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Abstract

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Abstract—The root cause of the instability is quantitatively identified for the explicit time-domain finite-element method that employs a time step beyond that allowed by the stability criterion. With the identification of the root cause, an unconditionally stable explicit time-domain finite-element method is successfully created. This method is unconditionally stable in the sense that it is stable for any time step no matter how large the time step is. The proposed method retains the strength of an explicit time-domain method in being matrix free while eliminating its shortcoming in time step. Numerical experiments have demonstrated the superior performance of the proposed method in computational efficiency as well as stability compared to the conditionally stable explicit method and the unconditionally stable implicit method. The essential idea of the proposed method for achieving unconditional stability in an explicit method is also applicable to other time domain methods.

Keywords— *explicit time-domain methods; unconditionally stable methods; time-domain finite-element methods; stability*

I. INTRODUCTION

The time-domain methods in computational electromagnetics can be categorized into two classes. One is the explicit time-domain method; the other is the implicit time-domain method. In an explicit time-domain method, the field solution at each time step is evaluated from the field solutions at previous time steps, which are known; whereas in an implicit time-domain method, the field solution at each time step involves the field solution that is unknown. Explicit methods can avoid solving a matrix, while implicit methods generally require a matrix solution.

Despite its advantage of being matrix free, an explicit method requires the time step to be restricted by the smallest space step for ensuring stability. For problems that have fine features relative to working wavelength like on-chip integrated circuits, explicit methods require a large number of time steps to finish one simulation, which is computationally expensive. Existing unconditionally stable methods (methods that permit the use of any large time step without becoming unstable) are all implicit methods. In the FDTD based methods, a family of implicit schemes [1-9] such as the ADI (alternating direction implicit)-FDTD [1-3], the CN (Crank-Nicolson)-FDTD [4], the LOD (locally one-dimensional)-FDTD [5], the Laguerre-FDTD [6], and the split-step FDTD [8] methods have been developed to achieve unconditional stability. In [7], it is shown that these unconditionally stable implicit FDTD methods can be derived from a general formulation based on generalized matrix operator equations pertaining to some classical splitting formulae, from which a variety of other unconditionally stable implicit schemes can also be deduced.

Similarly, a group of unconditionally stable time-domain finite-element methods (TDFEM) such as the Newmark method [10], ADI-FETD [11], the CN-FETD [12], and the backward difference method have also been developed. They require the solution of the sum of the mass matrix and the stiffness matrix, whereas the explicit TDFEM only requires the solution of the mass matrix, which is either diagonal in nature or can be diagonalized by the orthogonal vector basis functions [13-15], and hence becoming matrix free. In summary, the large time step provided by the existing unconditionally stable schemes is achieved by resorting to implicit time-domain methods that sacrifice in computational efficiency. Moreover, late-time instability has also been observed from implicit methods. In [16], a new FDTD method using the alternating-direction explicit (ADE) method was developed for efficient electromagnetic field simulation. The method is explicit. However, it is not unconditionally stable. Recently, research has also been done to extend the stability limit of the explicit FDTD method by spatial filtering [17]. As yet, no explicit methods have achieved unconditional stability.

The research question considered in this work is: can an explicit method be made unconditionally stable so that its matrix-free strength can be retained and its shortcoming in time step can be eliminated?

The contribution of this work is the successful development of an explicit time-domain method that is unconditionally stable, a capability that does not exist previously. We have done preliminary research on the proposed work in [18-19]. In this paper, we complete it from both theoretical and numerical perspectives. The paper is organized as follows. In Section II, we present the background of a time-domain finite-element method. In Section III, we describe the proposed theory for making an explicit time-domain method unconditionally stable. In Section IV, we propose an explicit time-domain finite-element method that is unconditionally stable. The linear computational complexity of an explicit method at each time step is preserved by the proposed method. Section V demonstrates the unconditional stability, accuracy, and efficiency of the proposed method. It is also shown that the proposed unconditionally stable *explicit* method outperforms both the conditionally stable explicit method and the unconditionally stable implicit method in computational efficiency. Although the proposed method is presented in the framework of a time-domain finite-element method, the essential idea can be applied to other time domain methods and, hence, contributing to the removal of one major computational bottleneck in time-domain electromagnetic analysis.

II. BACKGROUND OF A TIME-DOMAIN FINITE-ELEMENT METHOD

Consider the second-order vector wave equation

$$\nabla \times [\mu_r^{-1} \nabla \times \mathbf{E}(\mathbf{r}, t)] + \mu_0 \varepsilon \partial_t^2 \mathbf{E}(\mathbf{r}, t) = -\mu_0 \partial_t \mathbf{J}(\mathbf{r}, t), \quad (1)$$

where \mathbf{E} is electric field, μ_0 is free-space permeability, μ_r is relative permeability, ε is permittivity, and \mathbf{J} is current density. A time-domain finite-element based solution of (1) and its boundary conditions results in the following system of linear equations [20]:

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

in which \mathbf{T} is called a mass matrix, \mathbf{S} is called a stiffness matrix, u is the unknown field vector, and j is a current excitation vector. The \mathbf{T} and \mathbf{S} are sparse and symmetric. Typically they have only tens of nonzero elements in each row regardless of the matrix size N . These matrices can be assembled in linear time and storage from their elemental contributions as follows:

$$\begin{aligned} \mathbf{T}_{ij} &= \mu_0 \varepsilon \langle \mathbf{N}_i, \mathbf{N}_j \rangle_V, \\ \mathbf{S}_{ij} &= \mu_r^{-1} \langle \nabla \times \mathbf{N}_i, \nabla \times \mathbf{N}_j \rangle_V, \\ j &= -\mu_0 \langle \mathbf{N}_i, \partial_t \mathbf{J} \rangle_V, \end{aligned} \quad (3)$$

where \mathbf{N}_i and \mathbf{N}_j are the vector basis functions used to expand \mathbf{E} and $\langle \cdot, \cdot \rangle_V$ denotes a volume integration in each element.

Compared to other time-domain methods, a time-domain finite-element method possesses flexibility in both geometrical modeling and material modeling.

III. PROPOSED THEORY FOR MAKING AN EXPLICIT TIME-DOMAIN METHOD UNCONDITIONALLY STABLE

A. Quantitative Analysis on the Root Cause of the Instability When Using a Time Step beyond Stability Criterion

In this section, we will use the time-domain finite-element method as an example to develop a quantitative analysis on the root cause of the instability associated with an explicit time-domain method when a time step beyond stability criterion is used. However, the findings are equally applicable to other time-domain methods.

In an explicit time-domain finite-element method, to maintain stability, the time step is required to satisfy [21]

$$\Delta t \leq 2 / \sqrt{\rho(\mathbf{T}^{-1}\mathbf{S})}, \quad (4)$$

where $\rho(\mathbf{T}^{-1}\mathbf{S})$ denotes the spectral radius of $\mathbf{T}^{-1}\mathbf{S}$, which is the largest eigenvalue of $\mathbf{T}^{-1}\mathbf{S}$. Since the largest eigenvalue of $\mathbf{T}^{-1}\mathbf{S}$ that is supported by a numerical system is inversely proportional to the smallest space resolution, like the CFL condition in explicit FDTD-based methods [22], (4) also dictates that the time step for a stable simulation is dependent on the smallest space step. Since $\rho(\mathbf{T}^{-1}\mathbf{S})$ is nonzero, apparently, there is no obvious way to make an explicit scheme stable for any large time step, i.e., unconditionally stable. However, from the following quantitative analysis on the root cause of the instability, it will become clear that it is feasible to make an explicit time-domain method unconditionally stable.

The solution of (2) can be rigorously found by first solving the following generalized eigenvalue problem:

$$\mathbf{S} \phi = \lambda^2 \mathbf{T} \phi, \quad (5)$$

then expand the field solution vector u in the space formed by all the eigenvectors of (5), and then find the coefficient of each eigenvector in the field solution u [23]. This approach is also known as modal superposition method [24].

Let $[\Phi, \mathbf{D}]$ be the solution to the generalized eigenvalue problem shown in (5), in which the entries of diagonal matrix \mathbf{D} are eigenvalues $\lambda_1^2, \lambda_2^2, \dots, \lambda_N^2$, and the column vectors of Φ are eigenvectors $\phi_1, \phi_2, \dots, \phi_N$. Physically speaking, $\lambda_1, \lambda_2, \dots, \lambda_N$ are the angular resonance frequencies of the 3-D structure being simulated, which have the same unit as ω ; and the eigenvectors of (5) represent the 3-D resonance modes that can be intrinsically supported by the 3-D structure. Since \mathbf{T} is symmetric positive definite and \mathbf{S} is symmetric, the eigenvectors of (5) are \mathbf{T} - and \mathbf{S} -orthogonal [25]. As a result, we have

$$\Phi^T \mathbf{T} \Phi = \mathbf{I}, \quad \Phi^T \mathbf{S} \Phi = \mathbf{D}, \quad (6)$$

where \mathbf{I} is an identity matrix. The solution of (2) can then be rigorously expanded in the eigenspace Φ

$$u(t) = \Phi y(t), \quad (7)$$

where the unknown coefficient vector y contains all the weights of the eigenvectors in the field solution. From (7), it can be seen that the field solution at each time instant in an arbitrary 3-D problem is the superposition of the 3-D eigenvectors (modes). To obtain unknown coefficient y , we substitute (7) into (2). Multiplying both sides of (2) by Φ^T , and using the property shown in (6), we obtain

$$\frac{d^2 y}{dt^2} + \mathbf{D} y = \Phi^T j. \quad (8)$$

A central-difference based explicit solution to the above yields

$$y^{n+1} = 2y^n - y^{n-1} - \Delta t^2 \mathbf{D} y^n + \Phi^T b^n, \quad (9)$$

where $b^n = \Delta t^2 j^n$. To analyze the stability of (9), we set the excitation to be zero and perform a z -transform of (9), we obtain

$$(z-1)^2 + \Delta t^2 \mathbf{D} z = 0. \quad (10)$$

For an explicit time marching like (9) to be stable, $|z|$ of (10) should be bounded by 1. As a result, the following condition must be satisfied:

$$\Delta t^2 \lambda_i^2 \leq 4, \quad i=1, 2, \dots, N, \quad (11)$$

where eigenvalue λ_i^2 is the i -th entry of the diagonal matrix \mathbf{D} , and N is matrix size.

Due to the property of \mathbf{T} (positive definite) and \mathbf{S} (semi-positive definite), the eigenvalues of (5), λ_i^2 , are nonnegative. The smallest eigenvalue of (5) is zero, which is due to the null space of the stiffness matrix \mathbf{S} . These zero eigenvalues always exist. The corresponding eigenvector is called DC mode. Despite its zero eigenvalue, a DC mode can also have a complicated field distribution such as the DC mode of an integrated circuit made of multiple metallic wires immersed in dielectric materials. As for the largest eigenvalue of (5), although theoretically speaking, the resonance frequency of a 3-D structure, and hence the eigenvalues of (5), can be infinitely large, the largest eigenvalue that can be numerically found is limited by the smallest space resolution. To be

specific, the square root of the maximum eigenvalue of (5), λ_{\max} , is inversely proportional to the smallest space resolution Δ_{\min} as the following:

$$\lambda_{\max} \sim O(\pi c / \Delta_{\min}). \quad (12)$$

where c is speed of light. This is because given the smallest space step Δ_{\min} , the minimum wavelength that can be captured by the space discretization is $2\Delta_{\min}$. The angular frequency corresponding to such a wavelength is $\pi c / \Delta_{\min}$. From (12), it is clear that the smaller the space step, the larger the maximum eigenvalue that can be numerically supported by (5).

The meaning of (11) is significant. It demonstrates that when an explicit method becomes unstable, among all the eigenvectors ϕ_i (modes) that are contained in the field solution shown in (7), not every mode becomes unstable. Only a subset of the modes, whose eigenvalues are so large that (11) is violated, is unstable. The rest of the modes are stable. For example, the DC modes, whose eigenvalues are zero, are always stable irrespective of the choice of time step. Therefore, **we conclude that the set of modes that violate (11) in the field solution are the root cause of the instability associated with an explicit time-domain method when a large time step is used.** The λ_i in (11) is an angular resonance frequency of the 3-D system. When (11) is violated, $\Delta t > 2 / \lambda_i = 1 / (\pi f_i)$, where f_i is the frequency corresponding to λ_i . Therefore, **given a time step Δt , the unstable modes are also those modes which vary with space at such a high frequency that it cannot be accurately captured by the given time step based on sampling theorem.**

The remaining question is why these unstable modes exist? They exist because of fine discretization as can be seen from (12). A fine discretization cannot be avoided in problems having fine feature sizes relative to working wavelength. The finer the space discretization, the larger the maximum eigenvalue that can be intrinsically supported by (5). Once these unstable modes, which have eigenvalues beyond what can be accurately captured by the given time step, are supported by (5), even though the right hand side b does not have a projection onto them, the numerical round off error will have a projection onto them. This can be seen clearly from (9). The (9) is a diagonal system of equations with the i -th entry in vector y , y_i , representing the coefficient of the i -th mode of (5). It is clear that even though $\Phi_i^T b^n$ is zero, the round-off error can make y_i not zero. As a result, in the field expansion shown in (7), the coefficients of the unstable modes would not be zero, and hence the unstable modes exist in the field solution at each time instant. Meanwhile their eigenvalues are so large, i.e. these modes vary with space at such a high frequency that they cannot be accurately simulated by the given time step, and hence instability occurs.

The above analysis also shows clearly why in the case where fine features do not exist, and hence the space step can be solely determined by accuracy, the time step suggested by the stability criterion has a good correlation with that required by accuracy. In this case, the frequency corresponding to the maximum eigenvalue of (5) agrees well with the physically

important maximum frequency to be captured. Therefore, $\lambda_{\max} \sim 2\pi f_{\max}$, where f_{\max} is the physically important maximum frequency to be captured. As a result, the time step suggested by stability criterion (4) has a good correlation with that dictated by accuracy for sampling an f_{\max} -based system.

B. How to Make an Explicit Time-Domain Method Unconditionally Stable

From the aforementioned root cause analysis, it becomes clear how to make an explicit method unconditionally stable, i.e. stable for any large time step. **Given a time step Δt regardless of how large it is, one can correspondingly remove those modes whose field variation with space cannot be accurately simulated by the given time step based on sampling theorem. For a time-domain finite-element method, quantitatively, we remove those modes that violate (11), i.e., those modes whose eigenvalues are greater than $4 / \Delta t^2$, out of the numerical system.** By doing so, an explicit method can be made stable for any large time step. In the extreme case that $\Delta t = \infty$, one can, also, make an explicit method stable by simply keeping all the null-space modes whose eigenvalues are zero and removing all the modes having nonzero eigenvalues.

Denoting the coefficient vector y in (7) by

$$y = \begin{bmatrix} y_l \\ y_h \end{bmatrix}, \quad (13)$$

where y_h is a coefficient vector of unstable modes whose eigenvalues are greater than $4 / \Delta t^2$, and y_l is for the stable modes for the given time step Δt . To clean up the unstable modes, what one only needs to do is to set y_h to be zero at each time step:

$$y_h = 0, \quad (14)$$

for modes which vary with space at an angular frequency higher than $2 / \Delta t$.

C. How to Make an Explicit Time-Domain Method Unconditionally Stable and Accurate

To satisfy accuracy criterion, the time step cannot be chosen arbitrarily large, it has to satisfy sampling theorem, i.e.,

$$\Delta t < 1 / (2f_{\max}), \quad (15)$$

where f_{\max} corresponds to the smallest wavelength, and hence the maximum frequency of space variation that is physically important in a system response. For good accuracy, the time step is generally chosen as

$$\Delta t \leq 1 / (10f_{\max}). \quad (16)$$

In other words, in one wavelength, one should at least sample 10 points for achieving a good accuracy.

Based on the analysis given in previous section, for any given Δt , to make an explicit time-domain scheme stable, we should remove the modes having eigenvalues greater than $4 / \Delta t^2$. For a time step given in (16) that is solely

determined by accuracy, the modes that are removed are also physically negligible. This is because the removed modes have eigenvalues greater than $4/\Delta t^2$, by using (16), we have

$$\lambda_i^2 > 4/\Delta t^2 \geq 400f_{\max}^2 > (2\pi f_{\max})^2. \quad (17)$$

In other words, the removed modes vary with space at a frequency higher than f_{\max} . Since f_{\max} is the maximum frequency of space variation that is physically important in a system response, the beyond- f_{\max} modes are physically negligible. As a result, when Δt is chosen based on the accuracy criterion, if we remove the modes having eigenvalues greater than $4/\Delta t^2$, not only we make the explicit time marching stable, but also we preserve the accuracy of the field solution. If Δt is chosen conservatively that $4/\Delta t^2$ is larger than $(2\pi f_{\max})^2$, instead of only removing the modes having eigenvalues greater than $4/\Delta t^2$, we can remove more modes as long as their eigenvalues are greater than $(2\pi f_{\max})^2$ since the beyond- f_{\max} modes are physically negligible. In other words, the number of modes that need to be kept for a stable and accurate simulation is bounded by the number of modes whose resonance frequency is no greater than f_{\max} . These modes are termed *physically important modes* in this paper.

Why there exists a maximum frequency of space variation that is physically important in a system response? In other words, why removing beyond- f_{\max} modes does not affect the accuracy of the field solution? This can be understood from the following theoretical analysis.

Eqn. (7) shows that the field solution is a superposition of all the N eigenmodes of (5). However, given an input pulse that is band limited, the number of modes that make nontrivial contributions to the field solution is also limited. To see how many vectors in Φ should be included in the field solution (7), we can convert (2) to frequency domain for a quantitative analysis. In frequency domain, (2) becomes

$$(\mathbf{S} - \omega^2 \mathbf{T}) \tilde{\mathbf{u}} = \tilde{\mathbf{j}}. \quad (18)$$

From (5), the solution to the above can be written as:

$$\tilde{\mathbf{u}} = \Phi(\mathbf{D} - \omega^2 \mathbf{I})^{-1} \Phi^T \tilde{\mathbf{j}}, \quad (19)$$

which is the superposition of all the eigenmodes [23]. Although the eigenvectors (modes) do not depend on frequency, their weights in the field solution do depend on frequency. As can be seen from (19), the weight of each mode Φ_i in $\tilde{\mathbf{u}}$ is $(\lambda_i^2 - \omega^2)^{-1} \Phi_i^T \tilde{\mathbf{j}}$. Clearly, given a frequency ω or a band of frequencies, not all of the modes make important contributions in the field solution for the given spectrum. Only those modes that have a large weight are important, and other modes whose eigenvalues are so far away from the working frequency can be truncated based on prescribed accuracy. Thus, (19) can be computed as

$$\tilde{\mathbf{u}} = \Phi_{N \times k} (\mathbf{D}_{k \times k} - \omega^2 \mathbf{I})^{-1} (\Phi_{N \times k})^T \tilde{\mathbf{j}}$$

where,
$$\frac{\min\{|\lambda_i^2 - \omega^2|\}, i \in (1, N)\}}{|\lambda_k^2 - \omega^2|} < \varepsilon$$

with controlled accuracy ε , where $\Phi_{N \times k}$ is composed of k eigenmodes whose relative weights in the field solution is greater than ε for the given frequency or the given spectrum. The frequency corresponding to the maximum eigenvalue of these k modes represents the maximum frequency of space variation that is physically important in a system response, which is f_{\max} . It is clear that by removing beyond- f_{\max} modes, the accuracy of the field solution is not affected. This is true for the field solution at any point in the computational domain, no matter the point is far away from the source or close to the source since the weights of beyond- f_{\max} modes are negligible due to the large gap between their eigenvalues and working frequency square (ω^2) instead of the large gap in space.

D. Validation of the Proposed Theory

As a validation of the proposed theory for making an explicit time-domain method unconditionally stable, we simulated a parallel plate structure made of perfect conductors in free space. The structure was 10 μm in length, 16 μm in

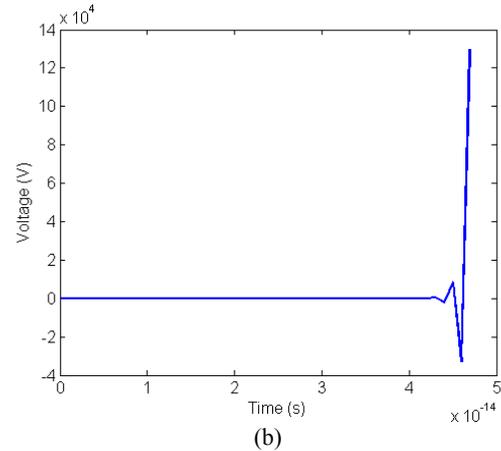
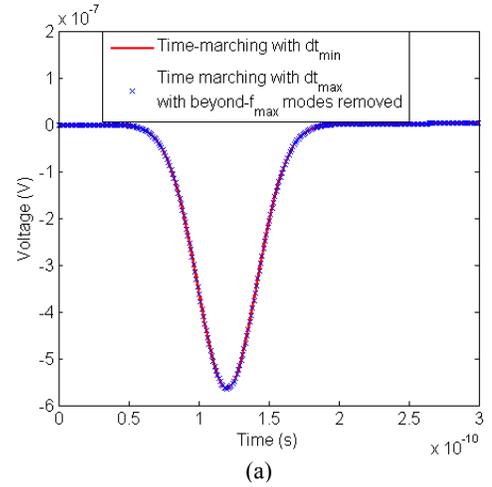


Fig. 1. (a) Comparison between the waveform generated by an explicit method with time step $dt_{\min}=10^{-16}$ s and that with a large time step $dt_{\max}=10^{-12}$ s with all unstable modes eliminated. (b) The waveform generated by the conventional explicit method for simulating (9) with a time step of 10^{-15} s.

width, and 8.5 μm in height. The voltages were sampled between two plates with a Gaussian derivative current source launched from one plate to the other at one end of the structure. The source pulse was $I(t) = 2(t-t_0)\exp(-(t-t_0)^2/\tau^2)$, where $t_0 = 4\tau$ and $\tau = 3 \times 10^{-11}$ s. Due to the small feature size of the structure, the time step permitted by a traditional central difference based explicit scheme was 10^{-16} seconds. With the proposed method, by setting y_h corresponding to unstable modes to be zero at each time step, we were able to obtain accurate and stable results using a central-difference based explicit scheme with a large time step of 10^{-12} seconds that was solely determined by accuracy. The result is shown in Fig. 1(a) in comparison with that generated by a traditional central-difference based scheme with 10^{-16} s time step. Excellent agreement can be observed. Without setting y_h to be zero, the simulation of (9) is unstable. In Fig. 1(b), we plot the voltage generated by simulating (9) with a time step of 10^{-15} s without setting y_h to be zero. Clearly, the result is unstable even in a short period of 50 time steps.

E. Comparison with Existing Unconditionally Stable Methods

In previous research, the approach used for achieving unconditional stability is to make the error amplification factor of a time stepping formula bounded by 1 regardless of the choice of time step. The source that is responsible for the instability is still kept in the numerical system. As a result, one has to resort to implicit methods to develop an unconditionally stable scheme. In contrast, in this work, the approach we create for achieving unconditional stability is to fix the problem from the root. In other words, we remove the source that generates the instability. With the source of instability removed, an explicit method can also be made unconditionally stable. It is worth mentioning that in [26], it is shown that an explicit linear multi-step method cannot be A-stable, thereby unconditionally stable. However, the underlying proof did not consider the scenario that the source that is responsible for instability is removed from the numerical system, like what is achieved in this work.

IV. PROPOSED EXPLICIT TIME DOMAIN FINITE ELEMENT METHOD THAT IS UNCONDITIONALLY STABLE

From the theoretical study given in the section above, it can be seen that the essential way to fix the instability of an explicit time-domain finite-element method with a large time step Δt is to eliminate eigenvectors whose eigenvalues are greater than $4/\Delta t^2$ out of the numerical system, i.e. eliminate resonance modes whose angular frequencies are greater than $2/\Delta t$, and hence cannot be accurately, and thus stably simulated by the given time step Δt . The proposed explicit time-domain finite-element method that is unconditionally stable therefore has two steps. The first step is a pre-processing step for building a complete and also accurate space that spans all the stable modes for a given time step Δt , i.e. the modes having eigenvalues no greater than $4/\Delta t^2$. This is described in Section IV.A. The second step is to perform a march-on in time with the given time step in an explicit time-

domain method without violating stability. This is described in Section IV.B. Both steps retain the strength of an explicit method in avoiding a matrix solution, and hence achieving unconditional stability without sacrificing the linear (optimal) complexity of an explicit method based time-domain simulation.

A. Pre-processing for Building a Complete and also Accurate Space Φ_l that Spans All the Stable Modes for a Given Time Step

Setting the coefficients of the unstable modes to be zero in the field solution at each time step as shown in (14) is equivalent to synthesizing the field solution in the space formed by stable modes only.

From Section III, it is clear that one straightforward approach to finding the stable eigenmodes is to solve the generalized eigenvalue problem shown in (5). After obtaining all the eigenvalues and eigenvectors of (5), one can identify those eigenvectors whose eigenvalues are no greater than $4/\Delta t^2$. The corresponding eigenvectors can then be used to form the space Φ_l that spans all the stable modes for the given time step, which can be written as

$$\Phi_l = \Phi_{N \times l}, \quad (20)$$

where $\Phi_{N \times l}$ denotes the matrix formed by l eigenvectors of (5) whose eigenvalues are no greater than $4/\Delta t^2$. The number of stable modes, i.e. the column dimension of Φ_l , is between 1 and the number of physically important modes whose resonance frequency is no greater than f_{\max} , and hence having eigenvalues no greater than $(2\pi f_{\max})^2$. We do not need to keep the rest of modes with higher eigenvalues even though they can be stably simulated by the given time step because these modes are physically negligible. When Δt is chosen based on accuracy, the Φ_l is also the union of physically important modes. The disadvantage of the aforementioned approach is that it requires an efficient solution of a generalized eigenvalue problem of $O(N)$.

To bypass the large-scale eigenvalue solution of $O(N)$, in this work, we develop a time-domain solution based fast eigenvalue solution of $O(k)$, where k is the number of physically important modes of (5). In general, k is orders of magnitude smaller than N in problems where the space discretization is much finer than that required by accuracy for sampling an f_{\max} -based system because many eigenvalues higher than f_{\max} will be generated. As shown in the Section of numerical results, k could be just 3 while N is large. In these problems, the time step issue of an explicit method is also the most critical.

In the proposed time-domain solution based fast eigenvalue solution of $O(k)$, with linear computational complexity, we transform the original large-scale generalized eigenvalue problem of $O(N)$ to a significantly reduced eigenvalue problem of $O(k)$, where k is orders of magnitude smaller than N . From the reduced eigenvalue problem of $O(k)$, we identify

the eigenvalues and eigenvectors of (5) that are physically important for a given spectrum, from which we select those eigenvectors whose eigenvalues are no greater than $4/\Delta t^2$ to form space Φ_l , where all the stable solutions for a give time step should reside. The details of this method are given below.

1) Transforming the Original Generalized Eigenvalue Problem of $O(N)$ to a Reduced Eigenvalue Problem of $O(k)$ by Field Solutions Obtained at a Small Number of Time Steps

We first employ a conventional explicit time-domain method to solve (2) at a small number of time steps. By doing so, we take advantage of the strength of an explicit method in being matrix free. Moreover, we do not suffer from the shortcoming of an explicit method in requiring many time steps for finishing one simulation. This is because compared to the total number of time steps required by the explicit method for finishing the entire simulation, the number of time steps to be simulated is small for revealing the physically important eigenvalues and eigenvectors from time-domain solutions.

When we solve (2), we collect the solution vector u at a few time instants. We store them in \mathbf{V} and also orthogonalize \mathbf{V} to make sure its column vectors are linearly independent with each other. The orthogonalization is done whenever a new solution vector u is added in \mathbf{V} . We develop the following method to quantitatively judge whether \mathbf{V} is complete or not for finding all the physically important modes.

We expand the field solution u in the space of \mathbf{V} as

$$u = \mathbf{V}x, \quad (21)$$

with x being the unknown coefficient vector, the i -th entry of which represents the weight of the i -th column vector in \mathbf{V} . Substituting (21) into (2) and multiplying (2) by \mathbf{V}^T , we obtain

$$\mathbf{V}^T \mathbf{T} \mathbf{V} \frac{d^2 x}{dt^2} + \mathbf{V}^T \mathbf{S} \mathbf{V} x = \mathbf{V}^T j, \quad (22)$$

which can be further written as

$$\mathbf{A}_{k' \times k'} \frac{d^2 x}{dt^2} + \mathbf{B}_{k' \times k'} x = \mathbf{V}^T j, \quad (23)$$

where

$$\mathbf{A}_{k' \times k'} = \mathbf{V}^T \mathbf{T} \mathbf{V}, \quad \mathbf{B}_{k' \times k'} = \mathbf{V}^T \mathbf{S} \mathbf{V}. \quad (24)$$

Assume the matrix system in (2) is of size N and there are k' vectors in \mathbf{V} , then \mathbf{V} is an $N \times k'$ matrix, where $k' \ll N$. As a result, both \mathbf{A} and \mathbf{B} are a small $k' \times k'$ matrix. Thus, instead of solving the $N \times N$ eigenvalue problem shown in (5), we only need to solve a reduced $k' \times k'$ eigenvalue problem as the following:

$$\mathbf{B}_{k' \times k'} \phi = \lambda^2 \mathbf{A}_{k' \times k'} \phi. \quad (25)$$

Denoting the union of the eigenvectors of (25) by Φ_r , and the eigenvalue matrix by \mathbf{D}_r . The solution of (23) can be expanded in the space of Φ_r . We hence have

$$x(t) = \Phi_r \tilde{y}(t), \quad (26)$$

where \tilde{y} contains the time-variant weights of the eigenvectors Φ_r , which is similar to y in (7) but with a significantly reduced size k' . Since \mathbf{A} is symmetric positive

definite and \mathbf{B} is symmetric, the following property holds true [25]:

$$\Phi_r^T \mathbf{A} \Phi_r = \mathbf{I}, \text{ and, } \Phi_r^T \mathbf{B} \Phi_r = \mathbf{D}_r. \quad (27)$$

Substituting (26) into (23), multiplying both sides of (23) by Φ_r^T , and using the property (27), we obtain

$$\frac{d^2 \tilde{y}}{dt^2} + \mathbf{D}_r \tilde{y} = \Phi_r^T \mathbf{V}^T j, \quad (28)$$

where \tilde{y} can be solved via a central-difference based scheme like (9).

2) Identify Physically Important Eigenvalues and Eigenvectors of the Original System from the Reduced Eigenvalue Problem of $O(k)$

One important fact is that the eigenvalues of physically important modes computed from the original system (5) will also satisfy the reduced system (25) as long as the space \mathbf{V} contains the information of these physically important modes. This is true because \mathbf{V} is formed by a set of solutions of (2) that are nothing but the superposition of the physically important modes. As a result, we can solve a $k' \times k'$ sytem shown in (25) to obtain the physically important modes of (5). In the appendix, we provide a theoretical proof to this fact.

During the time marching process, whenever we add a solution vector in space \mathbf{V} , we compute the eigenvalues from the reduced system (25). If the size of (25) is k' , we obtain k' eigenvalues. However, only a subset of the k' eigenvalues belongs to the set of k physically important eigenvalues of (5). We developed the following procedure to quantitatively identify the k physically important modes.

Our strategy is to monitor the weights of the eigenmodes in the time-marching process to identify physically important modes. The weight of the i -th mode is nothing but the i -th entry of \tilde{y} vector shown in (26). At the early time, very large eigenvalues are observed from (25). They correspond to the largest eigenvalues that are supported by the numerical system. These large eigenvalues can be observed at the early time because the frequency carried by the early-time response is the highest compared to the frequency carried by the system response in other time. As can be seen from (19), the field solution for a given frequency is dominated by eigenmodes whose eigenvalues are the closest to the given frequency because their weights in the field solution are the largest.

When the early time is passed and dominant frequency components that are no greater than f_{\max} set in, a set of eigenvectors whose eigenvalues are smaller than f_{\max} start to appear. Although f_{\max} can be estimated from the input spectrum, one may not know f_{\max} quantitatively in advance. The proposed method does not require users to quantitatively know f_{\max} either because f_{\max} can be numerically identified in the procedure of finding physically important modes. Without knowing the exact f_{\max} , what one observes is that after early time is passed, eigenvalues smaller than those observed in early time start to appear. When one enlarges the size of space \mathbf{V} by adding a new solution vector from time to time, one can observe that a set of common eigenvalues

reappear from time to time. When this set of eigenvalues start to have their weights \tilde{y} significantly larger than those of the rest of the eigenvalues which are larger, their corresponding eigenvectors are ready to be sampled as physically important eigenmodes. This is because once the weights of the modes having large eigenvalues become significantly small, in future time steps, the weights of these modes can only become smaller instead of larger because the frequency carried by the later time response can only be lower than higher. The relationship between eigenvalues, frequency, and weights in the field solution can be seen from (19).

In our implementation, we use the following condition to identify physically important eigenmodes systematically:

$$\tilde{y}_h < \varepsilon_1 \tilde{y}_l, \quad (29)$$

where ε_1 is a small parameter defined based on prescribed accuracy, \tilde{y}_l is the weight associated with the common eigenvalues that reappear from time to time, and \tilde{y}_h is that associated with larger eigenvalues. After identifying the physically important eigenmodes, the f_{\max} can be quantitatively determined from the largest eigenvalue among the set of physically important eigenvalues. As a result, we do not need to pre-assume f_{\max} based on empirical knowledge.

When the number of physically important eigenvalues does not increase in the time marching process, the space \mathbf{V} constructed can be considered complete. To obtain a complete as well as accurate space that spans all the physically important modes, we further apply the following accuracy requirement to each physically important eigenvalue λ_i :

$$\frac{|\lambda_{i,q}^{n+1} - \lambda_{i,q}^n|}{|\lambda_{i,q}^n|} < \varepsilon_2, \quad q = 1, 2, \dots, k, \quad (30)$$

where the superscript denotes the time index, ε_2 is a small parameter defined based on an accuracy requirement, and k is the number of λ_i . We select the eigenvectors of (25) corresponding to these λ_i , $\Phi_{r,l}$, to form the space Φ_k ,

$$\Phi_k = \mathbf{V}_{N \times k} (\Phi_{r,l})_{k \times k}, \quad (31)$$

which is the space that spans all the physically important modes. It is clear that the space \mathbf{V} that is formed by k field solution vectors cannot be used directly to construct Φ_k because not all the eigenvalues and eigenvectors contained in \mathbf{V} belong to the Φ_k space. We have to select only those eigenvalues that are the physically important eigenvalues of (5). This is accomplished by multiplying \mathbf{V} from right by $\Phi_{r,l}$. When both criteria (29) and (30) are satisfied, the Φ_k is complete as well as accurate.

3) Form Φ_l that Spans All the Stable Modes for a Given Time Step

With Φ_k obtained, the preprocessing can be terminated. For a given time step Δt , from the physically important modes, we select those modes whose eigenvalues are no greater than $4/\Delta t^2$ to form Φ_l . Thus,

$$\Phi_l = \mathbf{V}_{N \times k} (\Phi_{r,l})_{k \times l},$$

where $(\Phi_{r,l})_{k \times l}$ are the l physically important eigenvectors of (25) whose eigenvalues are no greater than $4/\Delta t^2$. When Δt is chosen based on accuracy, l is equal to k , i.e. all the physically important modes will be included in Φ_l . Hence, the simulation is not only stable but also accurate.

It is also worth mentioning that we store Φ_l by separately storing $\mathbf{V}_{N \times k}$ and $(\Phi_{r,l})_{k \times l}$, which has a linear cost. We do not need to multiply them together since their direct product is not required in the computation, which will be seen very clearly from the following section.

4) Discussion on the Choice of Simulation Parameters

Since k is generally less than N , when performing time-marching based on (2), one does not need to store the field solution at each time instant to construct the space \mathbf{V} . Instead, one can select the field solutions obtained at a few time instants to form \mathbf{V} . In our implementation, we selected the field solution every p steps to construct space \mathbf{V} . Which p to choose does not affect the accuracy of the proposed method. In other words, the proposed method is accurate regardless of how frequently one collects the field solution vectors as long as the resultant space is complete. However, a better choice of p can make the construction of Φ_l more efficient. Here, we provide a guideline on how to choose p . First, one can calculate the number of time steps required for the wave to traverse the entire computational domain once. One can also estimate the number of physically important modes that exist in the system response. Based on these two data, p can be determined by dividing the total number of time steps required for traversing the entire computational domain once by the number of modes. The aforementioned approach is not a unique way to construct \mathbf{V} . Based on the guideline that \mathbf{V} needs to contain all the physically important eigenmodes, one can also select field solution vectors in some other ways. For example, one can select the field solutions, the number of which is no less than the number of physically important modes, generated at the end of the pre-processing step, in which the field solution is dominated by the physically important modes and other modes with larger eigenvalues already become negligible.

B. Explicit Time Marching with Unconditional Stability

With Φ_l , the space formed by stable modes for a given time step Δt , obtained systematically, we can simulate (2) stably for the given Δt regardless of how large Δt is.

At each time step, we solve (2). To solve it, we first expand u in the space of $\Phi_l = \mathbf{V}_{N \times k} (\Phi_{r,l})_{k \times l}$, which is the same as the union of the eigenvectors of (5) corresponding to the l stable modes for the given time step. Thus, we obtain

$$u(t) = \mathbf{V} \Phi_{r,l} \tilde{y}_l(t). \quad (32)$$

Substituting (32) into (2) and multiplying $(\mathbf{V} \Phi_{r,l})^T$ on both sides of (2), we obtain

$$\Phi_{r,l}^T \mathbf{A} \Phi_{r,l} \frac{d^2 \tilde{y}_l}{dt^2} + \Phi_{r,l}^T \mathbf{B} \Phi_{r,l} \tilde{y}_l = \Phi_{r,l}^T \mathbf{V}^T j, \quad (33)$$

where \mathbf{A} and \mathbf{B} are the same as (24). Because of (27), we have

$$\Phi_{r,l}^T \mathbf{A} \Phi_{r,l} = \mathbf{I}, \text{ and, } \Phi_{r,l}^T \mathbf{B} \Phi_{r,l} = \mathbf{D}_l, \quad (34)$$

in which \mathbf{D}_l is a diagonal matrix that contains the l eigenvalues corresponding to stable modes. A central-difference based discretization of (33) thus yields

$$\tilde{y}_l^{n+1} = 2\tilde{y}_l^n - \tilde{y}_l^{n-1} - \Delta t_{\max}^2 \mathbf{D}_l \tilde{y}_l^n + \Delta t_{\max}^2 \Phi_{r,l}^T \mathbf{V}^T j^n. \quad (35)$$

After a time marching of (35) at all the time steps, if the field solution all over the structure is needed, it can be obtained by

$$\mathbf{u}^{n+1} = \mathbf{V} \Phi_{r,l} \tilde{y}_l^{n+1}. \quad (36)$$

Since $\Phi_{r,l}$ and \mathbf{V} are time independent, at each time step, we only need to update \tilde{y}_l and, also, from the reduced system of size l shown in (35), the cost of which is $O(l)$, and hence negligible.

C. Summary of the Overall Procedure and Cost Analysis

The overall procedure of the proposed unconditional stable explicit method can be summarized as follows.

Step I: Pre-processing for building a complete and also accurate space Φ_l that spans all the stable modes for a give time step

This is done by the proposed time-domain solution based fast eigenvalue solution of $O(k)$ described in Section IV.A, in which the following three sub-steps are performed.

- (I-1). Use the conventional explicit time-domain method to solve (2), and march on in time for a small number of steps. In this paper, we used an orthogonal prism vector basis based linear-complexity solution of the mass matrix developed in [15], and hence this step is performed in linear complexity.
- (I-2). Select the field solution vector \mathbf{u} every p steps and store them in \mathbf{V} . Orthogonalize the new solution vector with respect to other orthogonal vectors that are already stored in \mathbf{V} . If the new vector is independent of the other vectors in \mathbf{V} , then it is added in \mathbf{V} . The cost is linear for orthogonalizing k' vectors of length N .
- (I-3). Solve a reduced eigenvalue problem of size k' shown in (25). Solve the weight vector $\tilde{\mathbf{y}}$ from (28). Check whether (29) and (30) are satisfied. If not, go back to substep (I-1); if yes, stop, and then determine eigenvalues and eigenvectors corresponding to the stable modes. The cost of this step is negligible because of reduced system size.

Step II: Explicit time-marching with unconditional stability

- (II-1) Start time-marching. Compute the coefficient \tilde{y} of each mode from the reduced system (35) of size l at each time step. The cost at each time step is $O(l)$, where l is the number of stable modes, i.e. the eigenvectors whose eigenvalues are no greater than $4/\Delta t^2$. In addition, if the field distribution of only one specific mode is of interest, only the coefficient of this mode is updated at each time step. The cost is $O(1)$.
- (II-2) After \tilde{y} is obtained at each time step, the field solution \mathbf{u} can be recovered from (36) at each time instant. If only m selected field solutions \mathbf{u} are of interest, we can select

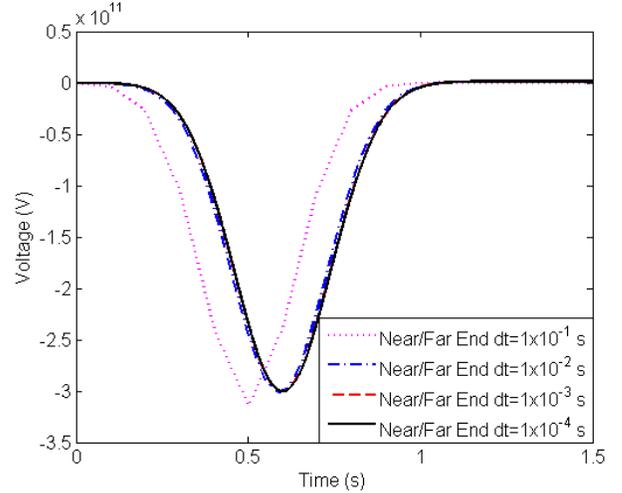


Fig. 2. Illustration of the unconditional stability of the proposed method.

those m rows corresponding to the selected locations for computing \mathbf{u} , the cost of which is $O(m)$.

V. NUMERICAL RESULTS

We have simulated a number of examples at both μm - and millimeter-scales to validate the unconditional stability, accuracy, efficiency, and late-time stability of the proposed unconditionally stable explicit time-domain finite-element method.

A. Demonstration of Unconditional Stability

First, we demonstrate the fact that the proposed method is stable regardless of the choice of time step. The example considered was a parallel plate structure that has an analytical solution. The fill-in material was air. The height (along x), width (along y), and length (along z) were set to be $1 \mu\text{m}$, $5 \mu\text{m}$, and $900 \mu\text{m}$, respectively. The space resolution along x , y , and z was $1 \mu\text{m}$, $1 \mu\text{m}$, and $100 \mu\text{m}$, respectively. A current source was launched from bottom plate to top plate at the near end while the voltages were extracted between the two plates at the near and far ends. The computational domain was truncated by a PEC (perfect electrically conducting) boundary condition on the top and at the bottom planes (yz -planes), a PMC (perfect magnetically conducting) boundary condition at the left and right boundaries (xz -plane boundaries), and the first-order absorbing boundary condition at the front and back ends. The parallel plate structure was excited by a current source launched from bottom plate to top plate at the near end while the voltages were extracted between the two plates at the near and far ends. The current source was 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 $\tau = 0.2$ s. For this example, the conventional explicit scheme has to use a time step of 10^{-15} s to maintain time-domain stability because of small space step. In contrast, as shown in Fig. 2, the proposed explicit unconditionally stable method permits the use of any large time step such as 0.0001 s, 0.001 s, 0.01s, and 0.1 s without becoming unstable. As described in Section III, the proposed method achieves

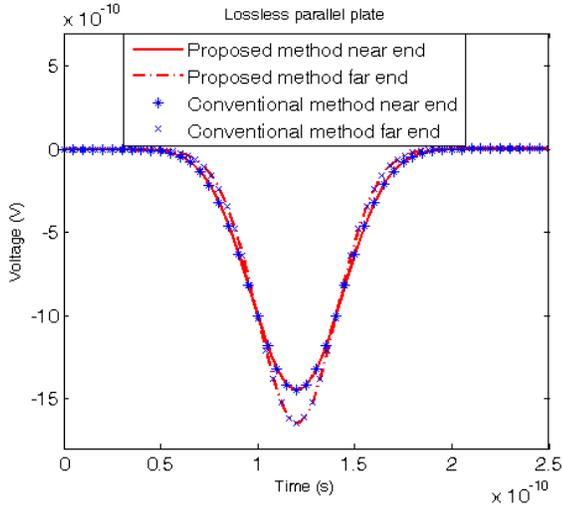


Fig. 3. Voltage waveforms of a μm -level parallel plate structure.

unconditional stability by removing unstable modes for the given time step. In this simulation, by only keeping the DC mode whose eigenvalue is zero from the reduced eigenvalue solution (25), we allow for the use of any large time step without making the simulation unstable. The same applies to other examples if one would like to use a time step that is infinitely large to examine stability.

B. Demonstration of Unconditional Stability, Accuracy, and Efficiency

With the unconditionally stability demonstrated, next we show that the proposed method is both unconditionally stable and accurate. In other words, given a time step determined solely based on accuracy, even though it could be orders of magnitude larger than that dictated by stability criterion, the proposed method is able to use it to produce both stable and accurate results. In addition, we show the efficiency of the proposed unconditionally stable explicit method is much better than that of the conventional explicit method that is conditionally stable.

1) Parallel plate structure of μm -dimension

The same parallel plate example simulated in Section V.A was simulated but with a different input pulse. The pulse was $I(t) = 2(t-t_0)\exp(-(t-t_0)^2/\tau^2)$ with $t_0 = 4\tau$ and $\tau = 3 \times 10^{-11}$ s. The maximum input frequency of the source was 34 GHz, at which the magnitude of the source's Fourier transform was 0.1% smaller than the maximum magnitude in the spectrum of the input signal. To simulate this example, a conventional explicit TDFEM or FDTD method required a time step as small as 10^{-15} s to maintain the stability of a time-domain simulation because the smallest space step was 1 μm . In contrast, the proposed explicit method was able to use a large time step of 5×10^{-13} s that is solely determined by accuracy to generate accurate and stable results. As shown in Fig. 3, the voltage waveforms simulated by the proposed method are in excellent agreement with those generated by the conventional central-difference based explicit method. The number of time steps simulated in the pre-processing was 4,400, which was

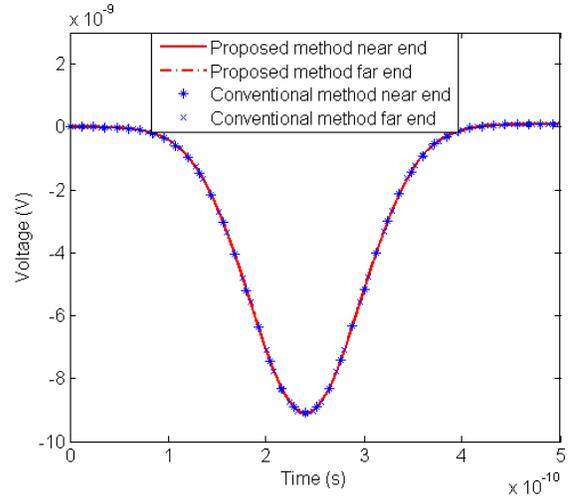


Fig. 4. Voltage waveforms of an on-chip interconnect.

automatically determined via criteria (29) and (30). Compared with the 2.5×10^5 steps required by the conventional explicit method, the speedup of the proposed method is 57.

In the pre-processing step, the ε_1 and ε_2 used in (29) and (30) were both chosen to be 10^{-3} . The proposed method systematically identified 5 physically important modes, whose eigenvalues were $\lambda_1 = 0$ (DC mode), $\lambda_2 = 3.02102 \times 10^{11}$, $\lambda_3 = 6.12116 \times 10^{11}$, $\lambda_4 = 9.38436 \times 10^{11}$, and $\lambda_5 = 1.28888 \times 10^{12}$ rad/s respectively. Therefore, $k = 5$. These eigenvalues were in excellent agreement with the first five eigenvalues found by solving the original eigenvalue problem (5) directly. The maximum relative error was shown to be less than 0.1%. This further verified our theoretical proof that the eigenvalues satisfying (5) also satisfy (25) as long as the corresponding eigenvectors are contained in the reduced space \mathbf{V} for generating (25). From the eigenvalues of the physically important modes, the f_{\max} , which corresponds to the largest eigenvalue of the physically important modes, was hence identified to be $1.29 \times 10^{12} / (2\pi)$ Hz. It is higher than the input maximum frequency 34 GHz. However, this is not contradictory to the fact that the spectrum of a linear system response should not go beyond the input spectrum because the f_{\max} represents how fast the field varies with space. The time step used by the proposed method for simulating this example, 5×10^{-13} s, was hence determined from $1/(10f_{\max})$ to ensure the accuracy of time-domain simulation although by removing unstable modes according to the given time step, the proposed method allows for the use of any large time step without becoming unstable. During the pre-processing step, the field solution was collected every 100 steps and then added into space \mathbf{V} . There is no need to collect the solution at every step since the number of physically important modes is not many. In addition, the accuracy of the proposed method is not affected by how frequently one collects the solution vectors as long as the resultant \mathbf{V} is complete. In total, 44 vectors were selected and 27 orthogonal vectors \mathbf{V} were built from these vectors, from which 5 physically important modes were identified.

2) 3D on-chip interconnect

The second example for demonstrating the unconditional stability as well as accuracy of the proposed method was a 600 μm long test-chip interconnect structure with 3 metal layers and 4 dielectric layers provided by Intel Corporation, where a PEC boundary condition was applied on the metal surface. The current source was again the derivative of a Gaussian pulse but with $t_0 = 3\tau$ and $\tau = 8 \times 10^{-11}$ s. The maximum input frequency of the source was 12.8 GHz, at which the source's magnitude was 0.1% smaller than the maximum magnitude in the spectrum of the input signal. Because of the fine feature size of the structure, which was at 0.1 μm -level, the time step allowed by the conventional central-difference based explicit method was only 1×10^{-16} s, whereas the proposed explicit method was able to use a time step of 8×10^{-13} s to generate accurate and stable results. The parameters ε_1 and ε_2 were chosen the same as the first example. Three physically important modes were detected from 14,800 time steps simulated in the pre-processing. Their eigenvalues were $\lambda_1 = 0$, $\lambda_2 = 7.00872 \times 10^{11}$, and $\lambda_3 = 7.20873 \times 10^{11}$ rad/s respectively. They again agreed very well with those obtained from (5) directly, with the maximum error being 0.3%. To simulate for 0.5 ns in time, the original central-difference scheme required 5 million steps to complete the simulation, whereas the proposed method only need 14,800 steps in pre-processing and the cost after pre-processing is negligible. Thus, the speedup is 330. Fig. 4 shows an excellent agreement between the proposed method and the conventional central-difference based method.

3) Millimeter-scale waveguide with thin films

Next example was a millimeter-scale waveguide with thin films as shown in Fig. 5. The dashed lines in Fig. 5(a) are

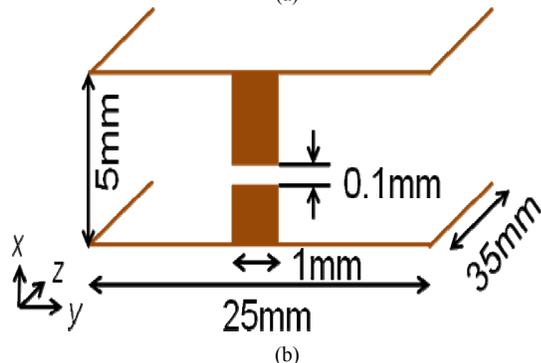
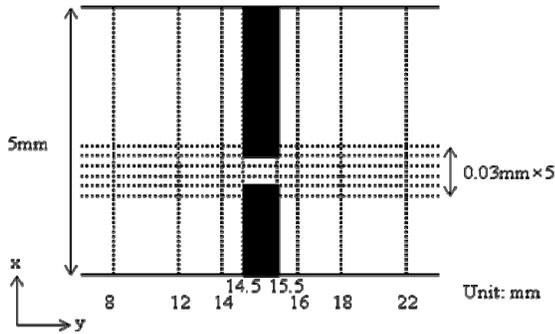


Fig. 5. Illustration of a millimeter-scale waveguide with thin films. (a) Cross-sectional view. (b). 3-D view.

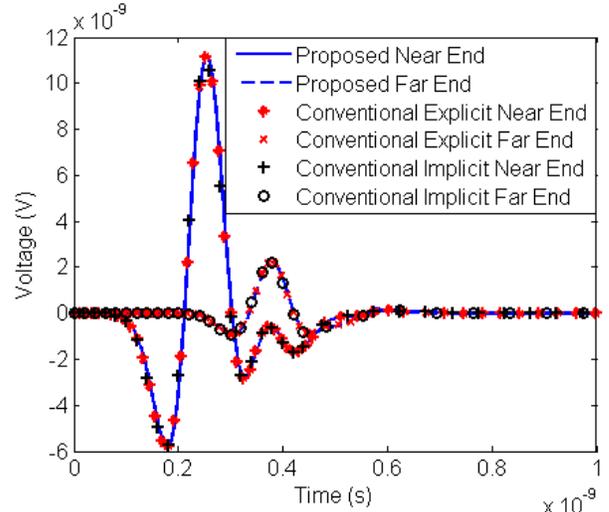


Fig. 6. Voltage waveforms of the waveguide with a thin film.

meshing lines. The PEC boundary condition was applied on the top plane, bottom plane, and the thin film. The first-order absorbing boundary condition was applied at the two ends of the waveguide. In order to accurately capture the geometry of the thin film and slit, a fine space discretization as small as 0.03 mm was used in the x - y plane as shown in Fig. 5(a). The waveguide was discretized to 7 layers along the 35 mm length and the film occupied one layer. The structure was excited by a Gaussian's derivative current source with $\tau = 6 \times 10^{-11}$ s and $t_0 = 4\tau$ from bottom plate to top plate at the near end of the waveguide. The voltages were extracted between the two plates at the near and far ends. To simulate this example, the conventional explicit scheme requires a time step of 6×10^{-14} s to maintain stability. Because of this small time step, over ten thousand steps were needed to finish the simulation. With the proposed explicit method, we were able to use a time step of 10^{-12} s solely determined by accuracy (because $f_{\max} = 10^{11}$ Hz) to generate accurate and stable results within 1,000 steps. We collected the field solution every 50 steps during the pre-processing. The solver automatically simulated for 3,000 time steps in pre-processing from which 60 vectors were sampled, among which 47 orthogonal vectors were constructed to form \mathbf{V} . Using the space \mathbf{V} , the original large eigenvalue problem was transformed to a small eigenvalue problem of size 47, from which 33 physically important modes were identified with the first two eigenvalues found to be $\lambda_1 = 0$ and $\lambda_2 = 1.87172 \times 10^{10}$ rad/s, the error of which was less than 1%. Since the conventional explicit method needs 1.7×10^4 steps and the proposed method only needs 3,000 steps in pre-processing, the speedup of the proposed method is 6. In this millimeter-scale example, because the space discretization is not significantly smaller than that required by accuracy, the gap between the time step allowed by accuracy and that permitted by the stability criterion is not that large. Therefore, the speedup of the proposed unconditionally stable explicit scheme is not as significant as that observed in previous examples that involve a space resolution much smaller than that required by accuracy due to the existence of fine features relative to working wavelength. In Fig. 6, we plot the voltages sampled at the near and far ends of the waveguide simulated by the proposed method in comparison with those generated by the

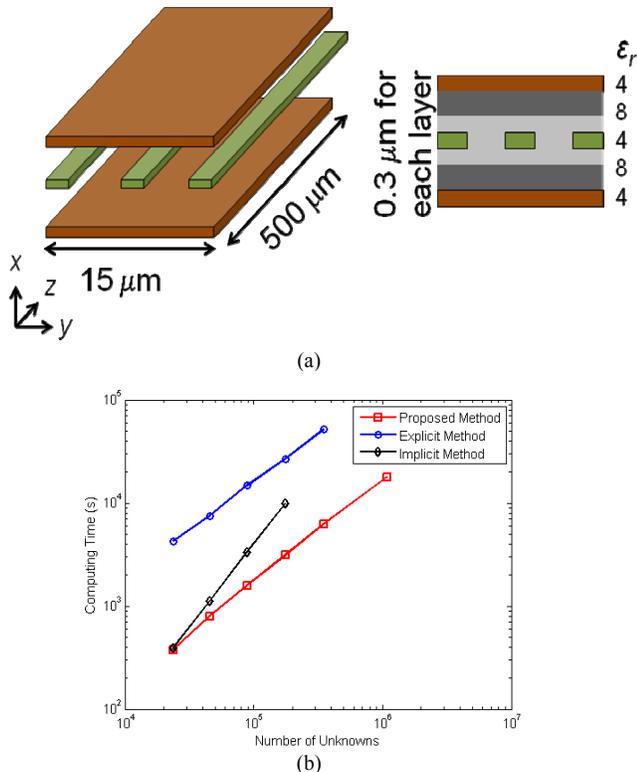


Fig. 7. Simulation of an on-chip bus. (a) Illustration of the structure and material. (b) Total CPU time comparison between 3 methods.

conventional explicit method as well as implicit Newmark-based unconditionally stable scheme. Excellent agreement is observed.

C. Comparison with Unconditionally Stable Implicit Method and Conditionally Stable Explicit Method

In addition to comparing the performance of the proposed method with that of the conditionally stable explicit method, we have also compared the performance of the proposed method with the unconditionally stable implicit method. The example considered was a 3-D on-chip bus with three parallel buses in M2 layer, one metal layer on the top, and the other at the bottom, as shown in Fig. 7(a). The width of each bus was 3 μm as well as the spacing between buses. The thickness of each dielectric and metal layer was 0.3 μm. There were 4 dielectric layers. The dielectric constant in the two layers adjacent to M2 layer was 4, and that for the other two dielectric layers was 8. The structure was excited by the same current source used in the example described in Section V.B.1). We simulated a suite of such 3-D bus structures, the discretization of which resulted in 23,677; 45,427; 88,927; 175,927; 349,927; and 1,089,427 unknowns, respectively. The total time simulated was 9×10^{-11} s. We compared the CPU time of the proposed unconditionally stable explicit method in comparison with the latest linear-complexity conditionally stable explicit method reported in [15] for integrated circuit simulation and the unconditionally stable implicit Newmark method [10] that used a state-of-the-art multi-frontal based sparse matrix solver [27]. In Fig. 7(b), we plot the total CPU time cost by the three methods versus N . The advantage of the proposed method can be clearly seen. The proposed explicit method and the explicit method in [15] both

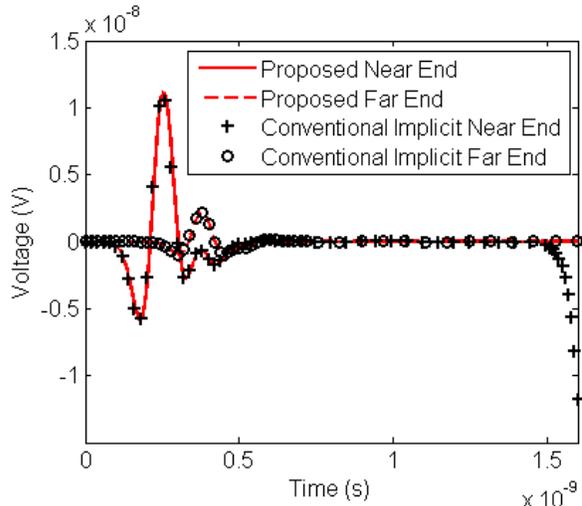


Fig. 8. Comparison of two method in late-time stability.

exhibit linear complexity. However, the proposed method was able to use 3000 steps to finish the entire simulation with a time step of 3×10^{-14} s whereas the conditionally stable explicit method in [15] required 300,000 steps to finish the simulation. As for the implicit Newmark method, although it permitted the same large time step as that used by the proposed method, it failed to factorize the matrix when matrix size is large.

D. Examination of Late-Time Stability

For all the examples simulated in this paper, we also performed simulations to very late time. No late-time instability is observed from the proposed method. This is well understood because at each time step, the field solution in the proposed method is strictly obtained from a space that spans the stable modes only. In contrast, we do observe late-time instability of implicit methods in some of the examples we simulated. For example, when simulating the millimeter-scale waveguide example described in Section V.B.3), we observed late-time instability from the Newmark-based implicit scheme, as shown in Fig. 8, whereas the proposed method is stable.

VI. CONCLUSIONS

In this work, we propose an explicit time-domain finite-element method that is unconditionally stable. Different from previous methods for achieving unconditional stability, in which one relies on a bounded error amplification factor to control stability, and hence has to resort to implicit methods, the proposed method completely eliminates the root cause that is responsible for the instability associated with an explicit time-domain method. As a result, an explicit method can also be made unconditionally stable, thus the time step is solely determined by accuracy requirement.

The proposed method has two steps to realize unconditional stability in the framework of an explicit time-domain finite-element method. In the pre-processing step, a time-domain solution based fast eigenvalue solution of $O(k)$ with $k \ll N$ was developed to build a complete and accurate space that spans all the stable modes for a give time step. This step has linear

computational complexity in which only the solution of mass matrix is required. In the second step, the field solution is spanned in the space constructed in the pre-processing step, which is equivalent to removing the unstable modes for the given time step. An explicit time marching can then be performed with unconditional stability for the given time step irrespective of its size. The cost of this step is negligible. As a result, in the proposed method, the strength of an explicit method in avoiding computationally intensive matrix solutions is retained, while its shortcoming of requiring a small time step is overcome for problems having fine features relative to working wavelength.

Numerical experiments have demonstrated that the proposed unconditionally stable explicit method outperforms both the conditionally stable explicit method and the unconditionally stable implicit method in computational efficiency. The method is also shown to be stable at late time, while late-time instability is observed in unconditionally stable implicit methods. Although the proposed method is presented in the framework of a time-domain finite-element method, the essential idea can be applied to other time domain methods.

APPENDIX

In the following, we prove that the eigenvalues of the large system (5) can be found from the reduced system (25) as long as the space \mathbf{V} used to reduce (5) to (25) contains the information of the eigenvectors corresponding to these eigenvalues.

Consider an eigenpair (λ_i^2, ϕ_i) of (5). It satisfies

$$\mathbf{S} \phi_i = \lambda_i^2 \mathbf{T} \phi_i. \quad (\text{A-1})$$

If the space \mathbf{V} contains the information of ϕ_i , the ϕ_i can be expanded in the space \mathbf{V} as the following

$$\phi_i = \mathbf{V} y, \quad (\text{A-2})$$

where y is a coefficient vector. Substituting (A-2) into (A-1) and testing both sides of (A-1) by \mathbf{V}^T , we obtain

$$\mathbf{V}^T \mathbf{S} \mathbf{V} y = \lambda_i^2 \mathbf{V}^T \mathbf{T} \mathbf{V} y. \quad (\text{A-3})$$

From (24), the above can be further written as

$$\mathbf{B} y = \lambda_i^2 \mathbf{A} y. \quad (\text{A-4})$$

As a result, the eigenpair (λ_i^2, y) is the solution of (25). Therefore, the eigenvalues that satisfy (5) also satisfy (25) as long as the \mathbf{V} used to reduce (5) to (25) contains the information of the eigenvectors corresponding to these eigenvalues. In addition, by front multiplying the eigenvector obtained from (25) corresponding to λ_i^2 by \mathbf{V} , one can obtain the eigenvector of (5) as can be seen from (A-2).

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