A Hybrid Explicit-Implicit Scheme for Spectral-Element Time-Domain Analysis of Multiscale Simulation

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Abstract ─ The multiscale simulation usually leads to dense meshes discretization for fine structures, thus making time step size of the spectral-element time-domain (SETD) method extremely small to ensure stability for explicit scheme. In this paper, a hybrid explicit-implicit scheme for SETD is proposed to deal with the simulation of multiscale electromagnetic problems. The central-difference is applied for the coarse region with large cells and the Newmark-Beta scheme is for the fine region with small cells. Then a large size of time step can be selected in the whole domain instead of the one limited by the smallest cell. When solving the matrix equation formed by the implicit scheme, two approaches are employed. One uses the sparse matrix solver UMFPACK directly and the other involves an explicit and iterative scheme. Numerical results show that the hybrid method is an efficient alternative to conventional SETD method for multiscale simulation.

Index Terms ─ Explicit-implicit, iterative Newmark-Beta, multiscale, spectral-element time-domain (SETD) method.

I. INTRODUCTION

When handling the multiscale electromagnetic simulations, traditional techniques face great challenges as some small grids may appear in very fine structures, which will result in a very small size of time step for the whole domains to obtain a stable solution [1]. Therefore, it will waste a lot of time because in other coarse domains a larger size of time step can be used. Unconditionally stable methods are often employed for the fine features as the time step size can be chosen in spite of the restriction between the time step size and the space step to guarantee stability [2]. However, most of the existing unconditionally stable techniques are implicit, which generally need a matrix solution. FDTD (finite-difference time-domain) is a very useful and simple time domain method [3]-[6], and some implicit methods are proposed based on FDTD such as the CN (Crank-Nicolson)-FDTD [5], ADI (alternating direction implicit)-FDTD [6]. Meanwhile, some FETD (finite-element time-domain) based methods [7]-[10] are also developed to reach unconditional stability such as the CN (Crank-Nicolson)-FETD [8], ADI (alternating direction implicit)-FETD [9], the Newmark-Beta scheme [10] and so on. If the implicit method is adopted for the whole domain, it will lead to a very large matrix, which is computationally expensive. Some hybrid time-stepping techniques are studied to improve the efficiency of the methods [11], [12]. Discontinuous Galerkin time-domain methods are very popular to deal with the multiscale simulations. The whole region is separated into a few subregions and different time-stepping scheme can be applied in these subregions [11]. However, the derivation is troublesome and additional cost is required on the interface for communicating fields among different subregions.

Here, a hybrid explicit-implicit scheme for spectral-element time-domain method is proposed and it is relatively simple and easy to implement. The spectral-element time-domain method makes use of Gauss-Lobatto-Legendre (GLL) polynomials and the mass matrix is diagonal or block-diagonal [13], so the inverse of the mass matrix can be easily obtained. One advantage of the proposed hybrid algorithm is that it is not derived with the help of the discontinuous Galerkin technique. As a result, the algorithm is easy to implement on the existing program without extra procedure for the interfaces of different subdomains. The simple central-difference is applied for the large elements region and the Newmark-Beta scheme is applied for the small elements region. Consequently, in the coarse region conditionally stability is realized and in the fine region unconditionally stability is realized. So the size of time step in the fine region could be chosen as large as the one in the coarse region instead of the one limited by the smallest mesh. Two approaches are used for the matrix solution in the fine region. The first one directly uses the sparse matrix solver UMFPACK [15] to solve the matrix equation. For the other, an iterative and explicit scheme is developed. Computational cost is also compared in the

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demonstrated example.

This paper is organized as follows. In Section II, the basic theory and formulations of explicit-implicit scheme for SETD are presented. Stability analysis is given in Section III and numerical results are given to demonstrate the validity of the proposed method in Section IV. Conclusions are summarized in Section V.

II. THEORY AND FORMULATIONS

To deal with the multiscale problem, we start from the vector wave equation:

$$\nabla\times\nabla\times\mathbf{E}+\mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2}=0\,. \tag{1}$$

The GLL element discretization is applied in SETD method, which can achieve the spectral accuracy. The Nth-order GLL basis function in a one-dimensional reference unit $\xi\in[-1,1]$ is defined by [13]:

$$\phi_j^{(N)}(\xi)=\frac{-1}{N(N+1)L_N(\xi_j)}\frac{(1-\xi^2)L_N'(\xi)}{\xi-\xi_j}. \tag{2}$$

Consequently, when applying the 3-D standard reference unit, the basis functions are described as:

$$\begin{aligned}\boldsymbol{\Phi}_{rst}^{\xi}&=\hat{\xi}\phi_r^{(N_\xi)}(\xi)\phi_s^{(N_\eta)}(\eta)\phi_t^{(N_\zeta)}(\zeta)\\ \boldsymbol{\Phi}_{rst}^{\eta}&=\hat{\eta}\phi_r^{(N_\xi)}(\xi)\phi_s^{(N_\eta)}(\eta)\phi_t^{(N_\zeta)}(\zeta)\,.\\ \boldsymbol{\Phi}_{rst}^{\zeta}&=\hat{\zeta}\phi_r^{(N_\xi)}(\xi)\phi_s^{(N_\eta)}(\eta)\phi_t^{(N_\zeta)}(\zeta)\end{aligned} \tag{3}$$

Therefore, the electric field can be expanded by the basis functions:

$$\mathbf{E}(\xi,\eta,\zeta)=\sum_{j=1}^{N}e_j\boldsymbol{\Phi}_j\,. \tag{4}$$

Then the Galerkin's test is used and we have a discretized system of equations:

$$\begin{aligned}&[S]e+[T]\frac{d^2e}{dt^2}=0\\ &S_{ij}=\frac{1}{\mu}\iiint_{V^e}\nabla\times\tilde{\boldsymbol{\Phi}}_i\cdot\nabla\times\tilde{\boldsymbol{\Phi}}_j dV\,.\\ &T_{ij}=\varepsilon\iiint_{V^e}\tilde{\boldsymbol{\Phi}}_i\cdot\tilde{\boldsymbol{\Phi}}_j dV\end{aligned} \tag{5}$$

Where $\tilde{\boldsymbol{\Phi}}$ represents the basis function in the physical domain and has the following mapping relationship with the basis function $\boldsymbol{\Phi}$ in the reference domain [14]:

$$\begin{aligned}\tilde{\boldsymbol{\Phi}}&=J^{-1}\boldsymbol{\Phi}\\ \nabla\times\tilde{\boldsymbol{\Phi}}&=\frac{1}{|J|}J^T\nabla\times\boldsymbol{\Phi}\end{aligned}\,. \tag{6}$$

In the conventional SETD method, the derivative in Equation (5) is substituted via the central-difference in the entire computation domain:

$$[T]e^{n+1}=\left(2[T]-\Delta t^2[S]\right)e^n-[T]e^{n-1}\,. \tag{7}$$

As the basis functions have the property of orthogonality and the GLL quadrature is used [16], the mass matrix [T] is diagonal or block-diagonal. Therefore, the inverse can be directly obtained. It could be a great advantage of the SETD method over the conventional FETD method whose mass matrix doesn't have the block-diagonal characteristic.

When handling some complicated electromagnetic problems such as the multiscale simulation, very small meshes usually appear in the fine features. Moreover, it is the same to other complex materials or structures because the curved hexahedrons are used and extremely small size meshes are unavoidably produced sometimes. Since the size of time step is limited by the spatial discretization of the simulation domain according to the CFL condition, the time step size may become very small because of small cells. It will result in a large number of simulation steps and the efficiency is low.

Here, a novel hybrid explicit-implicit spectral-element time-domain method is proposed to deal with this kind of problem. The fine structures can be wrapped by a proper box and treated as the fine region, the rest is treated as the coarse region. In the coarse region with large elements, the traditional central-difference is employed, which is displayed in Equation (7). In the fine region with very small elements, the Newmark-Beta scheme is used to guarantee unconditional stability with a large size of time step, which is the same as the one used in the coarse domain:

$$S\left(\beta e^{n+1}+(1-2\beta)e^n+\beta e^{n-1}\right)+T\frac{e^{n+1}-2e^n+e^{n-1}}{\Delta t^2}=0\,. \tag{8}$$

Navsariwala and Gedney [10] have demonstrated that when the parameter is chosen to be $\beta\geq 0.25$, the unconditional stability can be ensured. So the size of time step could be selected in spite of the stability condition:

$$\begin{aligned}\left([T]+\Delta t^2\beta[S]\right)e^{n+1}=&\left(2[T]-\Delta t^2(1-2\beta)[S]\right)e^n\\ &-\left([T]+\Delta t^2\beta[S]\right)e^{n-1}\end{aligned}\,. \tag{9}$$

As far as Equation (7) is concerned, the unknowns related to one node will form a block in the mass matrix, which is the characteristic of the spectral-element time-domain method. So each node in an element can be solved independently in one time step. In Fig. 1, assuming there are two elements, the nodes in the red dashed box are marked as the coarse region while the rest nodes are marked as fine region. The two different regions do not have overlapped nodes, so no extra procedure for the interfaces of different regions is needed. In the coarse region, Equation (7) is solved explicitly. In the fine region, because the mass matrix in the left-hand side of (9) does not have the characteristic of block-diagonal, a solver is required to solve the matrix equation. The first approach uses the sparse

matrix solver UMFPACK [15], [17] with the solving process illustrated in Fig. 1. When computing Equation (9), the electric field e^{n+1} in the adjacent large cells is needed as a known quantity. As a result, in each time step, Equation (7) is solved ahead of Equation (9).

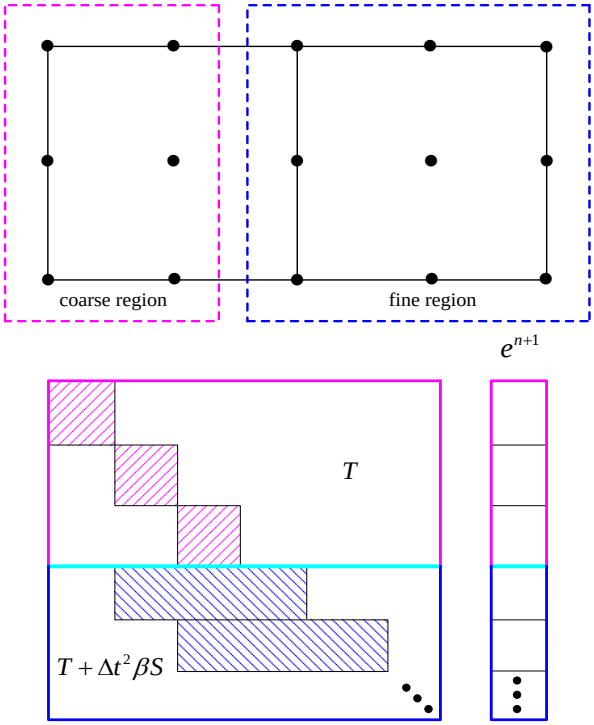

Fig. 1. Schematic diagram of the explicit-implicit scheme.

When dealing with a large problem, using the UMFPACK solver is quite time-consuming. Moreover, the solver costs additional memory because of the LU factorization. In the second scheme, a new splitting scheme is proposed, where [S] can be split into two parts, one is a block-diagonal matrix the same as [T] and is merged with [T] to form a new matrix marked as [T'], the rest is marked as [S'] and it is moved to the right-hand side of the equation:

$$\left[T'\right]e^{n+1}=\left(2\left[T\right]-\Delta t^2\left(1-2\beta\right)\left[S\right]\right)e^n-\left(\left[T\right]+\Delta t^2\beta\left[S\right]\right)e^{n-1}-\Delta t^2\beta\left[S'\right]e^{n+1}. \quad (10)$$

As the [T'] is block-diagonal, it possesses the advantage of the SETD method whose equations can be solved explicitly. Moreover, the linear system of (10) will be solved iteratively:

$$\left[T'\right]e_{k+1}^{n+1}=\left(2\left[T\right]-\Delta t^2\left(1-2\beta\right)\left[S\right]\right)e^n-\left(\left[T\right]+\Delta t^2\beta\left[S\right]\right)e^{n-1}-\Delta t^2\beta\left[S'\right]e_k^{n+1}. \quad (11)$$

Where the subscript k represents the kth iteration. Firstly, the initial value of e^{n+1} in the right-hand side of the equation is set to be the previous time step value e^n, after a few iterations for the solution e_{k+1}^{n+1}, the error is acceptable and it will then go to the next time step.

III. STABILITY ANALYSIS

The stability analysis of the system is divided into two parts. As for the coarse region, after applying the z-transform of Equation (7), we obtain:

$$\left(z-1\right)^2e\left(z\right)+\Delta t^2\mathbf{T}^{-1}\mathbf{S}ze\left(z\right)=0. \quad (12)$$

To make the scheme stable, z should be inside the unit circle of the complex z plane, which means the magnitude of z should be bounded by one. Further analysis results in the following equation:

$$\left(z-1\right)^2+\Delta t^2\lambda z=0, \quad (13)$$

where λ is the eigenvalue of $\mathbf{T}^{-1}\mathbf{S}$ and the eigenvalues are non-negative and real.

To make z in (13) bounded by 1, we can find that the time step should satisfy the condition:

$$\Delta t\le\frac{2}{\sqrt{\rho\left(\mathbf{T}^{-1}\mathbf{S}\right)}}, \quad (14)$$

where $\rho\left(\cdot\right)$ represents the spectral radius of matrix $\left(\cdot\right)$.

As for the fine region, when using the Newmark-Beta scheme, the system is unconditionally stable [10]. Convergence analysis is needed for the iterative Newmark-Beta method. If we describe the exact solution of Equation (9) as u^{n+1}, then the error of the kth iteration is [18]:

$$err_k^{n+1}=u^{n+1}-e_k^{n+1}. \quad (15)$$

From (10), we can get:

$$u^{n+1}=\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'u^{n+1}+b, \quad (16)$$

and from (11):

$$e_{k+1}^{n+1}=\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'e_k^{n+1}+b, \quad (17)$$

where

$$b=\left(2\mathbf{T}'\mathbf{T}-\Delta t^2\left(1-2\beta\right)\mathbf{T}'^{-1}\mathbf{S}\right)e^n-\left(\mathbf{T}'\mathbf{T}+\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}\right)e^{n-1}. \quad (18)$$

Substitute (16) and (17) into (15):

$$err_{k+1}^{n+1}=\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'err_k^{n+1}. \quad (19)$$

As a result,

$$\left\|err_{k+1}^{n+1}\right\|=\rho\left(\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'\right)^{k+1}\left\|err_0^{n+1}\right\|. \quad (20)$$

We can find that only when the $\rho\left(\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'\right)$ is smaller than one, the iterative method can be a convergent solver.

When Δt is chosen,

$$\Delta t<\frac{2}{\sqrt{\rho\left(\mathbf{T}'^{-1}\mathbf{S}'\right)}}, \quad (21)$$

and $\beta=0.25$, we can finally get:

$$\rho\left(\Delta t^2\beta\mathbf{T}'^{-1}\mathbf{S}'\right)=\Delta t^2\beta\rho\left(\mathbf{T}'^{-1}\mathbf{S}'\right)<1. \quad (22)$$

IV. NUMERICAL RESULTS

To verify the performance of the proposed method, we carried out the simulation of a cavity as shown in Fig. 2. It is a PEC cavity and there is a dielectric ring inside. The dielectric constant of the ring was 2.06. Because the thickness of the ring was very thin, it leaded to a multiscale problem with very small cells in the ring. The hybrid method, together with the traditional SETD were employed to do the simulation and compute the resonate frequencies of the cavity. The number of the total discretized hexahedron was 10440 with 240 for the fine domain and 10200 for the coarse domain. Unstructured hexahedron mesh grids are demonstrated in Fig. 3.

To simulate the example, the traditional SETD required a time step of 1ps and 25000 steps while the explicit-implicit SETD using the UMFPACK was able to use 3730 steps to finish the simulation with a time step as large as 6.7ps. As for the explicit-implicit SETD using the iterative Newmark-Beta scheme, time step was chosen to be 3.3ps and it needed 7575 steps. It can be seen from Fig. 4 that the electric field waveform in time domain of one observation point inside the cavity agrees well with each other among the three methods. After the Fourier transform, the frequency spectrums of the electric field were shown in Fig. 5.

Excellent agreements can also be observed. Finally, the computational costs of the three methods were listed in Table 1.

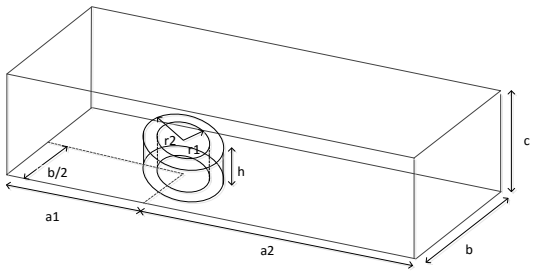

Fig. 2. A rectangular PEC cavity loaded with a dielectric ring: a1 = 207.25 mm, a2 = 440.75 mm, b = 242 mm, c = 43 mm, r1 = 9.5 mm, r2 = 10.0 mm, h=14.0 mm.

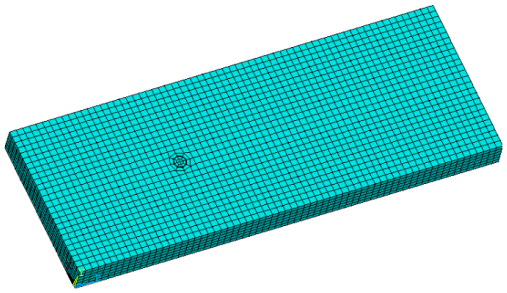

Fig. 3. Mesh grids used to model the cavity.

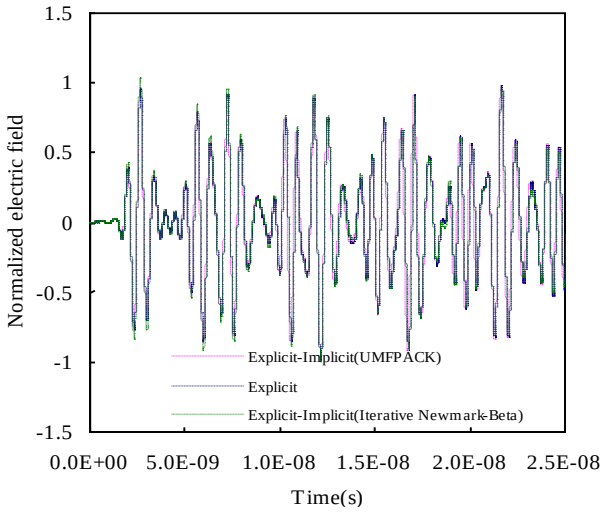

Fig. 4. Electric field in time domain calculated by three methods.

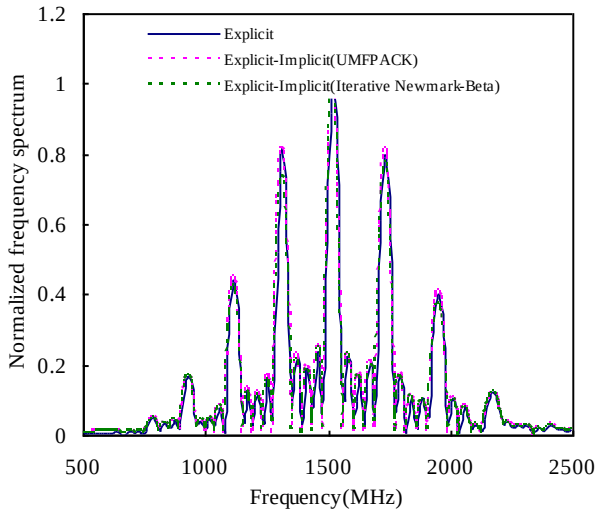

Fig. 5. Normalized frequency spectrum of the electric field.

Table 1: Comparison of the computational cost among the hybrid explicit-implicit SETD method and the traditional SETD method

	Time Step (ps)	CPU Time (min)	Memory (MB)
Explicit	1	67	1156
Explicit-Implicit (UMFPACK)	6.7	23	1639
Explicit-Implicit (Iterative Newmark-Beta)	3.3	25	1264

We can clearly find out that the proposed methods are more efficient in terms of the simulation time. The

explicit-implicit SETD with the UMFPACK solver cost approximate 1/3 simulation time of the traditional method while sacrificed more memory. The iterative Newmark-Beta scheme required a little more CPU time than the UMFPACK method as the time step couldn't be selected too large to ensure the convergence. In this example, the iterative number of the Equation is 8.

V. CONCLUSION

In this paper, we have proposed an explicit-implicit spectral-element time-domain method for the multiscale simulation. Explicit scheme is used in the coarse domain while implicit scheme is used in the fine domain. Explicit scheme can avoid solving the matrix equation. To solve the matrix equation generated by the implicit method, two schemes are developed. The first employs the UMFPACK and the second involves an iterative and explicit method. Comparisons have been made among different methods. The numerical results verify the correctness of the algorithm and demonstrate that the simulation time could be saved as the size of time step is much larger than the one chosen by conventional method. In addition, the method is very efficient when the unknowns of the fine domain are much smaller than those of the coarse domain. Because the discontinuous Galerkin technique is not involved in the proposed methods, conformal mesh grids must be ensured on the interface of different subdomains. How to use the nonconformal grids to make the methods more flexible will be our research topic in the future.

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