Alternative Method for Making Explicit FDTD Unconditionally Stable

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Abstract—An alternative method is developed to make an explicit FDTD unconditionally stable. In this method, given any time step, we find the modes that cannot be stably simulated by the given time step, and deduct these modes directly from the system matrix (discretized curl-curl operator) before the explicit time marching. By doing so, the original FDTD numerical system is adapted based on the desired time step to rule out the root cause of instability. The resultant explicit FDTD marching is absolutely stable for the given time step no matter how large it is, and irrespective of space step. The accuracy is also guaranteed for time step chosen based on accuracy. Numerical experiments have validated the accuracy, efficiency, and unconditional stability of the proposed new method for making an explicit FDTD unconditionally stable.

Index Terms—Explicit methods, finite-difference time-domain method (FDTD), stability, unconditionally stable methods.

I. Introduction

INITE-DIFFERENCE TIME-DOMAIN (FDTD) method [1], [2] is one of the most popular time domain methods for electromagnetic analysis. This is largely attributed to its simplicity and optimal computational complexity at each time step gained by not solving a matrix. However, the time step of a traditional FDTD is restricted by space step for stability, as dictated by the well-known Courant-Friedrichs-Lewy (CFL) condition. When the space step can be chosen based on accuracy for sampling the working wavelength, the time step dictated by the CFL stability condition agrees well with the time step required by accuracy. Hence, the dependence of time step on space step does not become a concern. However, when the problem being simulated involves fine features relative to working wavelengths such as an on-chip nanometer integrated circuit working at microwave frequencies, or a multiscaled system spanning a wide range of geometrical scales, the time step determined by space step for a stable FDTD simulation can become many orders of magnitude smaller than the time step required by accuracy. Due to such a small time step, a tremendous number of time steps must be simulated to reach the time corresponding to the working frequency, which is computationally prohibitive. From

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the accuracy point of view, such a choice of time step is not necessary, and hence the time step's dependence on space step is a numerical problem that must be overcome.

Implicit unconditionally stable FDTD methods [3]–[13] have been developed to overcome the dependence of time step on space step. In these methods, the time integration technique is changed to a different way such that the resulting time marching scheme has an error amplification factor bounded by 1, thus ensuring stability. However, the implicit methods require a matrix solution, the efficiency of which is not desired when a large problem size is encountered. In addition, it is observed that the accuracy of the implicit methods can degrade greatly with the increase of time step. Late-time instability has also been observed among existing implicit unconditionally stable FDTD methods.

Recently, advanced research [14]-[18] has been pursued to address the time step problem in the framework of the original explicit time-domain methods. In [15], [17], [18], the root cause of instability is identified for explicit time-domain methods, based on which an explicit and unconditionally stable time-domain finite-element method (TDFEM) is successfully developed in [15], [17] and the same capability is demonstrated for FDTD in [18]. The root-cause analysis shown in [15], [17], [18] is different from a conventional stability analysis [2], [19]. In a conventional stability analysis, the time step required for a stable time-domain simulation is derived and used to guide the choice of time step. From such a stability analysis, apparently, except for choosing the time step based on the stability criterion, there is no other way forward to make an explicit method stable. On the contrary, the root-cause analysis given in [17], [18] reveals that when an explicit time-domain method becomes unstable, not every eigenmode present in the field solution becomes unstable. Only a subset of eigenmodes is unstable, while the rest of the eigenmodes are still stable. This subset of eigenmodes is the root cause of instability, which are termed unstable modes. These modes have eigenvalues (characterizing the rate of field variation in space) greater than that can be accurately captured by the given time step, thus causing instability. When the time step is chosen based on accuracy, the unstable modes are not required by accuracy. Hence, they can be removed without affecting the accuracy.

Based on the root-cause analysis, in [18], an explicit FDTD that is unconditionally stable is developed. It has also been extended to analyze general lossy problems in [21], [22]. In this method, the field solution is expanded into stable eigenmodes, and the numerical system is also projected onto the space of stable eigenmodes. The resulting explicit time-marching is absolutely stable for the given time step no matter how large it

is. Comparisons with state-of-the-art implicit unconditionally stable FDTD methods have also shown clear advantages of the new explicit method in accuracy, dispersion error, and stability in addition to computational efficiency [22]. This is mainly because in an implicit unconditionally stable method, the root cause of instability that makes an explicit method unstable is not removed from the numerical system. When a large time step beyond CFL condition is used, the root cause, which is unstable modes, cannot be accurately simulated by the given time step. Although they are suppressed to be stable, they can still negatively affect the overall accuracy and stability of the implicit method. To preserve the advantage of the explicit FDTD in avoiding solving a matrix equation, a preprocessing algorithm is developed in [18] to extract the stable eigenmodes from the field solutions obtained from the traditional explicit FDTD. The time window simulated in the preprocessing step is much smaller than that of the entire time window to be simulated. However, since the time step required by a traditional FDTD method is used in the preprocessing step, the speedup of the overall scheme can become limited by the preprocessing step.

In this work, we develop a new explicit and unconditionally stable FDTD method. This new method eliminates the traditional FDTD-based preprocessing in [18]. Meanwhile, it permits the use of a large time step upfront in the explicit time marching by deducting the unstable modes directly from the FDTD system matrix. The unstable modes have the largest eigenvalues of the system matrix, and hence they can be efficiently found in $O(k^2N)$ complexity, with k the number of unstable modes. Using the proposed method, one only needs to perform a very minor modification on the traditional FDTD to make it unconditionally stable. Hence, the proposed method is convenient for use. The basic idea of this work has been presented in our IMS conference paper [20]. In this paper, we expand [20] to address aspects that have not been addressed before, including algorithm details, complexity and accuracy analysis, open-region problems, how to efficiently find unstable modes, and comparisons with the previous explicit and unconditionally stable FDTD method [18]. Extensive numerical experiments and comparisons with existing methods have demonstrated the unconditional stability, accuracy, and efficiency of the proposed alternative explicit and unconditionally stable method.

II. PRELIMINARIES

Before presenting the proposed work, it is necessary to review the root cause of instability [17], [18]. Using a matrix notation, we can rewrite the FDTD updating equations into the following compact form:

$$H^{n+\frac{1}{2}} = H^{n-\frac{1}{2}} - \Delta t \mathbf{D}_E E^n \tag{1}$$

$$E^{n+1} = E^n + \Delta t \mathbf{D}_H H^{n+\frac{1}{2}} - \Delta t j^{n+\frac{1}{2}}$$
 (2)

where E denotes the vector of electric field unknowns placed along the edges of the primary grid, H denotes the vector of magnetic field unknowns along the edges of the dual grid, j is the vector of current sources whose entry is J/ϵ with J being current density, Δt is time step, superscripts such as $n, n \pm (1)/(2)$, and n + 1 denote the time instant, \mathbf{D}_E and \mathbf{D}_H are

sparse matrices representing the discretized $(1)/(\mu)\nabla \times$, and $(1)/(\epsilon)\nabla \times$ operators, respectively. As can be seen from (1) and (2), the computations involved in the FDTD are sparse matrix-vector multiplications.

Equations (1) and (2) solve both E and H. We can also eliminate one field unknown to see the root cause of instability more easily. Rewriting (2) for E^n , we find

$$E^{n} = E^{n-1} + \Delta t \mathbf{D}_{H} H^{n-\frac{1}{2}} - \Delta t j^{n-\frac{1}{2}}.$$
 (3)

Subtracting (3) from (2), and using (1) to replace the term of $H^{n+(1)/(2)} - H^{n-(1)/(2)}$ in the resultant, we arrive at

$$\frac{E^{n+1} - 2E^n + E^{n-1}}{\Delta t^2} + \mathbf{D}_H \mathbf{D}_E E^n = f^n$$
 (4)

where $f^n=-(j^{n+(1)/(2)}-j^{n-(1)/(2)})/\Delta t$, which is actually $-(\partial j)/(\partial t)$ at the *n*-th time instant. Equation (4) is nothing but a central-difference based discretization of the following second-order wave equation

$$\frac{d^2E}{dt^2} + \mathbf{M}E = f \tag{5}$$

where

$$\mathbf{M} = \mathbf{D}_H \mathbf{D}_E. \tag{6}$$

The solution to (5) at any time is a time-dependent superposition of the eigenmodes of M. Performing a z-transform of (4), it can be found the eigenmodes, whose eigenvalues ξ_i satisfy the following condition, can always be stably simulated by the given time step Δt

$$\xi_i \le 4/\Delta t^2. \tag{7}$$

The root cause of instability is thus the eigenmodes whose eigenvalues ξ_i are greater than $4/\Delta t^2$, which are termed unstable modes.

In a traditional explicit time-domain method, the underlying numerical system and thereby the eigenmodes governing the field solution are not changed, but the time step is adjusted based on the CFL condition so that a time-domain simulation can be made stable. The CFL condition essentially requires the time step to be chosen based on the largest eigenvalue of \mathbf{M} , so that (7) is satisfied for all eigenmodes present in the numerical system. In an explicit and unconditionally stable method like [17], [18], the desired time step is not changed, but the numerical system is changed so that only those eigenmodes that can be stably simulated by the given time step are kept, while the unstable modes are discarded. In this way, the dependence of the time step on space step is removed, and an explicit method can also be made unconditionally stable.

III. PROPOSED METHOD

From the root-cause analysis reviewed in the previous section, it is evident that once a space discretization is done, whether there exist unstable modes or not is known for a given time step, regardless of time marching. Therefore, the source of instability is inherent in the system matrix resulting from the space discretization, rather than in the field solution. To completely remove such a source, the system matrix has to be

changed. In this section, we present proposed method, explain how it works, and analyze its complexity and accuracy. In addition, we also describe how to handle open-region problems in the proposed method.

A. Method

Let V_h denote the matrix formed by all the unstable modes, with each column being an eigenvector of M whose eigenvalue is greater than $4/\Delta t^2$. How to efficiently find V_h will soon be given in next section. Right now, assume V_h has been generated.

In the proposed method, we use V_h to directly change the original system matrix M to a new system matrix M_l

$$\mathbf{M}_l = \mathbf{M} - \mathbf{V}_h \mathbf{V}_h^T \mathbf{M}. \tag{8}$$

For an M that is Hermitian and positive semi-definite, the above is equal to

$$\mathbf{M}_l = \mathbf{M} - \mathbf{M} \mathbf{V}_h \mathbf{V}_h^T \tag{9}$$

i.e., multiplying \mathbf{M} by $\mathbf{V}_h \mathbf{V}_h^T$ from the right. We then perform an explicit FDTD simulation on the new system matrix \mathbf{M}_l . If a second-order based system shown in (4) is employed, we simply modify it to

$$\frac{E^{n+1} - 2E^n + E^{n-1}}{\Delta t^2} + \mathbf{M} \left(\mathbf{I} - \mathbf{V}_h \mathbf{V}_h^T \right) E^n = f^n \quad (10)$$

and march on in time step by step. If the original FDTD-based first-order system given in (1) and (2) is used, we update them to

$$H^{n+\frac{1}{2}} = H^{n-\frac{1}{2}} - \Delta t \mathbf{D}_{E} \left(\mathbf{I} - \mathbf{V}_{h} \mathbf{V}_{h}^{T} \right) E^{n}$$

$$E^{n+1} = E^{n} + \Delta t \mathbf{D}_{H} H^{n+\frac{1}{2}} - \Delta t j^{n+\frac{1}{2}}$$
(11)

which is the same as (10). This can be readily verified by eliminating H unknowns from (11).

One can also eliminate E unknowns to obtain an equation for H, which is the H-based counterpart of (10). In this case, \mathbf{M} becomes $\mathbf{D}_E \mathbf{D}_H$, and in (11), the $(\mathbf{I} - \mathbf{V}_h \mathbf{V}_h^T)$ term does not exist in the first row, but appears in front of H in the second row.

After obtaining the solution of E from (10) or (11), we need to add *one more important step* to make the solution correct, which is

$$E = E - \mathbf{V}_h \mathbf{V}_h^T E. \tag{12}$$

Obviously, the aforementioned method only requires a very minor modification in the traditional FDTD, and hence the method is convenient for use. Now, we shall explain how the proposed method works.

B. How It Works?

The new system matrix \mathbf{M}_l consists of the stable eigenmodes only, and hence the source of instability is completely removed. To prove, we first utilize the property of the eigenvectors of \mathbf{M} . Since \mathbf{M} is Hermitian positive semi-definite, its eigenvectors \mathbf{V} are orthogonal. Hence, the following property holds true:

$$\mathbf{V}^T \mathbf{V} = \mathbf{I}.\tag{13}$$

Since $MV = V\Lambda$, where Λ is the diagonal matrix of eigenvalues, using (13), we obtain

$$\mathbf{M} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T \tag{14}$$

which can further be written as

$$\mathbf{M} = \mathbf{V}_h \mathbf{\Lambda}_h \mathbf{V}_h^T + \mathbf{V}_l \mathbf{\Lambda}_l \mathbf{V}_l^T \tag{15}$$

where V_l is the eigenvector matrix of stable eigenmodes, Λ_l and Λ_h are diagonal matrices containing stable and unstable eigenvalues, respectively.

Multiplying both sides of (15) by $\mathbf{V}_h \mathbf{V}_h^T$, since \mathbf{M} 's eigenvectors are orthogonal, we obtain

$$\mathbf{V}_h \mathbf{V}_h^T \mathbf{M} = \mathbf{V}_h \mathbf{\Lambda}_h \mathbf{V}_h^T. \tag{16}$$

Thus, substituting (16) into (8) and using (15), (8) is nothing but

$$\mathbf{M}_l = \mathbf{V}_l \mathbf{\Lambda}_l \mathbf{V}_l^T \tag{17}$$

and hence the space of stable modes only.

Since \mathbf{M}_l is symmetric as can be seen from (17), (8) is the same as (9). However, for non-symmetric \mathbf{M} such as the one resulting from a lossy analysis [22], (8) is different from (9), and (8) is the correct one to use since it is still made of \mathbf{V}_l modes only, while (9) is not. In addition, in this case, the \mathbf{V}_h should be orthogonalized to satisfy $\mathbf{V}_h^H \mathbf{V}_h = \mathbf{I}$ before being removed from \mathbf{M} , and the $\mathbf{V}_h \mathbf{V}_h^T$ in (8) is replaced by $\mathbf{V}_h \mathbf{V}_h^H$.

After updating the system matrix from M to M_l that is free of the source of instability, we can perform the explicit FDTD time-marching on \mathbf{M}_l with absolute stability. However, after implementing (10) and (11), we found the result is indeed stable but not accurate. Interestingly, if V_h is found by first obtaining all eigenvectors of M, and then selecting V_h from them, the accuracy is good. However, if \mathbf{V}_h is found by computing the unstable eigenvectors of M only, the results do not match the reference data. Certainly, the first approach that finds all eigenvectors is not practical for use when problem size is large, and the second approach is the one that can truly make the proposed method useful in practice. To figure out the problem, we compare the V_h modes found by the second approach with those found by computing all eigenvectors of M. They show good agreement with each other. Therefore, the accuracy of V_h is not a problem. This has led to the finding that the updated matrix M_l has additional zero eigenvalues, the eigenvectors corresponding to these additional zero eigenvalues are not the eigenvectors of the original matrix \mathbf{M} , and they make the result wrong. To explain, the M_l as shown in (17) has rank k_l , where k_l is the number of stable eigenmodes of M. On the other hand, M_l is a matrix of size $N \times N$. Hence, the additional $N - k_l$ eigenvalues are zero, whose eigenvectors make an additional nullspace. As a result, when computing (10) or (11), the field solution is not only the superposition of the V_I modes, but also the additional nullspace (V_{oa}) modes as the following:

$$E = \mathbf{V}_l y_l + \mathbf{V}_{oa} y_{oa} \tag{18}$$

where y_l and y_{oa} are corresponding coefficient vectors. The true solution should satisfy $E = \mathbf{V}_l y_l$. Hence, the result of (18) is wrong. When \mathbf{V}_h is found by computing all the eigenvectors of

V and from them choosing V_h , (17) matches that in (15) very well. Hence, the contribution of the additional nullspace in (17) is almost zero. However, this is not the case when V_h is found from computing only the eigenvectors of M that violate (7).

To solve this problem, after obtaining the solution of E from (10) or (11), we need to add (12) to make the solution correct. This treatment removes the second term in (18). This is because \mathbf{V}_{oa} must be in the space of \mathbf{V}_h since it is not in \mathbf{V}_l . By deducting $\mathbf{V}_h\mathbf{V}_h^TE$ from E, all of the \mathbf{V}_h -components and thereby \mathbf{V}_{oa} -components are removed, making E's solution correct. It is also worth mentioning that if nullspace, whose eigenvectors are also termed DC modes, does not make an important contribution in the field solution such as in the case of an electrically large antenna, the step of (12) is not needed.

To use an infinitely large time step without making the FDTD unstable, we simply remove all the eigenmodes of **M** whose eigenvalues are nonzero. To use other time step sizes, we remove eigenmodes adaptively based on the given time step. As a result, the proposed method flexibly permits the use of any time step independent of space step, thus being explicit and unconditionally stable.

C. Complexity and Accuracy Analysis

1) Complexity Analysis: As compared to the original FDTD, the only additional computation involved in the proposed method is the computation of $\mathbf{V}_h\mathbf{V}_h^TE^n$ at each time step, as shown in (10) and (11). The $\mathbf{V}_h\mathbf{V}_h^TE^n$ can be efficiently evaluated by two matrix-vector multiplications: first, computing $\mathbf{V}_h^TE^n$, the cost of which is kO(N); second, multiplying the resultant by \mathbf{V}_h , the cost of which is also kO(N). If one computes $\mathbf{V}_h\mathbf{V}_h^T$ first, the resultant matrix is a dense matrix of size $N\times N$. Multiplying such a dense matrix by E^n would cost $O(N^2)$ operations, which is expensive when N is large. Therefore, the approach of doing two matrix-vector multiplications should be used to obtain $\mathbf{V}_h\mathbf{V}_h^TE^n$.

2) Accuracy Analysis: When the time step is chosen based on accuracy, the unstable modes are not required by accuracy, and hence they can be deducted from the system matrix without affecting accuracy. To explain, in the proposed method, we expand the space dependence of the field solution using the eigenmodes of M as follows:

$$E(\mathbf{r},t) = \sum_{i=1} \mathbf{V}_i y_i(t)$$
 (19)

where $y_i(t)$ is the time-dependent coefficient of the *i*-th eigenmode \mathbf{V}_i . In a source-free problem, the $y_i(t)$ is analytically known as [18]

$$y_i(t) = a_i \cos(\sqrt{\xi_i}t) + b_i \sin(\sqrt{\xi_i}t) \tag{20}$$

with a_i,b_i arbitrary coefficients. Hence, the square root of the eigenvalue is also the frequency of the field's time variation, i.e., $\omega=\sqrt{\xi_i}$. This is, in fact, dispersion relation. In free space, the $\sqrt{\xi_i}$ is analytically known as βc , where β is free-space wave number. In inhomogeneous problems, the $\sqrt{\xi_i}$ is not analytically known but can be numerically found. When the time step is chosen based on accuracy such as $\Delta t \leq 1/(10f_{\rm max})$. The unstable modes have $\xi_i > 4/\Delta t^2$, and

hence $\xi_i > 4/\Delta t^2 \ge 400 f_{\rm max}^2$, thus beyond the maximum frequency required to be captured by accuracy. The above accuracy analysis is for source-free problems. The same holds true for problems with sources, as shown by the analysis given in Section IV.B, and specifically (40) of [18].

D. Treatment of Open-Region Boundary Conditions

In open-region problems, the computational domain can be truncated by various Absorbing Boundary Conditions (ABC) such as Perfectly Matched Layers (PML). Since the field solution inside PML is fictitious, and there is no fine feature inside the PML region either, we do not perform any special treatment in the PML region, but to conduct the FDTD simulation as it is. In the solution domain, we update the system matrix by deducting the unstable modes from it. Basically, we divide the unknown E into two groups, one inside the solution domain denoted by E_S , and the other elsewhere such as boundary, PML or other ABCs, denoted by E_O . The same is done for unknown E. Subsequently, the sparse matrices E and E are cast into the following form:

$$\mathbf{D}_{E} = \begin{bmatrix} \mathbf{D}_{E,SS} & \mathbf{D}_{E,SO} \\ \mathbf{D}_{E,OS} & \mathbf{D}_{E,OO} \end{bmatrix}$$

$$\mathbf{D}_{H} = \begin{bmatrix} \mathbf{D}_{H,SS} & \mathbf{D}_{H,SO} \\ \mathbf{D}_{H,OS} & \mathbf{D}_{H,OO} \end{bmatrix}.$$
(21)

With the above, rewriting (11) separately for H_S, H_O, E_S and E_O , we obtain

$$H_{S}^{n+\frac{1}{2}} = H_{S}^{n-\frac{1}{2}} - \Delta t \mathbf{D}_{E,SS} \left(\mathbf{I} - \mathbf{V}_{h} \mathbf{V}_{h}^{T} \right) E_{S}^{n} - \Delta t \mathbf{D}_{E,SO} E_{O}^{n}$$

$$H_{O}^{n+\frac{1}{2}} = H_{O}^{n-\frac{1}{2}} - \Delta t \mathbf{D}_{E,OO} E_{O}^{n} - \Delta \mathbf{D}_{E,OS} E_{S}^{n}.$$

$$E_{S}^{n+1} = E_{S}^{n} + \Delta t \mathbf{D}_{H,SS} H_{S}^{n+\frac{1}{2}} + \Delta t \mathbf{D}_{H,SO} H_{O}^{n+\frac{1}{2}} - \Delta t j^{n+\frac{1}{2}}$$

$$E_{O}^{n+1} = E_{O}^{n} + \Delta t \mathbf{D}_{H,OO} H_{O}^{n+\frac{1}{2}} + \Delta \mathbf{D}_{H,OS} H_{S}^{n+\frac{1}{2}}.$$
(22)

IV. FINDING UNSTABLE MODES

For any given time step Δt , the unstable modes are the eigenmodes of ${\bf M}$ whose eigenvalues are greater than $4/\Delta t^2$. Hence, the unstable modes have the largest eigenvalues of ${\bf M}$. Since ${\bf M}$ is sparse, the computing task becomes how to find the largest eigenpairs of a sparse matrix. The Arnoldi method is particularly suited for this computing task [23]. In O(k) steps, it can find a complete set of k largest eigenvalues and eigenvectors. When the matrix is Hermitian, the Arnoldi process reduces to Lanczos method. A k-step Arnoldi method on matrix ${\bf M}$ is to carry out the following computation:

$$\mathbf{MQ}_{N \times k} = \mathbf{QH}_{k \times k} + ge_k^T \tag{23}$$

where \mathbf{Q} is a unitary matrix of size $N \times k$, \mathbf{H} is a small upper Hessenberg matrix of dimension $k \times k$, e_k is the k-th column of identity matrix \mathbf{I} , and g is a column vector of length N yielding ge_k^T an $N \times k$ matrix. When the norm of ge_k^T and hence the norm of g goes to zero, the eigenvalues of \mathbf{H} are the eigenvalues of the original matrix \mathbf{M} , and \mathbf{Q} multiplied by the eigenvectors of \mathbf{H} are the eigenvectors of \mathbf{M} . The detailed algorithm for realizing (23) can be found from Algorithm 3.7 of [23]. The overall computational cost is simply k sparse matrix-vector multiplications, each of which is \mathbf{M} multiplied by an intermediate vector

Algorithm 1: Algorithm for Finding Unstable Modes

Data: Matrix: M Lower bound of the eigenvalue: $(4/\Delta t^2)$ Random vector: ν_0 $k_{initial}$: initial eigenpair number; k_{step} : increment of kp: number of unwanted eigenvalues to be shifted. tol: accuracy of eigenvalue solution Result: V_h 1 k-step Arnoldi (Algorithm 3.7 of [23]) with initial ν_0 and $k = k_{initial}$, obtaining $\mathbf{MQ}_{N \times k} = \mathbf{QH}_{k \times k} + ge_k^T$ 2 while ||g|| > tol do Extend the k-step Arnoldi factorization to k + p steps $\mathbf{MQ}_{N\times(k+p)} = \mathbf{QH}_{(k+p)\times(k+p)} + ge_{k+p}^{T}$ Find eigenvalues of **H**, with $\mu_1, \mu_2, ..., \mu_p$ the smallest p eigenvalues to be shifted $r = e_{k+p}$ 5 for $j=1 \rightarrow p$ do QR factorize $\mathbf{H} - \mu_j \mathbf{I} = \tilde{\mathbf{Q}} \mathbf{R}$. 7 $\mathbf{H} = \tilde{\mathbf{Q}}^H \mathbf{H} \tilde{\mathbf{Q}}$ $\mathbf{V} = \mathbf{V} \tilde{\mathbf{Q}}$ $r = r^H \tilde{\mathbf{Q}}.$ 8 9 10 11 Update g, \mathbf{Q} , and \mathbf{H} as 12 $g = \mathbf{Q}(:, k+1)\mathbf{H}(k+1, k) + gf(k), \mathbf{Q} = \mathbf{Q}(:, 1:k),$

13 Find eigenvalues of $\mathbf{H}_{k \times k}$, check whether the smallest eigenvalue is less than $4/\Delta t^2$. If not, extend the k-step Arnoldi to $k+k_{step}$, update k to $k+k_{step}$, go back to 2. 14 $\mathbf{V}_h = \mathbf{Q}_{N \times k} \mathbf{V}_H$, where \mathbf{V}_H is the matrix formed by eigenvectors of small matrix $\mathbf{H}_{k \times k}$ not satisfying (7).

and $\mathbf{H} = \mathbf{H}(1:k,1:k)$.

generated during the k-step process, and the orthogonalization of the resulting k vectors. The complexity of the k sparse matrix-vector multiplications is kO(N), while the complexity of orthogonalization is $O(k^2N)$, and hence the overall complexity is $O(k^2N)$. This is much more efficient than a brute-force eigenvalue solution.

A straightforward k-step Arnoldi process cannot ensure the k largest eigenpairs to be found in O(k) steps. Spurious eigenvalues may also be produced. We hence employ the implicitly restarted Arnoldi method [23] to systematically drive the residual of (23) to be zero. For completeness of this paper, we give the algorithm of implicitly restarted Arnoldi method as shown in Algorithm 1, which is modified to suit the need of this work. In this algorithm, from Step 4 to 12 is to shift p unwanted eigenvalues so that the next initial vector is rich in the wanted eigenvectors. The computational cost from Step 4 to 12 is negligible as compared to Step 3, since these steps are performed on small matrices of size k + p. The computational complexity of Step 3 is $O(p^2N)$, where p is proportional to k. The cost of Step 13 is again negligible since it is performed on a small matrix of size $k \times k$. Overall, the complexity of Algorithm 1 is $O(k^2N)$ for finding k largest eigenpairs of M.

One may wonder why we do not use the same procedure to find the stable eigenmodes. The stable eigenmodes turn out to have the smallest eigenvalues of M. To find them efficiently,

one has to use a shift-invert technique to transform the eigenvalues of interest (now smallest eigenvalues) to the largest eigenvalues of a new matrix. This new matrix can be written as $(\mathbf{M} - \alpha \mathbf{I})^{-1}$, where α is a shift value chosen to be small so that the smallest eigenvalues can become the largest ones of the new matrix. It is evident that finding the eigenvalues of $(\mathbf{M} - \alpha \mathbf{I})^{-1}$ is computationally much more expensive as compared to finding the eigenvalues of M, since a matrix solution is involved. Furthermore, in O(k) steps, we cannot guarantee finding a complete set of k smallest eigenvalues since α is empirical. Moreover, M has a nullspace whose eigenvalues are zero. The size of nullspace grows with N. In other words, when matrix size increases, the number of eigenvectors whose eigenvalues are zero also increases. This further increases the computational cost. In contrast, the preprocessing algorithm developed in [18] is an efficient and reliable algorithm for finding a complete set of stable eigenmodes. The problem of the increasing size of the nullspace is also well handled in this preprocessing algorithm. This is because all the nullspace eigenvectors share the same eigenvalue (zero) in common. Given a right hand side (source) vector, the contributions from the nullspace eigenvectors are grouped together and become a single vector. Hence, the algorithm in [18] does not suffer from the issue of increasing nullspace size.

V. COMPARISON WITH PREVIOUS METHOD

First, we prove the proposed new method is mathematically equivalent to the previous method [18]. In previous method [18], the fields are expanded in the space of stable modes, and the numerical system is projected onto the space of stable modes. Consider the solution of (4), the E(t) is expanded as $E(t) = \mathbf{V}_l y_l(t)$, and the time-dependent unknown coefficient vector $y_l(t)$ is solved from the following equation:

$$\frac{y_l^{n+1} - 2y_l^n + y_l^{n-1}}{\Lambda t^2} + \mathbf{\Lambda}_l y_l^n = \mathbf{V}_l^T f^n. \tag{24}$$

In the proposed method, we solve (10). Substituting (17) into it, we obtain

$$\frac{E^{n+1} - 2E^n + E^{n-1}}{\Lambda t^2} + \mathbf{V}_l \mathbf{\Lambda}_l \mathbf{V}_l^T E^n = f^n.$$
 (25)

Here, let $E = \mathbf{V}y(t)$, since in the new method we do not explicitly expand the field solution in the \mathbf{V}_l space. Vector $y = [y_l, y_h]^T$ hence consists of the coefficients corresponding to both the \mathbf{V}_l , and the \mathbf{V}_h modes. Multiplying (25) by \mathbf{V}_l^T , with (12), we obtain $y_h = 0$, and y_l satisfying the same equation as (24). Hence, the proposed new method is mathematically equivalent to the previous method. Therefore, its accuracy and stability are both ensured.

However, the two methods are computationally different. In the previous method [18], a traditional FDTD-based preprocessing is developed to find the space of stable modes. In the proposed method, no such preprocessing is required, and hence the method is not subject to the constraint of the traditional FDTD's time step. In the previous method, the numerical system is projected onto the space of stable modes; in the proposed method, the unstable modes are directly deducted from the numerical system to eradicate the root cause of instability. In the

previous method, the explicit marching is performed on a reduced order system since the number of stable modes is smaller than the original system size; in the proposed method, there is no reduction in system order. In the previous method, if the number of stable modes is large, the modes can be broken into bands and found band by band independent of each other; in the proposed method, if the number of unstable modes k is many, the computational cost for finding them remains to be $O(k^2N)$ and, in general, cannot be made smaller.

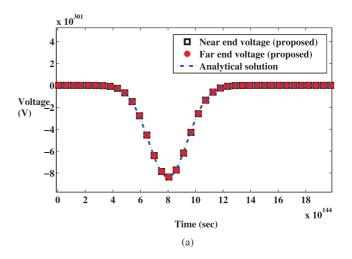
Overall, when the number of unstable modes is not large, the proposed method is efficient for use. This is typically true in many problems solved by the FDTD: the fine features only occupy a small portion of the entire space discretization. The proposed method is also much more convenient for implementation. In addition, by removing just one unstable mode whose eigenvalue is the largest, one already can use a time step larger than the CFL time step using the proposed method; by removing the highest two unstable eigenmodes, one can use an even larger time step; and so on. Hence, with negligible computational cost, the proposed method allows for the use of a time step beyond the stability criterion. In contrast, in the method of [18], the time step in the preprocessing procedure is restricted by the time step required by stability. The computational overhead is more for one to use a time step beyond the CFL condition.

Certainly, the two methods can be combined to accentuate the advantages of both methods. For example, when the number of unstable modes is many, from the proposed method, we can still remove a certain number of unstable modes within feasible run time, based on which the time step can be immediately enlarged although it has not been enlarged to the time step allowed by accuracy yet. Using the resulting updated system matrix, and hence a much increased time step, the preprocessing step in [18] can be accelerated greatly to identify the stable modes. The proposed method hence does not need to finish the simulation of the entire time window, but a small window simulated in the preprocessing step. The previous method can then be used to carry out explicit marching efficiently: the system has a much reduced order and is diagonal, in addition, the computation of the $\mathbf{V}_h \mathbf{V}_h^T E$ term in the proposed method is also avoided.

VI. NUMERICAL RESULTS

A. Demonstration of Unconditional Stability

First, we demonstrate the unconditional stability of the proposed method using an example that has an analytical solution. It is a 3-D parallel plate structure whose dimension is 900 μm , 6 μm , and 1 μm along x-, y-, and z-direction, respectively. The space step is 0.2 μm , 0.85714 μm , and 90 μm , respectively along z-, y-, and x-direction. This structure is excited at the near end by a current source that has a very low frequency pulse of $I(t)=2(t-t_0)\exp(-(t-t_0)^2/\tau^2)$ with $\tau=2\times 10^{144}$ s, and $t_0=4\tau$ s. The time step required by sampling accuracy thereby is at the level of 10^{144} s, while that dictated by the CFL condition for stability is 6.8221×10^{-16} s. Hence, there is a more than 160 orders of magnitude difference in the two time steps. With a time step of 6.6667×10^{144} s, the proposed method stably simulated the structure with excellent accuracy. As can be seen from Fig. 1(a), the voltages generated from the proposed method and



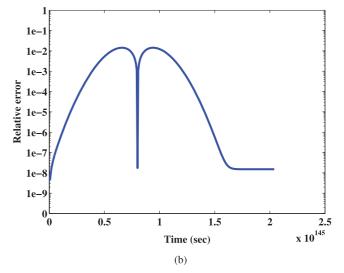


Fig. 1. Demonstration of unconditional stability. (a) Voltage waveforms. (b) Entire solution error as a function of time.

the analytical solution are on top of each other. Notice that the structure behaves as a capacitor at very low frequencies, and hence the near- and far-end voltages are identical to each other. The 6.6667×10^{144} s appears to be already an extremely large time step. In fact, the proposed method allows for a time step of infinity. The V_h includes all the eigenmodes whose eigenvalues are nonzero, leaving zero eigenvalues only, and hence permitting an infinitely large time step. The number of V_h modes is 561. In addition to examining the solution accuracy at selected points, we have also assessed the entire solution error by measuring $||E - E_{ref}|| / ||E_{ref}||$, where E consists of all electric field unknowns in the computational domain solved from the proposed method, whereas E_{ref} is obtained from the analytical solution. The entire solution error is shown in Fig. 1(b) as a function of time, verifying the accuracy of the proposed method at all points in the computational domain at each time instant. Notice that the error is plotted as it is instead of a percentage error. It takes the proposed method 2.99 s to finish the entire simulation including the time for finding unstable modes. To finish the same simulation, the FDTD would have to take more than 5×10^{17} s (the expanding universe time). This example appears to be dramatic, however, it is necessary to examine whether a

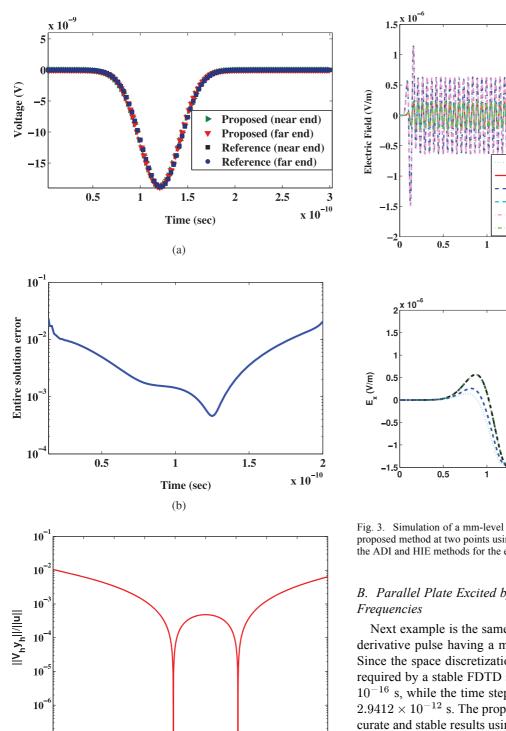


Fig. 2. Simulation of a 3-D parallel plate structure. (a) Voltage waveforms. (b) Entire solution error as a function of time. (c) The ratio of the unstable modes component to the entire field solution.

1.2

Time (sec)

(c)

1.4

1.6

1.8

x 10⁻¹⁰

10

0.2

0.4

0.6

0.8

method is truly unconditionally stable. This example also shows clearly that the dependence of time step on space step is a numerical problem, instead of a fundamental physical law one has to obey.

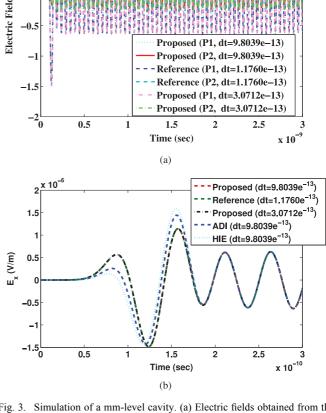
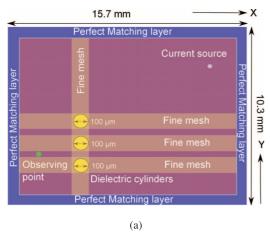


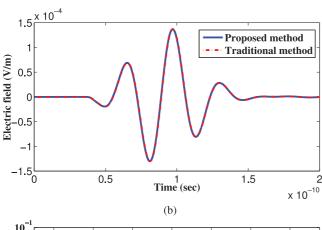
Fig. 3. Simulation of a mm-level cavity. (a) Electric fields obtained from the proposed method at two points using different tme steps. (b) Comparison with the ADI and HIE methods for the electric field simulated.

B. Parallel Plate Excited by a Current Source at Higher Frequencies

Next example is the same structure but with a fast Gaussian derivative pulse having a maximum input frequency 34 GHz. Since the space discretization remains the same, the time step required by a stable FDTD simulation remains to be $6.8221 \times$ 10^{-16} s, while the time step required by sampling accuracy is 2.9412×10^{-12} s. The proposed method is able to generate accurate and stable results using the time step of 2.9412×10^{-12} s. As shown in Fig. 2(a), the voltage waveforms simulated by the proposed method are in excellent agreement with those from the conventional explicit FDTD. The accuracy is further demonstrated by the entire solution error plotted in Fig. 2(b) as a function of time. The CPU time cost by the proposed method is approximately 6.013 s with 3.251 s for time marching, and the rest for finding the unstable modes. Compared with 6875.4 s required by the conventional explicit FDTD, the speedup of the proposed method is 1145.9.

In this example, we have also examined the weights of the unstable modes V_h in the field solution. Let the weights be denoted by y_h . It can be computed at each time step from $V_h^T u(t)$, where u(t) is the reference FDTD solution. As can be seen





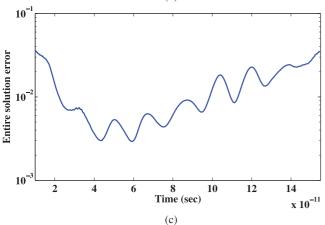


Fig. 4. Simulation of an open-region problem. (a) Structure. (b) Electric field at the observation point. (c) Entire solution error.

clearly from Fig. 2(c), the weights of the discarded unstable modes are small as compared to the entire field solution.

C. Millimeter-Level Cavity

Previous structures have very fine features relative to working wavelengths. Next, we consider a millimeter cavity whose space discretization is comparable to that required by the input spectrum. The overall dimension is $19.4 \text{ mm} \times 12.4 \text{ mm} \times 0.14118$ mm. The space step along x-, y-, and z-direction is respectively 1.8 mm, 1.8 mm, and 0.03529 mm. A current element of length 0.0334 mm is located in middle of the cavity along z-direction. The proposed method uses a time step of 9.8039×10^{-13}

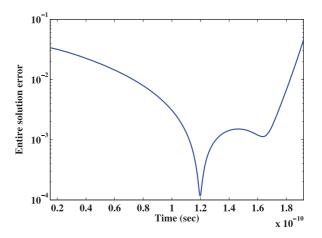
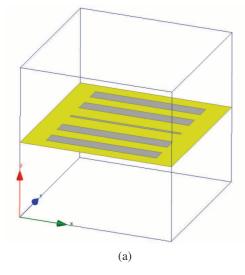


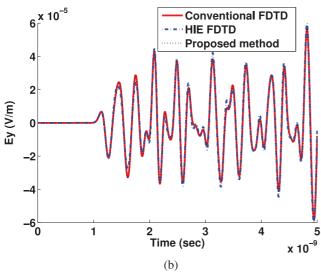
Fig. 5. Entire solution error for simulating a 3-D on-chip bus structure.

s solely determined by accuracy, whereas the time step used by the conventional FDTD is 1.176×10^{-13} s. The number of V_h modes removed is 288. In Fig. 3(a), we plot the electric fields at two points, P1 = (3.5, 7.1, 0.70588) mm, and P2 = (9.7, 7.1, 0.70588) mm, respectively, in comparison with the FDTD solutions. Excellent agreement can be observed. The total simulation time of the proposed method is 5.74 s including the time for finding V_h , and that for performing (11)–(12), in contrast to the 27.37 s cost by FDTD. The average entire solution error is found to be less than 3%. We have also simulated this example using the ADI and the HIE method [24] using the time step of 9.8039×10^{-13} s. In Fig. 3(b), we compare the voltages at point P1 simulated by the three methods, which further verifies the accuracy of the proposed method. The proposed method flexibly adapts the eigensystem based on the required time step. For example, if the required time step is 3.0712×10^{-13} s instead of 9.8039×10^{-13} s, the eigenvalues are accordingly removed from the largest down to 4.2907×10^{25} . The results are equally accurate as can be seen from Fig. 3(a). The CPU time for this case is 19.03 s.

D. Open-Region Radiation

Next, we simulate an open-region problem with a dipole antenna radiating in presence of multiple dielectric cylinders, as illustrated in Fig. 4(a). The solution domain is 15.7 mm by 10.3 mm, surrounded by a 10-layer PML region. The maximum space step size is 1.428×10^{-4} m. The smallest space step is 7.1429×10^{-6} m. There are three cylinders situated on the left side of the solution domain and a current source along z-direction located on the upper right corner. The pulse of the current source is a Gaussian derivative with a maximum input frequency of 1.05×10^{11} Hz. The cylinders have relative permittivity $\epsilon_r = 2$. The time step required by stability is $1.6836 \times$ 10^{-14} s, whereas the time step used by the proposed method is 3.3672×10^{-13} s. The proposed method takes 1.2493×10^3 s to finish the entire simulation, while the FDTD costs 1.9873×10^4 s. The electric field at the observation point shown in Fig. 4(a) is plotted and compared with that of traditional explicit FDTD in Fig. 4(b). The entire solution error is shown in Fig. 4(c). Excellent accuracy is observed.





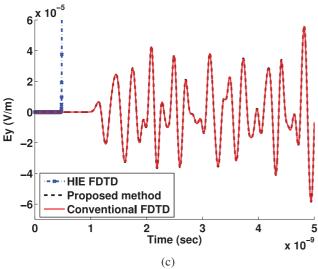


Fig. 6. Simulation of an EMI problem. (a) Illustration of the structure. (b) Electric field at the observation point using a time step of 0.166 ps. (c) Electric field at the observation point using a time step of 1.66 ps.

E. On-Chip 3-D Bus

Next, an on-chip 3D bus structure embedded in an inhomogeneous stack of dielectrics is simulated. The proposed method is

able to use the time step required by accuracy, 2.9412×10^{-12} s, to obtain accurate results. In contrast, the conventional FDTD must use a time step of 9.9355×10^{-16} s to ensure stability. The total CPU time of the proposed method is 7.12 s, whereas that of the conventional FDTD is 7 426 s. The speedup of the new method over the FDTD is approximately 1 043. The number of removed eigenmodes is 536 in this example. The entire solution error is plotted in Fig. 5 as a function of time, revealing good accuracy of the proposed method. The speedup of the method in [18] over the traditional FDTD is 47. Hence, the proposed method is more efficient in simulating this example.

F. Electromagnetic Interference (EMI) Example

In the last example, we simulate an EMI example as illustrated in Fig. 6(a), and compare the performance of the proposed method with the method of [24]. The structure is a cube of side length 11 cm truncated by perfect electric (PEC) boundary conditions all around. In the center, there is a PEC sheet with five slots. The thid slot has a width of 0.25 mm, and others are of width 1 cm. Then we set the total \mathbf{E}_y at the center point of the lower-half domain to be $\exp(-\alpha^2(t-t_0)^2)$ with $\alpha =$ 1.26×10^{10} s, and $t_0 = 1e - 9$ s. The third slot is discretized along y into 5 uniform cells. The cell size is 1 cm along x-, and z-direction, respectively, and 0.02 cm along y in the areas other than the third slot. We compare the results obtained from the conventional FDTD, the proposed method, and the HIE in [24], for a time step of 0.166 ps which is the time step of the conventional FDTD, and the time step of 1.66 ps, respectively. The \mathbf{E}_{y} obtained for the two choices of the time step at the center point of the upper domain are plotted in Fig. 6(b), and (c), respectively. The HIE is shown to be unstable for the time step of 1.66 ps, whereas the proposed method still generates stable and accurate results.

VII. CONCLUSION

In this paper, an alternative method is developed to achieve unconditional stability in an explicit FDTD simulation. It retains the strength of FDTD in avoiding matrix solutions, while eliminating its shortcoming in time step. The unstable modes are directly deducted from the original FDTD numerical system to eradicate the root cause of instability. Since the unstable modes have the largest eigenvalues and the FDTD system matrix is sparse, the unstable modes can be efficiently and reliably found in $O(k^2N)$ complexity, where k is the number of unstable modes. The proposed method only requires a very minor modification on the traditional FDTD to make it unconditionally stable. Its implementation is hence convenient. Numerical experiments and comparisons with existing explicit FDTD methods have demonstrated the superior performance of the proposed method in stability, accuracy, and efficiency. The essential idea of the proposed method can also be applied to other time domain methods. The proposed method complements the capability offered by the original explicit and unconditionally stable FDTD [18]. Recently, this work has also been extended for analyzing general lossy problems in [25].

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