Explicit Time-Domain Finite-Element Method Stabilized for an Arbitrarily Large Time Step

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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, which is stable and accurate for a time step solely determined by accuracy regardless of how large the time step is. The proposed method retains the strength of an explicit time-domain method in avoiding solving a matrix equation while eliminating its shortcoming in time step. Numerical experiments have demonstrated its superior performance in computational efficiency, as well as stability, compared with the conditionally stable explicit method and the unconditionally stable implicit method. The essential idea of the proposed method for making an explicit method stable for an arbitrarily large time step irrespective of space step is also applicable to other time domain methods.**

***Index Terms*—Explicit time-domain methods, stability, time-domain finite-element methods, unconditionally stable methods.**

I. Introduction

THE time-domain methods in computational electromagnetics can be categorized into two classes. One is the explicit time-domain method; the other being 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; 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 equation, while implicit methods generally require a matrix solution.

Despite its advantage of avoiding a matrix solution, 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. In an unconditionally stable method, there is no restriction between space step and time step for obtaining a stable solution. It also permits the use of an arbitrarily large time step without becoming unstable. Existing unconditionally stable methods 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 1-D)-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 further 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 have also been developed. These methods require the solution of a weighted 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], hence eliminating the need for solving a matrix equation. In summary, the large time step provided by the existing unconditionally stable scheme is achieved by resorting to implicit time-domain methods that sacrifice 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. Though the method is explicit, yet it is not unconditionally stable. In fluid dynamics, techniques have been developed to filter unstable high frequency waves to increase the time step of an explicit scheme [28]. However, the time step is only extended by a limited amount. The filtering technique has also been developed to extend the stability limit of the explicit FDTD method [17] in electromagnetics. As to-date, no explicit methods have been made unconditionally stable.

The research question considered in this work is: can an explicit method be made unconditionally stable so that its strength, which lies in avoiding a matrix solution, is retained while eliminating its shortcoming in time step?

The contribution of this work is the successful development of an explicit time-domain method that is unconditionally stable, a capability that previously did not exist. It is stable for any large time step without being restricted by the space step. If the time step is chosen based on accuracy, the proposed method produces not only stable but also accurate results no matter how large the time step is. We have already conducted preliminary research on the proposed method 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

Manuscript received August 10, 2011; revised November 02, 2011; accepted May 30, 2012. Date of publication July 10, 2012; date of current version October 26, 2012. This work was supported in part by a grant from Intel Corporation, in part by a grant from the Office of Naval Research under award N00014-10-1-0482, and in part by grants from the NSF under Awards 0747578, 0802178, and 1065318.

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Digital Object Identifier 10.1109/TAP.2012.2207666

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 the explicit method at each time step is preserved by the proposed method. Section V demonstrates the 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 as well as stability. 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, 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 $\mathbf{E}$, μ_0, μ_r, ε, and $\mathbf{J}$ are the electric field, free-space permeability, relative permeability, permittivity, and current density respectively. A time-domain finite-element based solution of (1) and its boundary conditions results in the following system of linear equations [20]:

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

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 stored in linear computational resources from their elemental contributions as follows:

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

where $\mathbf{N}_i$ and $\mathbf{N}_j$ are the vector basis functions used to expand $\mathbf{E}$ while $\langle .,. \rangle_V$ denotes a volume integration in each element. Compared to other time-domain methods, a time-domain finite-element method possesses flexibility in both geometrical 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, whenever a time step beyond the 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], [27]

$$\Delta t \le \frac{2}{\sqrt{\rho(\mathbf{T}^{-1}\mathbf{S})}} \quad (4)$$

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. 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:

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

The field solution vector u is then expanded in the space formed by all the eigenvectors of (5) followed by finding the corresponding coefficients of each eigenvector in the field solution of u [23]. This approach is also known as modal superposition method [24].

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

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

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

$$u(t) = \mathbf{\Phi} y(t) \quad (7)$$

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 problem is the superposition of the eigenvectors (modes). This is true for 1-D, 2-D, and 3-D problems. To obtain unknown coefficient y, we substitute (7) into (2). Multiplying both sides of (2) by $\mathbf{\Phi}^{\mathrm{T}}$, and using the property shown in (6), we obtain

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

A central-difference based explicit solution to the above yields

$$y^{n+1} = 2y^n - y^{n-1} - \Delta t^2 \mathbf{D} y^n + \mathbf{\Phi}^{\mathrm{T}} b^n \tag{9}$$

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), obtaining

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

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:

$$\Delta t^2 \lambda_i^2 \leq 4, \quad i = 1, 2, \ldots, N \tag{11}$$

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 a 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 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), $\lambda_{\max}$ (whose unit is angular frequency), is inversely proportional to the smallest space resolution $\Delta_{\min}$ as the following:

$$\lambda_{\max} \sim O\left(\frac{\pi c}{\Delta_{\min}}\right). \tag{12}$$

where c is speed of light. This is because given the smallest space step $\Delta_{\min}$, 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 identified from (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, the eigenvalues of which 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 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 number of these unstable modes is also finite.

The remaining question is why these unstable modes exist? They exist because of the 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 of (5). Once these unstable modes are inherent in (5), even though the right hand side b does not have a projection onto them, the numerical roundoff error will have a projection onto them. This can be seen clearly from (9), which 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 $\mathbf{\Phi}_i^{\mathrm{T}} b^n$ is zero, the roundoff error can make y_i nonzero. 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 clearly shows why in cases, 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. 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 the modes that violate (11), i.e., those modes whose eigenvalues are greater than $4/\Delta t^2$, from 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 nullspace modes whose eigenvalues are zero and removing the rest of the modes having nonzero eigenvalues.

To completely remove the unstable modes, we expand the field solution strictly in the space of stable modes; we also project the numerical system onto the space of stable modes. The detailed procedure is as follows.

Denoting the coefficient vector y in (7) by

$$y = \begin{bmatrix} y_l \\ y_h \end{bmatrix} \tag{13}$$

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, denoted by $\mathbf{\Phi}_l$. We expand the field solution in the space of stable modes, $\mathbf{\Phi}_l$, as the following:

$$u(t) = \mathbf{\Phi}_l y_l(t). \tag{14}$$

This is equivalent to setting y_h in (13) to be zero at each time instant. Meanwhile, we project the numerical system (2) onto the space of $\mathbf{\Phi}_l$, which is achieved by multiplying both sides of (2) by $\mathbf{\Phi}_l^{\mathrm{T}}$. We thereby obtain

$$\mathbf{\Phi}_l^{\mathrm{T}}\mathbf{T}\mathbf{\Phi}_l \frac{d^2 y_l}{dt^2} + \mathbf{\Phi}_l^{\mathrm{T}}\mathbf{S}\mathbf{\Phi}_l y_l = \mathbf{\Phi}_l^{\mathrm{T}} j. \tag{15}$$

By using the property shown in (6), we have

$$\frac{d^2 y_l}{dt^2} + \mathbf{D}_l y_l = \mathbf{\Phi}_l^{\mathrm{T}} j$$

and hence

$$y_l^{n+1} = 2y_l^n - y_l^{n-1} - \Delta t^2 \mathbf{D}_l y_l^n + \mathbf{\Phi}_l^{\mathrm{T}} b^n \tag{16}$$

where $\mathbf{D}_l$ is a diagonal matrix comprising the eigenvalues corresponding to stable modes, which are no greater than $4/\Delta t^2$. The resultant explicit marching of (16) is stable for the given time step Δt regardless of how large the time step is because (11) is always satisfied.

It is worth mentioning that by removing unstable modes from the field solution *only*, we cannot make a time-domain scheme stable for any large time step. This is because in this case, a central-difference based explicit marching of (2) can be written as

$$\begin{aligned} u^{n+1} = {} & 2u^n - u^{n-1} \\ & -\Delta t^2 \mathbf{T}^{-1}\mathbf{S}(u^n - \text{unstable part}) + \mathbf{T}^{-1} b^n, \end{aligned} \tag{17}$$

in which the unstable part of the field solution is excluded at each time instant. Although now u^n is free of unstable modes, $\mathbf{T}^{-1}\mathbf{S}$ constitutes a space that spans all the modes of (5) including both stable and unstable modes for a given time step. The roundoff error of $(u^n - \text{unstable part})$ can always project onto the unstable modes, causing instability. In other words, the source of instability is contained in system matrix $\mathbf{T}^{-1}\mathbf{S}$ instead of field solution. Without changing the system matrix to a matrix that only spans the space of stable modes, the source of instability still exists. That is why in this work, we find the space of stable modes ($\mathbf{\Phi}_l$) for a given time step, expand the field solution in this space and, also, project the system matrix onto this space, as shown by (15). The resultant numerical system (16) is absolutely stable for the given time step no matter how large it is.

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

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

$$\Delta t < \frac{1}{(2 f_{\max})}$$

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

$$\Delta t \le \frac{1}{(10 f_{\max})}. \tag{18}$$

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 (18) 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 (18), we have

$$\lambda_i^2 > \frac{4}{\Delta t^2} \ge 400 f_{\max}^2 > (2\pi f_{\max})^2. \tag{19}$$

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 do we make the explicit time marching stable, but also 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.

Equation (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 $\mathbf{\Phi}$ should be included in the field solution (7), we can convert (2) to frequency domain for a quantitative analysis. In frequency domain, (2) becomes

$$(\mathbf{S} - \omega^2 \mathbf{T})\tilde{u} = \tilde{j}. \tag{20}$$

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

$$\tilde{u} = \mathbf{\Phi}(\mathbf{D} - \omega^2 \mathbf{I})^{-1} \mathbf{\Phi}^{\mathrm{T}} \tilde{j} \tag{21}$$

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 vary with frequency. As can be seen from (21), the weight of each mode $\mathbf{\Phi}_i$ in $\tilde{u}$ is $(\lambda_i^2 - \omega^2)^{-1} \mathbf{\Phi}_i^{\mathrm{T}} \tilde{j}$. 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, whereas the modes, whose eigenvalues are so far away from the working frequency, can be truncated based on prescribed accuracy. Thus, (21) can be computed as

$$\tilde{u} = \mathbf{\Phi}_{N\times k}(\mathbf{D}_{k\times k} - \omega^2\mathbf{I})^{-1}(\mathbf{\Phi}_{N\times k})^{\mathrm{T}}\tilde{j}$$
$$\text{where, } \frac{\left|\lambda_k^2 - \omega^2\right|}{\min\{|\lambda_i^2 - \omega^2|, i \in (1,N)\}} < \frac{1}{\varepsilon} \qquad (22)$$

with controlled accuracy ε, where $\mathbf{\Phi}_{N\times k}$ is composed of k eigenmodes whose relative weights in the field solution are 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 how far or close the point is from 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).

In addition, as can be seen from (12), if the space step is chosen based on the accuracy requirement, i.e., capturing a space variation up to $f_{\max}$ frequency, then the maximum eigenvalue $\lambda_{\max}$ of (5) does not go beyond that associated with $f_{\max}$. Then, no beyond-$f_{\max}$ modes exist in the numerical system. Once beyond-$f_{\max}$ modes exist, that is because the space step is finer than that required by accuracy for discretizing an $f_{\max}$-based system. Therefore, they are not necessary for the required accuracy, and hence can be eliminated without affecting accuracy.

IV. Proposed Explicit Time Domain Finite Element Method That is Unconditionally Stable

The proposed explicit time-domain finite-element method that is stable for any large time step has two steps. The first step is a preprocessing step for building a complete and also accurate space that spans all the stable modes for a given time step Δt. 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. Both steps retain the strength of an explicit method in avoiding a matrix solution, and hence achieving stability for any time step without sacrificing the linear (optimal) complexity of an explicit method based simulation.

A. Preprocessing for Building a Complete and Accurate Space $\mathbf{\Phi}_l$ That Spans all the Stable Modes for a Given Time Step

From Section III, it is clear that one straightforward approach for 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, $\mathbf{\Phi}_{N\times l}$, can then be used to form the space $\mathbf{\Phi}_l$ that spans all the stable modes for the given time step, which can be written as

$$\mathbf{\Phi}_l = \mathbf{\Phi}_{N\times l}. \qquad (23)$$

The number of stable modes, i.e., the column dimension of $\mathbf{\Phi}_l$, 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 remaining modes with higher eigenvalues even though they can be simulated in a stable manner by the given time step as these modes are physically negligible. When Δt is chosen based on accuracy, the $\mathbf{\Phi}_l$ 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 size $O(N)$.

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 will be shown in the numerical results, k could be as small as 3 while N is large. In these problems, the time step issue of an explicit method is also the most critical. 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 (terminating criterion will be discussed in Section IV-A-2). By doing so, we take advantage of the strength of an explicit method in avoiding a matrix solution. Meanwhile, 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 store the solution vector u in $\mathbf{V}$ and also orthogonalize $\mathbf{V}$ to ensure its column vectors are linearly independent of each other. The orthogonalization is done whenever a new u is added in $\mathbf{V}$. Since k is generally less than N, we do not need to store the field solution at each time instant to construct $\mathbf{V}$. Instead, we can select a subset of the obtained field solutions to form $\mathbf{V}$. We develop the following method to quantitatively judge whether $\mathbf{V}$ is complete enough to find all the physically important modes.

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

$$u = \mathbf{V}x \qquad (24)$$

with x being the unknown coefficient vector. Substituting (24) into (2) and multiplying (2) by $\mathbf{V^T}$, we obtain

$$\mathbf{A}_{k'\times k'}\frac{d^2x}{dt^2} + \mathbf{B}_{k'\times k'}x = \mathbf{V^T}j \qquad (25)$$

where

$$\mathbf{A}_{k'\times k'} = \mathbf{V}^{\mathrm{T}}\mathbf{T}\mathbf{V},\ \mathbf{B}_{k'\times k'} = \mathbf{V}^{\mathrm{T}}\mathbf{S}\mathbf{V}. \qquad (26)$$

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

$$\mathbf{B}_{k' \times k'} \phi = \lambda^2 \mathbf{A}_{k' \times k'} \phi. \tag{27}$$

Denoting the union of the eigenvectors of (27) by $\mathbf{\Phi}_r$, and the eigenvalue matrix by $\mathbf{D}_r$. The solution of (25) can be expanded in the space of $\mathbf{\Phi}_r$. We therefore have

$$x(t) = \mathbf{\Phi}_r \tilde{y}(t) \tag{28}$$

where $\tilde{y}$ contains the time-variant weights of the eigenvectors $\mathbf{\Phi}_r$, 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, we have [25]

$$\mathbf{\Phi}_r^{\mathbf{T}} \mathbf{A} \mathbf{\Phi}_r = \mathbf{I}, \text{ and, } \mathbf{\Phi}_r^{\mathbf{T}} \mathbf{B} \mathbf{\Phi}_r = \mathbf{D}_r. \tag{29}$$

Substituting (28) into (25), multiplying both sides of (25) by $\mathbf{\Phi}_r^{\mathrm{T}}$, and using the property (29), we obtain

$$\frac{d^2 \tilde{y}}{dt^2} + \mathbf{D}_r \tilde{y} = \mathbf{\Phi}_r^{\mathbf{T}} \mathbf{V}^{\mathbf{T}} j \tag{30}$$

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: One important fact is that the eigenvalues of physically important modes computed from the original system (5) will also satisfy the reduced system (27) 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 $k' \times k'$ system shown in (27) to obtain the physically important modes of (5). A theoretical proof of this is given in the appendix.

During the time marching process, whenever we add a solution vector in space $\mathbf{V}$, we compute the eigenvalues from the reduced system (27). If the size of (27) 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 (28). At the early time, very large eigenvalues are observed from (27). They correspond to the largest eigenvalues that are supported by the numerical system. These large eigenvalues can be observed at an 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 (21), the field solution for a given frequency is dominated by eigenmodes whose eigenvalues are the closest to the given frequency as 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 starts to have its weights $\tilde{y}$ significantly larger than those of the rest of the eigenvalues which are larger, the 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, instead of becoming larger, can only become smaller because the frequency carried by the later time response can only be lower than higher.

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

$$\tilde{y}_h < \varepsilon_1 \tilde{y}_l \tag{31}$$

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_l:

$$\frac{\left|\lambda_{l,q}^{n+1} - \lambda_{l,q}^{n}\right|}{|\lambda_{l,q}^{n}|} < \varepsilon_2, \ q = 1, 2, \ldots, k \tag{32}$$

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_l. We select the eigenvectors of (27) corresponding to these λ_l, $\mathbf{\Phi}_{r,l}$, to form the space $\mathbf{\Phi}_k$

$$\mathbf{\Phi}_k = \mathbf{V}_{N \times k'} (\mathbf{\Phi}_{r,l})_{k' \times k} \tag{33}$$

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 $\mathbf{\Phi}_k$ because not all the eigenvalues and eigenvectors contained in $\mathbf{V}$ belong to the $\mathbf{\Phi}_k$ 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 $\mathbf{\Phi}_{r,l}$. When both criteria (31) and (32) are satisfied, the $\mathbf{\Phi}_k$ is complete as well as accurate.

3) Form $\mathbf{\Phi}_l$ That Spans all the Stable Modes for a Given Time Step: With $\mathbf{\Phi}_k$ 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 $\mathbf{\Phi}_l$. Thus

$$\mathbf{\Phi}_l = \mathbf{V}_{N\times k'}(\mathbf{\Phi}_{r,l})_{k'\times l}$$

where $(\mathbf{\Phi}_{r,l})_{k'\times l}$ are the l physically important eigenvectors of (27) whose eigenvalues are no greater than $4/\Delta t^2$. When Δt is chosen based on accuracy requirement, l is equal to k, i.e., all the physically important modes will be included in $\mathbf{\Phi}_l$. Hence, the simulation is not only stable but also accurate.

It is also worth mentioning that we store $\mathbf{\Phi}_l$ by separately storing $\mathbf{V}_{N\times k'}$ and $(\mathbf{\Phi}_{r,l})_{k'\times l}$, 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 Section IV-B.

B. Explicit Time Marching Stable for Any Given Time Step

With $\mathbf{\Phi}_l$, the space formed by stable modes for a given time step Δt, obtained systematically, we can simulate (2) in a stable fashion for the given Δt regardless of how large Δt is.

At each time step, we solve (2). We first expand u in the space of $\mathbf{\Phi}_l = \mathbf{V}_{N\times k'}(\mathbf{\Phi}_{r,l})_{k'\times l}$, 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

$$u(t) = \mathbf{V}\mathbf{\Phi}_{r,l}\tilde{y}_l(t). \tag{34}$$

Substituting (34) into (2) and multiplying $(\mathbf{V}\mathbf{\Phi}_{r,l})^{\mathrm{T}}$ on both sides of (2), we obtain

$$\mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{A}\mathbf{\Phi}_{r,l}\frac{d^2\tilde{y}_l}{dt^2} + \mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{B}\mathbf{\Phi}_{r,l}\tilde{y}_l = \mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{V}^{\mathbf{T}}j \tag{35}$$

where $\mathbf{A}$ and $\mathbf{B}$ are the same as (26). Because of (29), we have

$$\mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{A}\mathbf{\Phi}_{r,l} = \mathbf{I}, \text{ and, } \mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{B}\mathbf{\Phi}_{r,l} = \mathbf{D}_l \tag{36}$$

in which $\mathbf{D}_l$ is a diagonal matrix that contains the l eigenvalues corresponding to stable modes. A central-difference based discretization of (35) thus yields

$$\tilde{y}_l^{n+1} = 2\tilde{y}_l^n - \tilde{y}_l^{n-1} - \Delta t^2\mathbf{D}_l\tilde{y}_l^n + \Delta t^2\mathbf{\Phi}_{r,l}^{\mathbf{T}}\mathbf{V}^{\mathbf{T}}j^n. \tag{37}$$

After a time marching of (37) at all the time steps, if the field solution all over the structure is needed, it can be obtained by

$$u^{n+1} = \mathbf{V}\mathbf{\Phi}_{r,l}\tilde{y}_l^{n+1}. \tag{38}$$

Since $\mathbf{\Phi}_{r,l}$ and $\mathbf{V}$ are time independent, at each time step, we only need to update $\tilde{y}_l$ and, also, from the reduced system shown in (37), the cost of which is $O(l)$, and hence negligible.

C. Summary of the Overall Procedure and Cost Analysis

The overall procedure is as follows.

Step I: Preprocessing for building a complete and accurate space $\mathbf{\Phi}_l$ that spans all the stable modes for any given time step irrespective of its size:

(I-1). Use the conventional explicit time-domain method to solve (2), and march on in time by one step. This can be performed in linear complexity.

(I-2). At selected time instants, the number of which is $O(k)$ (which instants to select does not affect the accuracy because the criteria (31) and (32) will ensure accuracy):

Add field solution vector u in $\mathbf{V}$. Orthogonalize the new solution vector with respect to the other vectors that have been already stored in $\mathbf{V}$. The cost is linear for orthogonalizing k' vectors of length N.

Solve a reduced eigenvalue problem of size k' shown in (27). Solve the weight $\tilde{y}$ from (30). Check whether (31) and (32) are satisfied. If not, go back to substep (I-1); if yes, stop, and then determine eigenvalues and eigenvectors of the stable modes. The cost of this step is negligible because of the reduced system size.

Step II: Explicit time-marching stable for any given time step

(II-1) Perform time-marching. Compute the coefficient $\tilde{y}$ of each mode from the reduced system (37) of size l at each time step. The cost is $O(l)$, where l is the number of stable modes.

(II-2) After $\tilde{y}$ is obtained at all time steps, the field solution u can be recovered from (38) at each time instant. If only m selected field solutions are of interest, we can select the m rows corresponding to the selected locations to compute u, the cost is $O(m)$.

V. Numerical Results

We have simulated a number of examples of both μm- and millimeter-scales to validate the unconditional stability, accuracy, efficiency, and late-time stability of the proposed method.

A. Demonstration of Unconditional Stability

First, we demonstrate the fact that the proposed method is stable regardless of the space step and 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 μm, 5 μm, and 900 μm, respectively. The space resolution along x, y, and z was 1 μm, 1 μm, and 100 μm, 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 current source was the derivative of a Gaussian pulse with $I(t) = 2(t\text{-}t_0)\exp(\text{-}(t\text{-}t_0)^2/\tau^2)$, 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. 1, the proposed method permits the use of any large time step such as 0.0001 s, 0.001 s, 0.01 s, and 0.1 s without becoming unstable. As described in Section III, the proposed method achieves stability for any large time step courtesy a representation of field solution strictly by stable modes for the given time step. In this simulation, by keeping only the DC

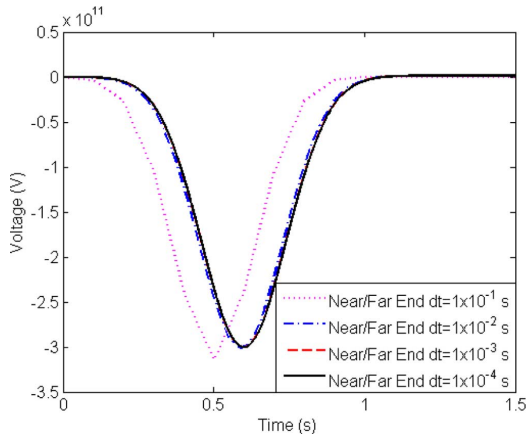

Fig. 1. Illustration of the unconditional stability of the proposed method.

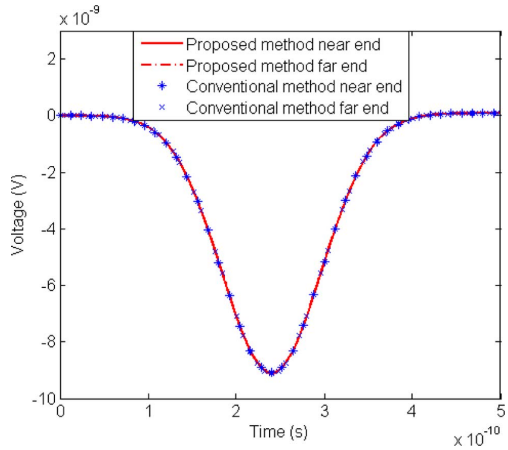

Fig. 2. Voltage waveforms of an on-chip interconnect.

mode whose eigenvalue is zero from the reduced eigenvalue solution (27), 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. In addition, in this example, since the time step of 0.0001 s, 0.001 s, and 0.01 s also satisfies accuracy requirements for the given input source, the results shown in Fig. 1 for these three time steps are not only stable but also accurate, which reveal that the voltages at the near and far end of the parallel plate operating in the input spectrum are nothing but the integration of the input current divided by a capacitive parameter of the structure. With 0.1 s time step, the proposed method still generates a stable result. But the result is not accurate because the time step of 0.1 s is greater than that required by accuracy.

B. Demonstration of Unconditional Stability, Accuracy, and Efficiency

1) Three-Dimensional On-Chip Interconnect: The first 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. 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 magnitude of the source 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 used in (31) and (32) were both chosen to be 10^{-3}. Three physically important modes were detected from 14,800 time steps simulated in the preprocessing. Their eigenvalues were $\lambda_1 = 0$, $\lambda_2 = 7.00872 \times 10^{11}$, and $\lambda_3 = 7.20873 \times 10^{11}$ rad/s respectively. These values 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 preprocessing and the cost after preprocessing is negligible. Thus, the speedup is 330. Fig. 2 shows an excellent agreement between the proposed method and the conventional central-difference based method.

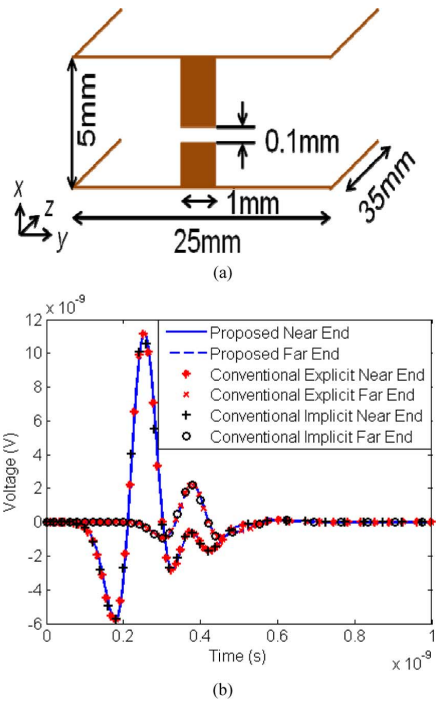

Fig. 3. Simulation of a millimeter-scale waveguide with thin films. (a) Structure. (b). Voltage waveforms.

2) Millimeter-Scale Waveguide With Thin Films: Next example was a millimeter-scale waveguide with thin films as shown in Fig. 3(a). 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. The waveguide was discretized to seven 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 preprocessing. The solver automatically simulated for 3,000 time steps in preprocessing 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, with error being less than 1%. Since the conventional explicit method needs 1.7×10^4 steps and the proposed method requires only 3,000 steps in preprocessing, 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 scheme is not as significant as that observed in previous example that involves a space resolution much smaller than that required by accuracy due to the existence of fine features relative to working wavelength. In Fig. 3(b), 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 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. 4(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 a current source $I(t) = 2(t\text{-}t_0)\exp(-(t\text{-}t_0)^2/\tau^2)$ with $t_0 = 4\tau$ and $\tau = 3 \times 10^{-11}$ s. 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 interval simulated was 9×10^{-11} s. We compared the CPU time of the proposed 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 multifrontal based sparse matrix solver [26]. In Fig. 4(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

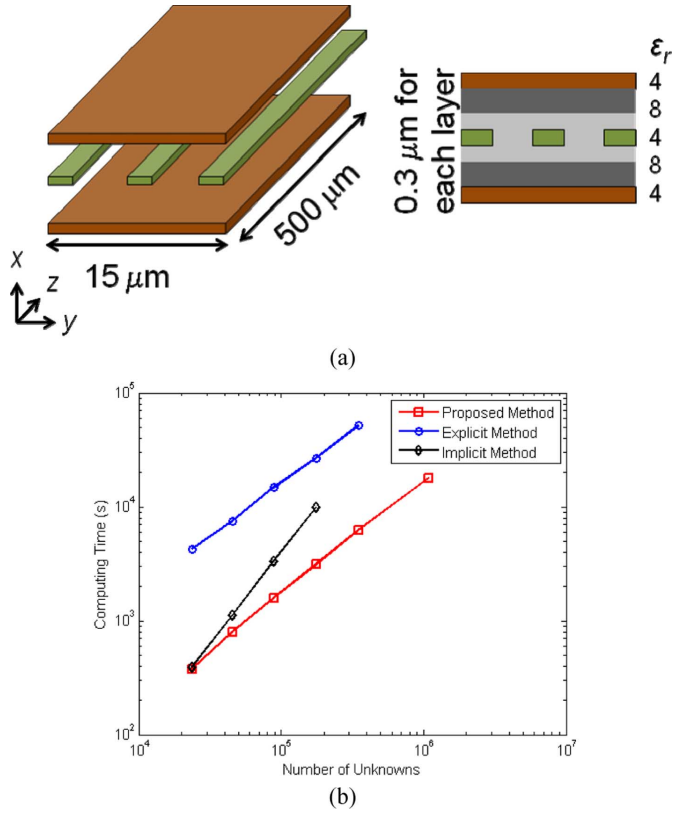

Fig. 4. Simulation of an on-chip bus. (a) Illustration of the structure and material. (b) Total CPU time comparison between 3 methods.

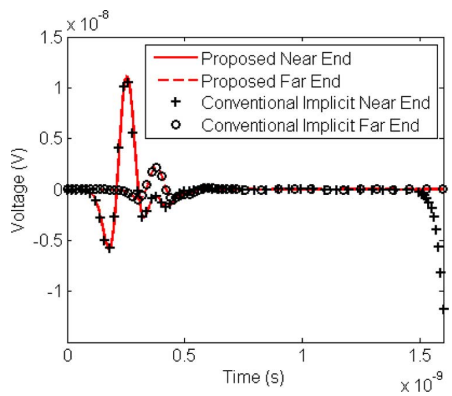

Fig. 5. Comparison of two methods in late-time stability.

explicit method and the explicit method in [15] both employ orthogonal prism vector bases and hence 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 for large problem sizes.

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-2), we observed late-time instability from the Newmark-based implicit scheme, as shown in Fig. 5, whereas the proposed method is stable.

VI. Conclusion

In this work, we propose an unconditionally stable explicit time-domain finite-element method that removes the dependence of the time step on the space step. It is stable for an arbitrarily large time step. If the time step is chosen based on accuracy, the proposed method is not only stable but also accurate no matter how large the time step is. The method is applicable to general 3-D problems with inhomogeneous materials and irregular structures. Different from previous methods for achieving such a capability, in which the source that is responsible for the instability still remains in the numerical system, and hence one has to resort to implicit methods to bound the error amplification factor by 1 to ensure stability, 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, allowing the time step to be solely determined by accuracy requirements.

The complete removal of the unstable modes for a given time step is achieved by strictly expanding the field solution in the space of stable modes, and also projecting the numerical system onto the space of the stable modes. By doing so, the original system matrix that spans both stable and unstable modes is transformed to a system of stable modes only. The stable modes are found in the preprocessing step by a time-domain solution based fast eigenvalue solution of $O(k)$, with $k \ll N$. This also allows the explicit marching to be efficiently performed in a reduced system of $O(k)$.

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 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 a time-domain finite-element method, the essential idea can be applied to other time domain methods.

Appendix

Here, we prove that the eigenvalues of the large system (5) can be found from the reduced system (27) as long as the space $\mathbf{V}$ used to reduce (5) to (27) contains the information of the eigenvectors corresponding to these eigenvalues.

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

$$\mathbf{S}\phi_i = \lambda_i^2 \mathbf{T}\phi_i. \tag{A-1}$$

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:

$$\phi_i = \mathbf{V}y \tag{A-2}$$

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

$$\mathbf{V}^{\mathrm{T}}\mathbf{S}\mathbf{V}y = \lambda_i^2 \mathbf{V}^{\mathrm{T}}\mathbf{T}\mathbf{V}y. \tag{A-3}$$

From (26), the above can be further written as

$$\mathbf{B}y = \lambda_i^2 \mathbf{A}y. \tag{A-4}$$

As a result, the eigenpair (λ_1^2, y) is the solution of (27). Therefore, the eigenvalues that satisfy (5) also satisfy (27) as long as the $\mathbf{V}$ used to reduce (5) to (27) contains the information of the eigenvectors corresponding to these eigenvalues. In addition, by front multiplying the eigenvector obtained from (27) 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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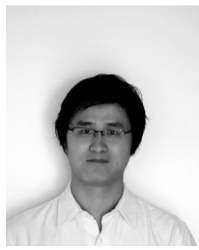

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