

Explicit and Unconditionally Stable Time-Domain Finite-Element Method with a More Than “Optimal” Speedup

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Abstract *The “optimal” speedup of an explicit and unconditionally stable time-domain method, without sacrificing accuracy, is the ratio of the time step required by accuracy to the time step determined by stability. In this work, by significantly accelerating the explicit time-marching-based revealing of the stable modes for any given time step, it is demonstrated that it is feasible to achieve a more than optimal speedup.*

Keywords explicit methods, time-domain methods, unconditionally stable methods, finite-element methods

1. Introduction

Driven by the design of advanced engineering systems, there exists a continued need to accelerate the methods in computational electromagnetics. An explicit time-domain method can be matrix free, i.e., requiring no matrix solution. However, its time step is traditionally restricted by the smallest space step to ensure the stability of a time-domain simulation. When the structure being simulated involves fine features relative to the working wavelength, the time step required for stability can be orders of magnitude smaller than the time step required by accuracy. As a result, one has to simulate a tremendous number of time steps to finish one simulation, which is computationally expensive, although the complexity of the explicit time-domain method is linear (optimal) at each time step.

In time-domain finite-element methods (TDFEMs), a number of unconditionally stable schemes have been developed to remove the dependence of the time step on the space step. Examples include the Newmark method (Gedney & Navsariwala, 1995), the alternation-direction implicit (ADI) finite-element time-domain (FETD; Movahhedi & Abdipour, 2007), the backward difference scheme (Jiao & Jin, 2002), etc. All of these methods are implicit methods that require a matrix solution. They achieve unconditional stability by sacrificing in computational efficiency. Recently, in He et al. (2012) and He and Jiao (2012), an explicit unconditionally stable TDFEM is developed. This method

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retains the strength of an explicit time-domain method in avoiding solving a matrix equation while eliminating its shortcoming in time steps. A significant speedup in CPU time has been accomplished over the conditionally stable explicit TDFEM as well as the unconditionally stable implicit TDFEM.

An explicit and unconditionally stable time-domain method removes the dependence of the time step on the space step. Apparently, the “optimal” speedup of an explicit and unconditionally stable time-domain method, without sacrificing accuracy, is $\Delta t_a/\Delta t_s$, where Δt_a is the time step required by accuracy, and Δt_s is the time step required by stability. Such a speedup is proportional to Δ_a/Δ_{\min} , the ratio of the space step required by accuracy (Δ_a) to the finest space step actually used for discretization (Δ_{\min}). The contribution of this article is the development of an explicit and unconditionally stable TDFEM that has a more than optimal speedup. Numerical experiments have demonstrated its superior efficiency without sacrificing accuracy.

The remaining of this article is organized as follows. Section 2 analyzes the feasibility of achieving a more than optimal speedup; Section 3 presents the proposed method. In Section 4, numerical examples are presented to demonstrate the accuracy and efficiency of the proposed method, and Section 5 concludes this article.

2. On the Feasibility of Achieving a More Than “Optimal” Speedup

A time-domain finite-element-based solution of the second-order vector wave equation and its boundary conditions results in the following linear system of equations (Jiao & Jin, 2002):

$$\mathbf{T} \frac{d^2 u}{dt^2} + \mathbf{S} u = j, \quad (1)$$

in which \mathbf{T} is a mass matrix, \mathbf{S} is a stiffness matrix, u is the unknown field solution vector, and j is a current excitation vector.

The explicit and unconditionally stable TDFEM presented in He et al. (2012) and He and Jiao (2012) has two steps. The first step is a preprocessing step, in which the stable modes are found for the given time step irrespective of its size. In this step, a conventional explicit time-domain method is employed to solve Eq. (1) at a small number of time steps. The resulting time-domain solutions are then used to synthesize the stable modes by an efficient algorithm. By doing so, advantage is gained of the strength of an explicit method in avoiding a matrix solution. Meanwhile, there is no suffering from the shortcoming of an explicit method in requiring many time steps to finish one simulation. This is because compared to the total number of time steps required by the explicit method to finish the entire simulation, the number of time steps is small for revealing the stable modes from the time-domain solutions. The detailed procedure of the aforementioned preprocessing step (He et al., 2012) is as follows.

Step I. Preprocessing for building a complete and accurate space that spans all the stable modes for any given time step irrespective of its size.

Step I-1. Use the conventional explicit time-domain method to solve Eq. (1) and march on in time by one step. This can be performed in linear complexity.

Step I-2. At selected time instants, the number of which is $O(k)$, where k is the number of physically important modes contained in Eq. (1), perform the following.

Step I-2-a. Add the field solution vector u in \mathbf{V} as a column vector. Matrix \mathbf{V} is initialized to be zero. Orthogonalize the new solution vector with respect to the other vectors that have already been stored in \mathbf{V} . The column dimension of the orthogonalized \mathbf{V} is denoted by k' . The computational cost is linear for orthogonalizing $O(k')$ vectors of length N .

Step I-2-b. Solve a reduced eigenvalue problem of size k' shown below:

$$\mathbf{B}_{k' \times k'} \phi = \lambda^2 \mathbf{A}_{k' \times k'} \phi, \quad (2)$$

where

$$\mathbf{A}_{k' \times k'} = \mathbf{V}^T \mathbf{T} \mathbf{V}, \quad \mathbf{B}_{k' \times k'} = \mathbf{V}^T \mathbf{S} \mathbf{V}. \quad (3)$$

Solve the weight \tilde{y} of each mode in the field solution from Eq. (30) in He et al. (2012). Weight \tilde{y} can also be determined by writing the field solution u as

$$u = \Phi_r \tilde{y}, \quad (4)$$

where Φ_r denotes the eigenvector matrix of Eq. (2). Multiplying both sides of Eq. (4) by $\Phi_r^T \mathbf{A}$, and utilizing the property of $\Phi_r^T \mathbf{A} \Phi_r = \mathbf{I}$, the weight \tilde{y} can be obtained as

$$\Phi_r^T \mathbf{A} u = \tilde{y}. \quad (5)$$

Then it is determined whether or not two criteria are satisfied to terminate the preprocessing step. The first terminating criterion is to assess whether or not the repeating eigenmodes are dominant in the field solution. When progressively enlarging \mathbf{V} and solving Eq. (2) step by step, some eigenvalues will repeatedly appear from the solution of Eq. (2). Denoting the weights of their corresponding eigenvectors in the field solution by \tilde{y}_l and the weights of the other eigenvectors by \tilde{y}_h , the first terminating criterion is

$$|\tilde{y}_h^T \tilde{y}_h| < \varepsilon_1 |\tilde{y}_l^T \tilde{y}_l|, \quad (6)$$

in which ε_1 is a small parameter defined based on prescribed accuracy. When Eq. (6) is satisfied, the repeating eigenmodes can be identified as physically important modes in the field solution. But to ensure the accuracy of the identified physically important eigenmodes, the second terminating condition is added as follows:

$$\frac{|\lambda_l^{q+1} - \lambda_l^q|}{|\lambda_l^q|} < \varepsilon_2, \quad (7)$$

where λ_l denotes the eigenvalues that repeatedly appear from the solution of Eq. (2), and ε_2 is the other user-defined accuracy parameter. In Eq. (7), the difference between the repeating eigenvalues at two adjacent steps, q and $q + 1$, is examined. When both Eqs. (6) and (7)

are satisfied, the corresponding repeating eigenmodes can be identified as accurate, physically important eigenmodes of the original physical problem, from which those eigenmodes that are stable for the given time step are selected to build the space of stable modes. The preprocessing step is then terminated. If either Eq. (6) or (7) is not satisfied, return to Step I-1. The cost of the above step (Step I-2-b) is negligible because of the reduced system size.

In the second step of the method in He et al. (2012), an explicit and unconditionally stable time marching for the given time step is performed, regardless of how large it is. The simulation is performed on a reduced and also *diagonal* system of $O(k)$, and hence, the cost of the second step is negligible as compared to the cost of the first step.

As can be seen from the above overview of the explicit and unconditionally stable TDFEM in He et al. (2012), the speedup of this method over the traditional explicit method is

$$\text{Speedup} \sim N_t/p, \quad (8)$$

where p is the number of time steps simulated in the preprocessing step, and N_t is the total number of time steps required to finish the entire explicit-marching-based simulation.

The optimal speedup of an explicit and unconditionally stable time-domain method over a traditional explicit method, as noted in Section 1, is

$$\text{Optimal Speedup} \sim \Delta_a/\Delta_{\min}. \quad (9)$$

To analyze the relationship between Eqs. (8) and (9), one should begin with the total time T to be simulated. T is proportional to l_{\max}/c , where l_{\max} is the largest physical dimension of the structure being simulated, and c is the speed of light. In other words, in general, in a time-domain analysis, the entire structure of the underlying problem needs to be traversed at least once by the input pulse. With a time step chosen based on stability, N_t is proportional to $l_{\max}/(c\Delta t_s)$, and hence, l_{\max}/Δ_{\min} . Therefore, N_t/p is proportional to

$$\text{Speedup} \sim N_t/p \sim l_{\max}/(p\Delta_{\min}). \quad (10)$$

Comparing Eq. (10) to Eq. (9), it is evident that by minimizing p , a more than optimal speedup can be achieved.

3. Proposed Method

To minimize the number of time steps p simulated in the preprocessing step, a theoretical analysis is first conducted on what prevents early identification of the stable modes in an explicit time-marching-based scheme. The preprocessing scheme in He et al. (2012) was analyzed, and it was found that its explicit time-marching-based revealing of stable modes can be viewed as an iterative process of finding the stable modes. Although it is matrix free, it has a slow convergence rate, which prevents an early identification of the stable modes, thereby achieving an optimal or even more than optimal speedup. Based on this finding, a new algorithm is developed that significantly increases the convergence rate of each non-DC stable mode while preserving the merit of the explicit-method-based revealing of the stable modes in avoiding solving a matrix. Moreover, it was found that the DC mode, the analytical eigenvalue of which is zero, has the slowest convergence

rate, which cannot be increased by changing time-stepping formulas. It is hence proposed to extract the DC mode and then remove the DC mode from the procedure of identifying other non-DC stable modes. As a result, the number of time steps simulated in the preprocessing step p is significantly reduced. The details of the proposed work are presented in what follows.

3.1. Theoretical Analysis

The solution of Eq. (1) at any time instant is a superposition of the eigenmodes of the following generalized eigenvalue problem:

$$\mathbf{S}v = \lambda \mathbf{T}v. \quad (11)$$

Since \mathbf{S} is semi-positive definite and \mathbf{T} is positive-definite, the eigenvalues λ are non-negative real values. The smallest eigenvalues are zero, and their corresponding eigenvectors are called DC modes. Let Φ be the eigenvector matrix of Eq. (11), Λ be the diagonal matrix comprised of the eigenvalues of Eq. (11), and \mathbf{I} be an identity matrix. The following properties hold true:

$$\Phi^T \mathbf{T} \Phi = \mathbf{I}, \quad \Phi^T \mathbf{S} \Phi = \Lambda. \quad (12)$$

In He et al. (2012), the stable modes were synthesized from the following traditional central-difference-based explicit marching of Eq. (1):

$$\mathbf{T}(u^{n+1} - 2u^n + u^{n-1}) + \Delta t^2 \mathbf{S}u^n = \Delta t^2 j^n. \quad (13)$$

Expanding the field solution u in Φ as

$$u = \Phi y \quad (14)$$

and multiplying Eq. (13) by Φ^T gives

$$(y^{n+1} - 2y^n + y^{n-1}) + \Delta t^2 \Lambda y^n = \Delta t^2 \Phi^T j^n, \quad (15)$$

where the properties shown in Eq. (12) are utilized. Setting the source to be zero and performing a z -transform of Eq. (15) gives

$$(z - 1)^2 + \Delta t^2 \lambda_i z = 0, \quad (16)$$

where λ_i is an eigenvalue of Eq. (11). The roots of Eq. (16) can be written as

$$z = \frac{(2 - \Delta t^2 \lambda_i) \pm \sqrt{\Delta t^2 \lambda_i (\Delta t^2 \lambda_i - 4)}}{2}. \quad (17)$$

To make Eq. (13) stable, $|z| \leq 1$ must be satisfied, from which $\Delta t^2 \lambda_i < 4$ can be deduced. When this happens, it can be seen from Eq. (17) that

$$|z| = 1. \quad (18)$$

Thus, for every eigenmode of Eq. (11), the magnitude of z is the same.

In Eq. (15), not only is z related to the stability, it also signifies the convergence rate of each eigenmode in the time-marching procedure. To explain, take one frequency

component contained in the input spectrum as an example. For such a single-frequency sinusoidal input, in Eq. (15), when the z -transform of y converges to a constant, the solution of y reaches its steady state. Since $\tilde{Z}(y^{n+1}) - \tilde{Z}(y^n) = z[\tilde{Z}(y^n) - \tilde{Z}(y^{n-1})]$, where $\tilde{Z}(\cdot)$ denotes the z -transform of a set, by recursively applying the equality, the following can be obtained:

$$\tilde{Z}(y^{n+1}) - \tilde{Z}(y^n) = z^n [\tilde{Z}(y^1) - \tilde{Z}(y^0)]. \quad (19)$$

Therefore, the smaller $|z|$ is, the faster the convergence is. In other words, the convergence of the z -transform y can be achieved with a smaller n , thus a smaller number of steps. As a result, it is found that when using a central-difference-based explicit marching, like that in Eq. (13), the convergence rate of every eigenmode in the field solution, as shown in Eq. (18), is the same and is also equally slow.

3.2. Proposed Method for Achieving a More Than Optimal Speedup

Based on the above finding, increasing the convergence rate of the eigenmodes is proposed. The reason is straightforward. If an eigenmode converges earlier, it will show up earlier in the reduced eigenvalue problem in Eq. (2) as a repeating eigenmode. Therefore, this eigenmode can be identified in a reduced number of steps. To increase the convergence rate, performing the following backward-difference-based time marching is proposed:

$$(\mathbf{T} + \Delta t^2 \mathbf{S})u^{n+1} + \mathbf{T}(-2u^n + u^{n-1}) = \Delta t^2 j^n, \quad (20)$$

but by using a central-difference based time step. By doing so, on one hand, expensive matrix solutions are avoided because the solution of $(\mathbf{T} + \Delta t^2 \mathbf{S})$ can be found from the solution of \mathbf{T} , the mass matrix that is either diagonal or can be solved in linear complexity (White, 1999; Jiao & Jin, 2003; Chen & Jiao, 2009). This is because choosing a central-difference-based time step satisfies $\|\Delta t^2 \mathbf{T}^{-1} \mathbf{S}\| < 1$, and thereby $(\mathbf{T} + \Delta t^2 \mathbf{S})^{-1} = (\mathbf{I} + \mathbf{B} + \mathbf{B}^2 + \dots) \mathbf{T}^{-1}$ with $\mathbf{B} = -\Delta t^2 \mathbf{T}^{-1} \mathbf{S}$, which can converge in a few terms. The computational cost of multiplying $(\mathbf{T} + \Delta t^2 \mathbf{S})^{-1}$ by any vector is simply the cost of a few matrix-vector multiplications of either $\mathbf{T}^{-1}b$ or $\mathbf{S}b$ type, with b being a vector. By taking $\mathbf{B}\mathbf{T}^{-1}f$ as an example, with f being a vector, it can be done in sequence from right to left, which consists of one linear-complexity computation of $f_1 = \mathbf{T}^{-1}f$, since \mathbf{T} is either diagonal in nature or can be solved in linear complexity, with one sparse matrix-vector multiplication $\mathbf{S}f_1$ denoted by f_2 and another linear-complexity computation for obtaining $f_3 = -\Delta t^2 \mathbf{T}^{-1}f_2$. After computing $\mathbf{B}\mathbf{T}^{-1}f$, the result of which, denoted by f_3 , can be reused for the following computation, since $\mathbf{B}^2 \mathbf{T}^{-1}f$ can be computed as $\mathbf{B}f_3$ instead of starting from scratch. The same approach applies to the following terms.

In addition to avoiding expensive matrix solutions, the scheme shown in Eq. (20) also accelerates the convergence of the eigenmodes, since now

$$|z| = \frac{1}{\sqrt{(1 + \Delta t^2 \lambda_i)}}, \quad (21)$$

which can be obtained by performing a z -transform of Eq. (20). As a result, the convergence of all the non-DC eigenmodes of Eq. (11) is accelerated. However, the DC eigenmodes, whose analytical eigenvalues are zero, have the same slow convergence rate as that in the original central-difference-based explicit marching. As a result, even

though non-DC modes converge in a much smaller number of time steps, as long as the DC mode has not converged to its accurate value, the inaccurate DC mode can delay the accurate identification of other non-DC modes. In addition, the DC mode must still be accurately obtained before terminating the preprocessing step for applications where DC modes play an important role in the field solution. If the DC modes can be removed from the preprocessing step, the preprocessing time to identify the non-DC stable modes can greatly be shortened, while the DC mode can be separately extracted. Hence, it is proposed to update the preprocessing scheme for finding the stable modes by changing Step I-2-a as follows.

In Step I-2-a shown in Section 2, instead of adding the field solution vector u in \mathbf{V} , field solution u is added with its DC-mode component excluded. Thus,

$$\mathbf{V} = [u(t_1) - u_0(t_1); u(t_2) - u_0(t_2); \dots], \quad (22)$$

where $u_0(t_i)$ denotes the DC-mode component of the field solution at time instant t_i . $u_0(t_i)$ can be found in the following way. The field solution $u(t)$ at any time can be written as

$$u(t) = \Phi_0 y_0 + \Phi_h y_h = u_0(t) + \Phi_h y_h, \quad (23)$$

where Φ_0 denotes the eigenvectors corresponding to the zero eigenvalues of Eq. (11), thus being DC modes; Φ_h denotes the rest of the eigenvectors; and

$$u_0(t) = \Phi_0 y_0. \quad (24)$$

Multiplying $\Phi_0^T \mathbf{T}$ on both sides of Eq. (23) and utilizing the property of $\Phi^T \mathbf{T} \Phi = \mathbf{I}$ gives

$$\Phi_0^T \mathbf{T} u(t) = y_0. \quad (25)$$

Substituting Eq. (25) into Eq. (24),

$$u_0(t) = \Phi_0 \Phi_0^T \mathbf{T} u(t). \quad (26)$$

The number of DC modes can be large since the nullspace of Eq. (11) is large. However, all eigenvectors in the nullspace (Φ_0) share a common zero eigenvalue. For a given right-hand side b , their contributions to the field solution can be represented by a single vector, $\mathbf{V}_0 \mathbf{V}_0^T b$, for any frequency and at any time (Zhu & Jiao, 2012). Denoting this single vector by w_0 , it is orthogonalized with respect to \mathbf{T} . $u_0(t)$ in Eq. (26) can then be obtained as

$$u_0(t) = w_0 w_0^T \mathbf{T} u(t). \quad (27)$$

Next, it is shown how to quickly obtain w_0 .

The single vector w_0 , which carries the contributions to the field solution from all null-space eigenvectors for a given right-hand side, can be obtained by solving the frequency-domain counterpart of Eq. (1) at one relatively low frequency (Zhu & Jiao, 2012) as follows:

$$(S - \omega^2 \mathbf{T}) \tilde{u} = \tilde{j}, \quad (28)$$

where \tilde{u} and \tilde{j} are the frequency-domain counterparts of u and j , respectively. When the problem size is large, solving Eq. (28) can still be a computational challenge. This

challenge can be overcome by a rigorous divide-and-conquer algorithm for fast DC-mode extraction (He & Jiao, 2013). In this algorithm, the original large-scale system matrix shown in Eq. (28) is rigorously decomposed into small sparse matrices that are fully decoupled, and then the solution of Eq. (28) is synthesized from the null-space of the small sparse matrices.

Except for the change of Step I-2-a based on the aforementioned algorithm, the other steps in the preprocessing scheme of He et al. (2012), summarized in Section 2, remain the same. With the aforementioned algorithm, all non-DC stable modes are found in a significantly reduced number of time steps, thus reducing p . Combining the non-DC stable modes identified from the updated preprocessing scheme with the DC-mode w_0 separately extracted from Eq. (28), the space of stable modes is completed based on the second step; i.e., explicit and unconditionally stable time marching can be performed.

4. Numerical Results

The first example is a parallel plate whose height, width, and length are 1, 2, and 900 μm , respectively. The computational domain is truncated by a perfect electric conductor (PEC) on the top and at the bottom, a perfect magnetic conductor (PMC) on the left and right boundaries, and two air regions backed by the first-order absorbing boundary conditions in the front and at the back. The space resolution along x , y , and z is 1, 1, and 300 μm , respectively. The parallel plate structure is excited by a current source launched from the bottom plate to the top plate at the near end, while the voltages are extracted between the two plates at the near and far ends. The current source is the derivative of a Gaussian pulse with $I(t) = 2(t - t_0) \exp(-(t - t_0)^2/\tau^2)$, where $t_0 = 3\tau$ and $\tau = 8 \times 10^{-11}$ sec.

The time step required by accuracy is 10^{-13} sec, and that by stability is 10^{-15} sec, yielding an optimal speedup of 100. The method in He et al. (2012) requires 1,900 steps of explicit time marching in the preprocessing procedure to build an accurate and complete space of stable modes for the given time step of 10^{-13} sec. In contrast, the proposed fast method only costs 600 time steps in finding the same set of non-DC stable modes. The accuracy parameters ε_1 and ε_2 , used in Eqs. (6) and (7), are chosen as 10^{-3} and 10^{-2} , respectively. The time-domain solutions are sampled every 50 steps to perform the computing tasks in Step I-2 shown in Section 2. The square roots of the non-DC stable modes are found to be 3.684×10^{11} , 7.965×10^{11} , 1.141×10^{11} , 1.827×10^{12} , and 1.849×10^{12} rad/s, respectively. The DC mode for the given right-hand side is extracted by the fast DC-mode extraction algorithm (He & Jiao, 2013) at 5 GHz with negligible cost. To finish the entire time-domain simulation in a time window of 0.5 ns, the conventional explicit time-domain method must simulate 5×10^5 steps. The speedup of the proposed method, $\sim 5 \times 10^5/600$, is over 800 as compared to the conventional explicit time-domain method and is hence much more than the optimal speedup 100 in this example. The voltages waveforms sampled at the near and far ends of the structure, as shown in Figure 1, agree very well with those obtained from the conventional explicit time-domain method.

The second example is a 600- μm -long on-chip interconnect with three metal layers and four dielectric layers, as shown in Figure 2 (He et al., 2012). The relative permittivity ε_r is given on the left-most side of the figure from the bottom layer to the top layer. The thickness of each layer is shown on the right-most side, with the unit

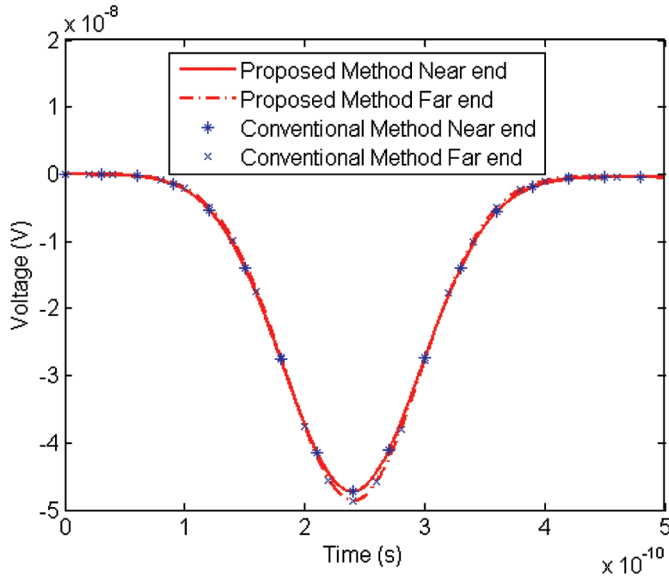


Figure 1. Voltage waveforms of parallel-plate structure simulated from the proposed method in comparison with reference solutions.

being $0.1 \mu\text{m}$. The width of each segment along the horizontal y -direction is also listed in Figure 2. The current source is the same as that used in the first example, and it is launched from the bottom metal plate to the center wire as well as from the top metal plate to the center wire, as shown by the arrows in middle of the figure. The computational domain is truncated by the same conditions as used in the first example. The time step required by accuracy is 8×10^{-13} sec, and that by stability is 10^{-16} sec, yielding an optimal speedup of 8,000. The method in He et al. (2012) requires 14,800 steps of explicit marching in the preprocessing procedure to build an

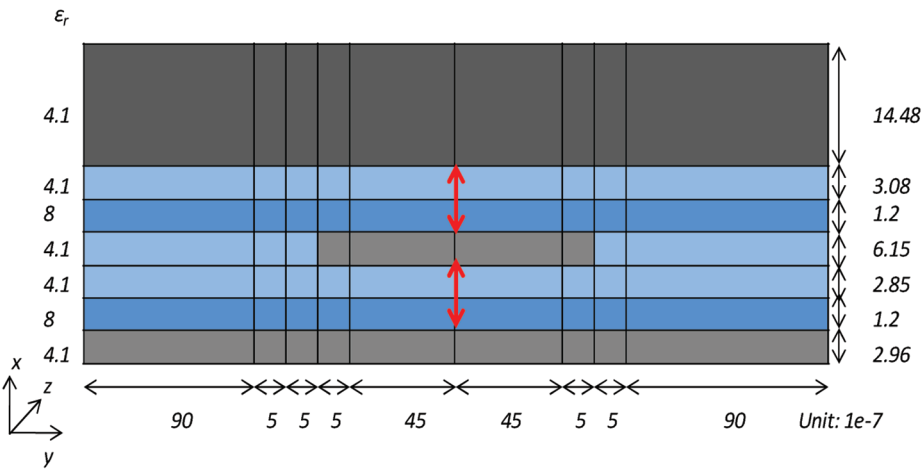


Figure 2. Cross-sectional view of 3D on-chip interconnect (geometrical unit is $0.1 \mu\text{m}$).

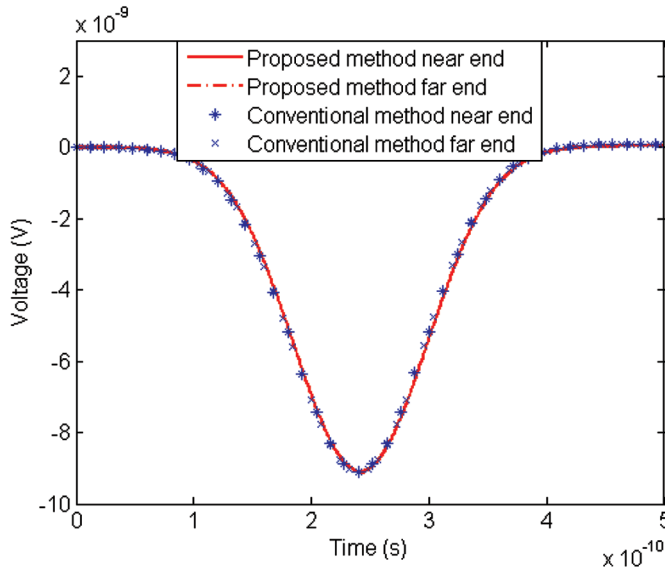


Figure 3. Voltage waveforms of 3D on-chip interconnect simulated from the proposed method in comparison with reference solutions.

accurate and complete space of stable modes for the given time step of 8×10^{-13} sec. In contrast, the proposed fast method only needs 1,800 time steps to find the same space of stable modes accurately. The accuracy parameters ε_1 and ε_2 are both chosen as 10^{-3} . Two non-DC stable modes are identified from the updated preprocessing step, the square roots of whose eigenvalues are 7.20873×10^{11} and 1.57404×10^{12} rad/s, respectively. The DC-mode is separately extracted by solving Eq. (28) at 5 GHz using the fast algorithm in He and Jiao (2013). To finish the entire time-domain simulation in a time window of 2 ns, the speedup of the proposed method is approximately $2 \times 10^7/1,800$ over the conventional explicit time-domain simulation, which is more than optimal. Once again, excellent agreement with reference solutions is observed in the time-domain results, as can be seen from Figure 3.

5. Conclusions

The optimal speedup of an explicit and unconditionally stable time-domain method, without sacrificing accuracy, is the ratio of the time step required by accuracy to the time step determined by stability. This work develops an explicit and unconditionally stable TDFEM with a speedup greater than optimal speedup. Numerical experiments have demonstrated its superior performance.

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