation, implementation, optimisation, and parameters tuning, has an obvious influence in concluding the most suitable in respect of the computational efficiency.

IV. PRE-CONDITIONERS

Two pre-conditioners are applied to solve for the FD-CN-FDTD method: incomplete LU with no fill-in ILU(0) and Sparse Approximate Inverse (SAI). ILU(0) did not give any improvement in convergence (rather convergence deteriorated). However SAI gave slight improvement in reducing the number of iterations to converge but there were two major setbacks making it unsuitable for use. The time to compute the approximate inverse pre-conditioner is too long which makes the total CPU time for the FD-CN-FDTD simulation longer than that without any pro-conditioner. [8] showed SAI can reduce iteration numbers but did not mention the total CPU time. A second problem is that memory requirements of SAI restricted the maximum computational space to only $30^3$ cells. SAI also showed lack of robustness in our case.

V. CONCLUSION

In this paper, we have presented Krylov-based approaches to solve the three dimensional CN-FDTD method for frequency dependent Debye dispersive media. Two best-known iterative methods, GMRES and BiCGStab, were compared in terms of the number of iteration requirements for convergence with different $CFLN$, and in terms of CPU-time and memory requirements. BiCGStab outperforms GMRES when used with the FD-CN-FDTD method in every aspect of the study. It has also been pointed out that the diagonal-dominance of the coefficient matrix, which degrades when $CFLN$ increases, is a main reason for the increase of the CPU time.

<table>
<thead>
<tr>
<th>Computational Size (cells)</th>
<th>40$^3$</th>
<th>60$^3$</th>
<th>80$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiCGStab</td>
<td>145Mb</td>
<td>487Mb</td>
<td>1.1Gb</td>
</tr>
<tr>
<td>GMRES</td>
<td>151Mb</td>
<td>507Mb</td>
<td>1.2Gb</td>
</tr>
</tbody>
</table>

TABLE I

MEMORY REQUIRED BY BICGSTAB AND GMRES FOR DIFFERENT COMPUTATIONAL SPACES
needed by the solvers. Furthermore it was found that ILU(0) and SAI pre-conditioners can not improve the computational efficiency of the FD-CN-FDTD method. Many of these findings about the frequency dependent CN-FDTD method do not match with the existing literature on frequency independent CN-FDTD method and possible reasons for this are also mentioned. Since the commonly used pre-conditioners do not seem to improve the solution time of the FD-CN-FDTD sparse matrix system, further research is needed to tailor suitable pre-conditioners which will provide the ultimate benefit of using higher $CFLN$.

REFERENCES


