Model Order Reduction and Stability Enforcement of Finite-Difference Time-Domain Equations Beyond the CFL Limit

by

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Abstract

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The Finite-Difference Time Domain (FDTD) method is a versatile and popular method for solving Maxwell’s equations. As a consequence of the explicit time integration, the maximum stable time-step of FDTD is constrained by the Courant-Friedrichs-Lewy (CFL) limit. This thesis focuses on two interdependent topics: model order reduction (MOR) of explicit FDTD equations and stability enforcement above the CFL limit. The combination of these two topics leads to the proposed CFL extension technique which has been demonstrated for 2D and 3D simulations. In addition, the proposed method has also been applied to the FDTD sub-gridding application. Comparisons have been made with existing implicit and explicit CFL extension techniques with respect to versatility, computational efficiency, and numerical dispersion errors. While there exist computation and memory limitations, the proposed method has demonstrated excellent versatility and accuracy for all test cases while having significant speed-ups over standard FDTD.
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Chapter 1

Introduction

1.1 Motivation

The Finite-Difference Time-Domain (FDTD) method is a versatile and efficient technique for solving Maxwell’s equations [2]. FDTD, along with the Finite-Element Method (FEM) [3] and the Method of Moments (MoM) [4], is one of the most widely used simulation techniques in commercial electromagnetic simulators. Conventional FDTD utilizes centred finite difference approximations of temporal and spatial derivatives, leading to a finite spatial resolution. The basic FDTD technique utilizes uniform orthogonal meshing, leading to rectangular cells in space. The main distinction of the FDTD method is the use of explicit time integration and the staggered leap-frog update of electric and magnetic field nodes. A key advantage of standard FDTD is that the simulation domain may be directly discretized and updated without matrix formulations due to the simplicity of the FDTD update equations. The implicit FEM and MoM methods instead require the formulation and solution of large linear systems containing all discretized nodes. While computationally efficient, the explicit characteristic of FDTD results in a number of constraints and practical limitations.

One of the main constraints of explicit FDTD is the Courant-Friedrichs-Lewy (CFL) stability condition [2]. The CFL condition is a numerical stability limit general to explicit time integration schemes and is given in 1D as

\[ \Delta t \leq \frac{\Delta x}{c} \]

where \( \Delta t \) is the maximum stable time-step, \( \Delta x \) the smallest spatial cell size, and \( c \) the maximum speed of light in the medium. The exact terms and derivations of the CFL limit will be covered in Chapter 2. The main premise of the CFL limit is that the maximum stable time-step decreases as the spatial
cell size decreases. This implies that an increase in spatial resolution will result in a decrease of the allowable time-step.

The CFL limit is particularly limiting in simulations requiring fine spatial resolutions relative to the minimum wavelength of interest. Examples of such simulations include cell phone patch antennas and on-chip interconnects. The FDTD spatial discretization imposes two practical limitations: spatial resolution and numerical dispersion [5]. Due to the finite spatial resolution of the orthogonal spatial mesh, approximation errors will always be introduced when modelling smooth continuous surfaces. Minimizing the spatial approximation error has been a main area of research ever since the introduction of the original FDTD algorithm. A large number of techniques have been proposed [6, 7, 8], with some achieving commercial usage.

For a given frequency of interest, the well known Nyquist criterion dictates a minimum requirement of two points per wavelength in space. This is a necessary but not sufficient condition in the case of standard FDTD simulations. A simulation using this minimum required spatial discretization size will result in an unacceptable level of numerical dispersion errors, rendering the output results completely inaccurate. For all practical implementations, FDTD simulations must be significantly oversampled beyond the Nyquist criterion, leading to a finer mesh then necessary to accurately capture the interested frequency information.

Numerical dispersion is an undesirable non-linear error introduced through the finite-difference approximation. Numerical dispersion changes the phase velocity of propagation of a sinusoidal wave and is a function of the effective wave velocity and spatial discretization size. Decreasing the spatial discretization size results in three issues: increased memory usage, increased computations per time-step, and decreased maximum time-step. The last issue is a direct consequence of the CFL limit. The ultimate goal of this thesis is to make FDTD less sensitive to the three issues discuss above. We will achieve this aim through two concepts:

- overcoming the CFL limit: by extending the stability limit of FDTD, we will be able to use larger time steps while maintaining late time stability. This first contribution will reduce the performance decay that FDTD experiences in presence of fine geometrical details, and will provide a first source of speed-up.

- model order reduction: with model order reduction, we will further improve the efficiency of FDTD for fine grids and complicated structures, reducing its computational cost per time-step.
1.1.1 Overcoming the CFL Limit: State of the Art

Due to the previously described limitations imposed by the CFL limit, overcoming or removing of the CFL limit has been an active research topic for the past two decades. While an extensive amount of research and techniques have been made in academia, no commercial simulation software currently utilizes these techniques. As we will cover in this thesis, this aversion may be attributed to the increased computational cost and decreased overall accuracy associate with existing CFL extension methods. The general CFL extension techniques may be divided into two categories: implicit methods [9, 10, 1, 11, 12], and explicit methods [13, 14, 15, 16]. Implicit CFL extension methods utilize implicit time integration, leading to unconditional stability at any time-step. Although in principle still a “finite-difference” and “time-domain” method, the implicit methods differ dramatically from the original explicit FDTD technique in both theory and implementation. Similar to the implicit MOM and FEM methods, implicit FDTD methods require the solution of a large linear system at each update. The unconditional stability of implicit methods come at the cost of dramatically increased computational costs and uniformly decreased accuracy over standard FDTD as a function of the CFL used [17].

The most straightforward implicit technique is the direct solution of Maxwell’s equations using implicit time integration [1]. This implementation requires the solution of a large set of linear equations at each time-step and is prohibitively expensive even for modest simulation sizes. More recent developments such as the Alternating-Direction Implicit FDTD (ADI-FDTD) [11] and the Locally 1-D Finite-Difference Time-Domain (LOD-FDTD) [12] methods attempt to improve the efficiency of the linear system solution process. Both ADI-FDTD and LOD-FDTD involve the splitting of the single time-step update equations into implicit and explicit half steps, leading to the inversion of a tridiagonal matrix at each time-step and significantly decreasing computational requirements. As a consequence of the matrix inversion requirements, the direct use of implicit techniques in large scale problems may be problematic. Implicit CFL extension methods trade a dramatic increase in per time-step computation cost for the use of an arbitrarily large time-step. In addition to computational tradeoffs, additional numerical dispersion errors are introduced when above the CFL limit [17].

Explicit CFL extension aims to remove unstable spatial harmonics from the standard FDTD simulations at unstable CFL ratios. Explicit CFL extension methods are often referred to as enforceably stable methods, where the stability of the simulation is enforced through some additional algorithm. Explicit CFL extension is based upon the assumption that stable and unstable harmonics of a FDTD simulation may be identified and separated. The foundation of explicit methods are that relevant simulation information can be maintained and extracted even when the overall simulation is run at an unstable
CFL ratio. In the Spatial Filtering technique [13], the exact frequencies of the unstable harmonics are identified and removed using a frequency domain transformation and low-pass filtering. The authors of Spatial Filtering made an interesting observation regarding CFL stability: as the CFL limit is exceeded, the high frequency wavenumbers become imaginary, thus resulting in overall instability. The frequency cut-off for stability may be derived from the numerical dispersion equations. As long as the cutoff frequency is above the frequency of interest, removing unstable harmonics will have negligible impact on the accuracy of the simulation. This property will always hold for standard FDTD simulations due to the oversampling in space. Similar to the implicit case, additional numerical dispersion errors are introduced above the CFL limit. Implicit and explicit CFL extension methods exhibit different numerical dispersion characteristics at unstable CFL ratios. In addition, the frequency domain filtering introduces additional aliasing errors across discontinuous material boundaries, thus requiring special care in the implementation.

Using the same principles derived in [13], a different approach was proposed in [14] to make an explicit FDTD algorithm stable beyond the CFL limit. Rather than removing unstable harmonics at runtime through a low-pass filter, the FDTD equations can be perturbed to guarantee stability by construction. FDTD update equations can be seen as a dynamical system which, above the CFL limit, has some unstable eigenvalues (poles). By perturbing or removing these eigenvalues, one can eliminate the root cause of instability directly on the equations rather than at runtime. In theory this is an intuitive and simple process, consisting of eigenvalue decomposition and perturbation. In practice the computational cost of eigenvalue decomposition renders the process prohibitive for any practical simulation. To overcome this, a model order reduction step is first used in both cases [14, 18] to generate a set of reduced FDTD update equations to facilitate the application of eigenvalue decomposition. The unstable high frequency eigenvalues may then be directly removed. The MOR technique used is a time sampling algorithm, where a short simulation is ran at a stable CFL ratio to extract a set of dominant eigenvalues and eigenvectors. Unstable eigenvalues can then be discarded. Stable eigenvectors are instead used to form a projection matrix and obtain, from the large and unstable FDTD equations, a compact reduced model which will be stable by construction. The methods presented in [14, 18] have two main downsides. The first is the efficiency of the MOR technique in generating an accurate reduced model. For resonating structure with high Q factors, the initial time sampling algorithm must be run for a significant fraction of the full simulation. This may raise questions as to why the CFL extension and subsequent CFL extended simulation run is even required. In addition, the time sampling algorithm has problems identifying damped eigenvalues due to their attenuation. As a result of these limitations, the simulation test cases presented in [14, 18] have mainly focused on simply time domain propagation cases.
Chapter 1. Introduction

with little resonance or loss. The second limitation is the derivation of the stability criteria. In [14, 18] it is found that the introduction of conductivities has a negative impact on the derived stability limit. This is counter intuitive to the conclusion of the standard FDTD technique, since it is well established that the CFL limit in standard FDTD does not depend on conductivities [5, 19].

1.1.2 Application of CFL Extension Techniques: Sub-gridding

One of the most popular methods of compensating for the spatial approximation and numerical dispersion error is through the use of non-uniform meshing techniques. These include the non-uniform FDTD method, conformal FDTD method [6], and the FDTD sub-gridding method [7]. It is known that conformal FDTD meshing is used in commercial FDTD simulation tools such as CST and XFDTD, while FDTD sub-gridding has been experimented with by both software vendors. Such methods utilize an overall coarse mesh with local fine cell sizes to increase the spatial resolution where necessary. Such methods result in significant reductions in the overall memory requirements compared to a uniform rectangular mesh with similar resolutions. A major downside is that the maximum time-step is constrained by the minimum cell size of the simulation domain. While it is possible to run different simulation domains at different time-steps, this is difficult to implement and introduces additional time interpolation errors.

Since the time-step of the FDTD sub-gridding techniques is restricted by the CFL limit of the fine cell domains, the application of the CFL extension method to the fine domain will have significant computational advantages. Through overcoming the CFL limit of the fine mesh domains, the simulation may be run at the larger time-step of the coarse mesh. The local application of CFL extension methods also alleviates the increased computational costs of such methods. The stability of the basic FDTD sub-gridding method is a developed field with analytical proofs of overall stability [8]. However, the application of CFL extension techniques to the FDTD sub-gridding problem has so far been only moderately successful. Implicit CFL extension methods have been applied to the sub-gridding application in multiple instances [9, 10, 20]. However, the full CFL time-step of the coarse mesh cannot be used without introducing instability. This implies that the connection of stable implicit and stable explicit simulation domains is not a sufficient condition for the stability of the overall simulation. The explicit spatial filtering technique has been applied to the FDTD sub-gridding method with more success [21]. Test cases have demonstrated late time stability at the full CFL limit of the coarse mesh for homogeneous problems. No analytical derivation of overall stability has been made for both implicit and explicit CFL extension sub-gridding.
1.2 Objectives

The main objective of this thesis is the development of a CFL extension technique for the Finite-Difference Time-Domain method using a combination of model order reduction and stability enforcement. The main objective may be divided into three main parts:

1. The development of an efficient and accurate MOR technique for the FDTD equations that is fully applicable to practical FDTD simulations. This will reduce the memory and computational requirements of the FDTD simulation, as well as facilitate the application of eigenvalue and singular value decomposition for stability enforcement.

2. The development of a stability enforcement technique for the FDTD method at unstable CFL values. Breaking the CFL barrier represents one of the main focuses of past and present research on the FDTD method. It allows the acceleration of the standard FDTD techniques through faster time marching.

3. The application of the developed MOR and stability enforcement techniques to the FDTD sub-gridding technique. The FDTD sub-gridding technique represents an ideal application of both the MOR and stability enforcement techniques. The MOR technique will reduce the memory and computational requirements of dense local meshes, while the CFL extension process will ensure overall stability with the use of a coarse mesh time-step.

1.3 Outline

This thesis will cover three main topics: extension of the CFL limit via eigenvalue perturbation, model order reduction of FDTD equations, and the application of both techniques to FDTD sub-gridding. The proposed method of CFL extension is performed through first reducing the FDTD update system to a manageable size, followed by the application of system level CFL extension.

This thesis will first derive the CFL conditions for the conventional FDTD method using the discrete-time system stability criteria. As performed in [15] and [5], the leap-frog updates of electric and magnetic field nodes may be written in the form of a discrete-time linear system. The discrete stability criteria of this update system is equivalent to the CFL condition. Using eigenvalue perturbation, the stability of the discrete system can be enforced at a time-step beyond the CFL limit. This stability enforcement is equivalent to the low-pass filtering process of spatial filtering. In [19, 16], a more refined formulation and stability criteria is utilized that maintains the leap-frog structure of FDTD. A direct
relationship between the CFL limit, wave velocity, and spatial difference approximation is made. Using this relationship, it is sufficient to only filter the spatial difference terms to allow a time-step beyond the CFL limit, a theoretically intuitive result. An evaluation of the numerical dispersion characteristics has been made for the proposed and existing CFL extension techniques.

The stability enforcement process will be followed by the introduction of the model order reduction (MOR) process. Although sequentially performed before stability enforcement, the MOR step serves a supporting role by reducing the total system size, facilitating the use of eigenvalue decomposition. The introduced system formulation [16] is fully compatible with existing Krylov projection based MOR techniques [22, 23]. When below the CFL limit, the MOR step preserves the stability of the FDTD equations. A number of test cases have demonstrated the proposed method’s accuracy, computational efficiency, and scalability to 3D problems. In addition, the proposed technique has also been extended to the sub-gridding with CFL extension combination. Through the connection of multiple systems with different cell sizes, a set of stability criteria for the non-uniform sub-gridding mesh scheme has been derived. It will be shown that the stability of the sub-gridding scheme is more restrictive than that of a stand alone simulation. This developments offers analytically stable sub-gridding at the coarse mesh CFL limit, a vital development not seen in previous publications.

Chapter 2 reformulates the standard FDTD equations into a single discrete update system. Limitations of the FDTD method such as the CFL limit and numerical dispersion error are introduced.

Chapter 3 covers the overcoming of the CFL limit for the FDTD update equations. The eigenvalues of the discrete update system of Chapter 2 are perturbed such that the FDTD simulation can be ran at any time-step. This chapter covers the derivation, verification, and discussion of accuracy tradeoffs associated with the stability enforcement as well as comparisons to existing CFL extension techniques.

Chapter 4 introduces the model order reduction of FDTD equations which serve to overcome the computation bottlenecks of the stability enforcement step. A revised formulation of the FDTD update equations is used to allow the use of existing model order reduction techniques. The MOR technique used is the Krylov subspace projection method which has been optimized for the discrete-time FDTD system. The revised formulation not only leads to stability preservation through the reduction process, but also provides a more intuitive stability criteria and enforcement process.

Chapter 5 verifies the proposed method of Chapter 4 for a number of 2D and 3D test cases including waveguide, focusing PEC structures, and microstrip filters.

Chapter 6 applies the proposed method to the FDTD sub-gridding scheme. An extended system formulation is introduced to facilitate the generation and connection of multiple FDTD meshes. To satisfy overall stability, a more constrained set of stability conditions has been derived and enforced.
Verification and comparisons have been made between the proposed method and existing FDTD sub-gridding techniques for 2D PEC cavity and 2D waveguide test cases.

Chapter 7 concludes this thesis and summarizes the main developments of this work. A short discussion is included with respect to potential future research topics and open problems.
Chapter 2

The FDTD Method in Discrete System Form

One of the key characteristics of FDTD is the ability to avoid the construction of large matrices. Fields at the grid nodes are directly stored and updated in memory using simple equations. This characteristic may be viewed as an implementation optimization taking advantage of the simplicity of the explicit FDTD update equations, a result of the second-order temporal and spatial finite difference approximations. While useful from an implementation point of view, key characteristics of the FDTD system become accessible only when all update equations are cast in update system form. Not surprisingly, all theoretical works regarding the FDTD technique have universally utilized the discrete-time linear system form of FDTD equations [5, 7, 8, 9, 19]. This chapter will introduce the basic FDTD method along with the discrete-time system formulation. Basic characteristics and limitations of the FDTD method will be introduced, including the CFL limit and numerical dispersion. This chapter will provide the background and notations used for the rest of this thesis.

2.1 The Standard FDTD Technique in Matrix Form

In FDTD, Maxwell’s equations in differential form

\[
\begin{align*}
\mu \frac{\partial H}{\partial t} &= -\nabla \times E - M \\
\epsilon \frac{\partial E}{\partial t} &= \nabla \times H - J
\end{align*}
\]  

(2.1a) (2.1b)
are discretized through the application of centred finite difference approximations with second order accuracy. The electric and magnetic field nodes are staggered in both time and space. The application of the temporal difference approximation is equivalent to an explicit forward-Euler time integration scheme. The explicit nature of the update equations is the main foundation for the relative computational efficiency of FDTD. Applying substitution and rearranging, we arrive at the standard leap-frog FDTD equations for lossy inhomogeneous media, which for the 1D case read

\[
\begin{align}
\left( \frac{\varepsilon}{\Delta t} + \frac{\sigma_e}{2} \right) E_{k}^{n+1} &= \left( \frac{\varepsilon}{\Delta t} - \frac{\sigma_e}{2} \right) E_{k}^{n} - \frac{1}{\Delta x} \left( H_{k+\frac{1}{2}}^{n+\frac{1}{2}} - H_{k-\frac{1}{2}}^{n+\frac{1}{2}} \right) - J_{k}^{n+\frac{1}{2}} \\
\left( \frac{\mu}{\Delta t} + \frac{\sigma_m}{2} \right) H_{k+\frac{1}{2}}^{n+\frac{3}{2}} &= \left( \frac{\mu}{\Delta t} - \frac{\sigma_m}{2} \right) H_{k+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{1}{\Delta x} \left( E_{k+1}^{n+1} - E_{k}^{n+1} \right) - M_{k+\frac{1}{2}}^{n+1}.
\end{align}
\]

where \( E_{k}^{n} \) and \( H_{k+\frac{1}{2}}^{n+\frac{1}{2}} \) represent the discrete electric and magnetic field nodes, while \( n \) and \( k \) are the temporal and spatial indices. The variables \( \Delta t \) and \( \Delta x \) represent the temporal and spatial discretization sizes. The variables \( \varepsilon, \mu, \sigma_e \) and \( \sigma_m \) represent permittivity, permeability, electric conductivity, and magnetic conductivity values, respectively. Terms \( J_{k}^{n+\frac{1}{2}} \) and \( M_{k+\frac{1}{2}}^{n+1} \) represent electric and magnetic sources.

2.1.1 FDTD equations as a Discrete-Time System

In casting the FDTD equations into matrix form, it is first necessary to identify five matrices that will make up the full update system

- **\( D_{\varepsilon} \)** and **\( D_{\mu} \)** are diagonal matrices containing the electric permittivity and magnetic permeability values at each cell (\( \varepsilon_r, \mu_r \)),

- **\( D_{\sigma_e} \)** and **\( D_{\sigma_m} \)** are diagonal matrices containing the electric and magnetic conductivity values at each cell (\( \sigma_e, \sigma_m \)),

- **\( K \)** contains the finite difference approximation of the spatial curl operator of Maxwell’s equations, and contains terms in the form (\( \pm 1/\Delta x, \pm 1/\Delta y, \pm 1/\Delta z \)).
Table 2.1: Discrete-time FDTD system matrix size and properties.

<table>
<thead>
<tr>
<th>Matrix Symbol</th>
<th>Size</th>
<th>Elements</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_e )</td>
<td>( N_e \times N_e )</td>
<td>( \epsilon_r )</td>
<td>Diagonal</td>
</tr>
<tr>
<td>( D_\mu )</td>
<td>( N_m \times N_m )</td>
<td>( \mu_r )</td>
<td>Diagonal</td>
</tr>
<tr>
<td>( D_{\sigma_e} )</td>
<td>( N_e \times N_e )</td>
<td>( \sigma_e )</td>
<td>Diagonal</td>
</tr>
<tr>
<td>( D_{\sigma_m} )</td>
<td>( N_m \times N_m )</td>
<td>( \sigma_m )</td>
<td>Diagonal</td>
</tr>
<tr>
<td>( K )</td>
<td>( N_e \times N_m )</td>
<td>( \pm 1/\Delta x, \pm 1/\Delta y, \pm 1/\Delta z )</td>
<td>-</td>
</tr>
</tbody>
</table>

Using these matrix definitions, the spatial index \( k \) may be removed and the standard FDTD equations may be rewritten as

\[
\frac{D_e}{\Delta t} + \frac{D_{\sigma_e}}{2} \begin{pmatrix} E^{n+1} \\ H^{n+\frac{3}{2}} \end{pmatrix} = \begin{pmatrix} \frac{D_e}{\Delta t} - \frac{D_{\sigma_e}}{2} \end{pmatrix} \begin{pmatrix} E^n \\ H^{n+\frac{1}{2}} \end{pmatrix} - KH^{n+\frac{1}{2}} - J^{n+\frac{1}{2}} \tag{2.3a}
\]

\[
\frac{D_\mu}{\Delta t} + \frac{D_{\sigma_m}}{2} \begin{pmatrix} M^{n+1} \\ H^{n+\frac{3}{2}} \end{pmatrix} = \begin{pmatrix} \frac{D_\mu}{\Delta t} - \frac{D_{\sigma_m}}{2} \end{pmatrix} \begin{pmatrix} M^n \\ H^{n+\frac{1}{2}} \end{pmatrix} + K^T E^{n+1} - M^{n+1}. \tag{2.3b}
\]

The \( E^n \) and \( H^{n+\frac{1}{2}} \) matrices are state space vectors containing all electric and magnetic field nodes. From this point on we will denote the size of the full \( E^n \) and \( H^{n+\frac{1}{2}} \) state space vectors as \( N_e \) and \( N_h \).

The presence of \( K \) and \( K^T \) in the two equations shows the reciprocity between the electric and magnetic field update equations. Boundary conditions imposed at the limits of the simulation domain can also be incorporated in this matrix form. In the case of PEC nodes, the associated rows of the \( K \) matrix are left zero. The left hand side matrices of (2.3) are the summation of diagonal matrices and may be eliminated through multiplying both sides with their inverse. A short summary of the size and properties of the five system matrices in (2.3a) and (2.3b) are given in Table 2.1. In order to write (2.3a) and (2.3b) in the form of a state space system, we substitute the \( E^{n+1} \) term of (2.3a) into (2.3b), obtaining

\[
\begin{bmatrix}
E^{n+1} \\
H^{n+\frac{3}{2}} \\
x^{n+\frac{3}{4}}
\end{bmatrix} =
\begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22} + M_{21}M_{12}
\end{bmatrix}
\begin{bmatrix}
E^n \\
H^{n+\frac{1}{2}} \\
x^n
\end{bmatrix}
+ \begin{bmatrix}
M_{12} \\
M_{22}
\end{bmatrix} Bu^{n+1}
\]

\[
y^{n+1} = L^T \begin{bmatrix} E^{n+1} \\ H^{n+\frac{1}{2}} \end{bmatrix}.
\]

where

\[
M_{11} = \left( \frac{D_e}{\Delta t} + \frac{D_{\sigma_e}}{2} \right)^{-1} \left( \frac{D_e}{\Delta t} - \frac{D_{\sigma_e}}{2} \right) \quad M_{12} = -\left( \frac{D_e}{\Delta t} + \frac{D_{\sigma_e}}{2} \right)^{-1} K \quad M_{21} = \left( \frac{D_\mu}{\Delta t} + \frac{D_{\sigma_m}}{2} \right)^{-1} K^T \quad M_{22} = \left( \frac{D_\mu}{\Delta t} + \frac{D_{\sigma_m}}{2} \right)^{-1} \left( \frac{D_\mu}{\Delta t} - \frac{D_{\sigma_m}}{2} \right). \tag{2.5}
\]
The column vector

\[ \mathbf{x}^n = \begin{bmatrix} \mathbf{E}^n \\ \mathbf{H}^{n+\frac{1}{2}} \end{bmatrix}, \]  

(2.6)

is the discrete-time state space vector, while the \( \mathbf{M}_{11} \), \( \mathbf{M}_{12} \), \( \mathbf{M}_{21} \), and \( \mathbf{M}_{22} \) matrices make up the full discrete-time update matrix \( \mathbf{A} \). The size of matrix \( \mathbf{A} \) is \((N_e + N_m) \times (N_e + N_m)\). The \( \mathbf{B} \) matrix contains 1’s at the location of transparent electric and magnetic current sources, while the matrix \( \mathbf{u}^{|n+1} \) contains the scalar source values at each time-step. The \( \mathbf{L} \) matrix contains 1’s at the location of the probes, while \( \mathbf{y}^{|n+1} \) represents the probe outputs at each time-step. Due to the explicit formulation, all operations needed to compute \( \mathbf{A} \) require only the inversion of diagonal matrices, thus having negligible computation cost. In addition, the \( \mathbf{A} \), \( \mathbf{B} \), and \( \mathbf{L} \) matrices to be multiplied at each time step are also extremely sparse.

### 2.1.2 Discrete-time z-Domain Stability

In (2.4) the FDTD update equations have been cast into the form of a discrete-time update system. The discrete stability condition dictates that the system of (2.4) is stable if and only if all the eigenvalues \( \lambda_i \) of \( \mathbf{A} \) are on or within the unit circle on the complex plane

\[ |\lambda_i| \leq 1. \]  

(2.7)

It will be shown later that the discrete-time z-domain stability criteria (2.7) is equivalent to the CFL limit.

### 2.2 The Courant-Friedrichs-Lewy Condition

One of the major limitations of standard FDTD is the Courant-Friedrichs-Lewy (CFL) stability condition. The CFL limit is a numerical limit present in a wide range of explicit solution methods. The CFL limit for the 1D, 2D, and 3D standard FDTD are

\[ \Delta t \leq \frac{\Delta x}{c}, \]  

(2.8a)

\[ \Delta t \leq \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}, \]  

(2.8b)

\[ \Delta t \leq \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}, \]  

(2.8c)
where $c$ is the speed of light in the medium. The CFL limit is often written in the form of $\text{CFL} \leq 1$, where CFL is defined as

\begin{align}
\text{CFL} &= \frac{c \Delta t}{\Delta x} \quad (2.9a) \\
\text{CFL} &= c \Delta t \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}} \quad (2.9b) \\
\text{CFL} &= c \Delta t \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \quad (2.9c)
\end{align}

for the 1D, 2D, and 3D cases. A derivation of the CFL limit from discrete stability criteria of (2.7) has been performed in [5].

The second-order finite difference approximation restricts the update information to one cell per wavelength per axis. By multiplying both sides of (2.8) by $c$, the CFL limit becomes equivalent to a causality constraint. The relation $c \Delta t \leq \Delta x$ states that the maximum time-step must be less than the time taken for the propagating wave to traverse one spatiality discretization.

Since the wave velocity is proportional to $\frac{1}{\sqrt{\epsilon_r \mu_r}}$, the CFL limit may be relaxed in areas with increased permittivity, permeability, and spatial discretization size. The maximum stability limit may therefore vary across inhomogeneous FDTD domains. FDTD simulation tools use the most restrictive CFL limit across the entire simulation domain. In general, the CFL limit introduces additional computational complexity for simulations requiring small spatial discretization sizes.

### 2.3 Analytical Numerical Dispersion

Aside from the CFL limit, one of the major limitations of the FDTD method is the numerical dispersion error. Numerical dispersion is a computational phenomenon where the effective numerical wave velocity in free space $v_p$ is different from the speed of light $c$. Numerical dispersion is a non-linear function of both temporal and spatial discretization sizes and results in a shifting of the frequency spectrum harmonics of the extracted frequency results. The numerical dispersion errors stem from the finite spatial discretization, along with the second-order finite difference approximation. The use of higher order difference approximation has been shown to decrease the relative numerical dispersion error [24].
The numerical dispersion equations for 1D, 2D, and 3D FDTD are

\[
\sin^2 \omega \Delta t = (c \Delta t)^2 \left( \frac{\sin^2 \tilde{k}_x \Delta x}{\Delta x^2} \right), \tag{2.10a}
\]

\[
\sin^2 \omega \Delta t = (c \Delta t)^2 \left( \frac{\sin^2 \tilde{k}_x \Delta x}{\Delta x^2} + \frac{\sin^2 \tilde{k}_y \Delta y}{\Delta y^2} \right), \tag{2.10b}
\]

\[
\sin^2 \omega \Delta t = (c \Delta t)^2 \left( \frac{\sin^2 \tilde{k}_x \Delta x}{\Delta x^2} + \frac{\sin^2 \tilde{k}_y \Delta y}{\Delta y^2} + \frac{\sin^2 \tilde{k}_z \Delta z}{\Delta z^2} \right), \tag{2.10c}
\]

where \(c\) is the speed of light in free space, \(\Delta t\) is the time-step, and \(\Delta x, \Delta y, \Delta z\) are the spatial discretization sizes along each axis. The terms \(\tilde{k}_x, \tilde{k}_y, \tilde{k}_z\) are the numerical spatial wavenumbers along each axis while \(\omega\) is the temporal angular frequency. Equation (2.10) is a direct relationship between the temporal angular frequency and the numerical spatial wavenumbers within the simulation domain for a plane wave in free space. The spatial wavenumber \(k\) is the result of Fourier transformation with respect to space of the propagating plane wave. For analysis purposes we make a simplifying assumption that the effective spatial wavenumbers along each axis are equal. For 2D, this implies \(\tilde{k}_x = \tilde{k}_y = \frac{1}{\sqrt{2}} \tilde{k}_{max}\), while for the 3D case \(\tilde{k}_x = \tilde{k}_y = \tilde{k}_z = \frac{1}{\sqrt{3}} \tilde{k}_{max}\). In the ideal dispersion-less case, the relationship between \(w\) and \(\tilde{k}_{max}\) is

\[
\tilde{k}_{max} = \frac{w}{c}. \tag{2.11}
\]

It may be seen from Equation (2.10) that the dispersion-less case occurs as the spatial discretization sizes become infinitesimally small. Using this simplifying assumption, the approximate numerical dispersion error as a function of the phase velocity normalized by the speed of light (\(\frac{v_p}{c}\)) verses wavelength per spatial discretization (\(\frac{\lambda}{\Delta x}\)) has been plotted in Figure 2.1.
A number of useful observations may be drawn from the Figure 2.1 numerical dispersion curves with square cells $\Delta x = \Delta y = \Delta z = \Delta$. The accuracy of the FDTD simulation results are heavily dependent upon the spatial discretization size. Numerical dispersion errors accumulate as the number of time-steps increase. The spatiality cell size is chosen to keep the introduced numerical dispersion errors beneath a set limit for the total number of time-steps ran. A general minimum limit is $\frac{\lambda}{\Delta x} \geq 10$. Therefore, all FDTD simulations are oversampled in space to limit the numerical dispersion error to an acceptable limit. For any stable time-step, the effective wave velocity $v_p$ will be less than the theoretical speed of light. To minimize the numerical dispersion error, a CFL as close to 1 as possible should be used regardless of the spatial cell size. From Figure 2.1, the numerical dispersion errors decrease from 1D to 3D for the same $\Delta$. The numerical dispersion errors introduce numerical anisotropy in the case of 2D and 3D simulations. For a time-step greater than the CFL limit, the normalized numerical phase velocity $\frac{v_p}{c}$ of standard FDTD becomes greater than one while the actual angular velocity $\omega$ becomes complex. This signifies that in the case of explicit CFL extension, the effective numerical wave velocity $v_p$ will be greater than the theoretical speed of light.

2.4 Summary

This chapter introduces the standard FDTD formulation along with the CFL limit and numerical dispersion equations. The explicit FDTD equations can be formulated into a discrete update system comprised of five main sub-matrices. The discrete system stability limit is equivalent to the CFL limit. The CFL limit dictates that the maximum stable time-step is inversely proportional to the spatial cell size. The numerical dispersion equations dictate that the amount of introduced numerical dispersion error is directly proportional to the spatial cell size. Therefore, the CFL limit and the finite spatial resolution represent numerical constraints that must be fulfilled for any FDTD simulation. The FDTD cell size must be set to minimize spatial resolution and numerical dispersion errors. As a consequence, the CFL limit decreases the maximum stable time-step $\Delta t$ to introduce additional computation costs on top of the costs incurred by the larger mesh size. This chapter provides a discrete-time system formulation of FDTD equations. The stability criteria of the discrete-time system is equivalent to the CFL limit, which may be overcome through eigenvalue perturbation. Chapter 3 will introduce the basis of the CFL extension techniques, which serves to overcome the CFL limitations at the cost of some numerical dispersion error.
Chapter 3

Overcoming the CFL Limit of the FDTD Method

This chapter will cover the derivation and extension of the CFL limit for the discrete-time FDTD update system presented in Chapter 2. The derivations will outline the theoretical foundations and limitations of explicit CFL extension with respect to propagating wavenumbers, eigenvalues, and the CFL limit. Existing implicit and explicit CFL extension techniques will be briefly covered. Special emphasis will be given in connecting the proposed method with existing explicit CFL extension techniques. The theory and accuracy of the eigenvalue perturbation technique is demonstrated using a 2D PEC cavity example. The accuracy of the eigenvalue perturbation based CFL extension has been benchmarked against both implicit and explicit CFL extension methods. The contents of this chapter were presented in [15] and represent the first approach taken in the initial stages of the research process.

3.1 Extension of the CFL limit

This section will introduce the procedures for overcoming the CFL limit through eigenvalue perturbation. In order to establish a background on the topic of CFL extension methods, a short overview of existing implicit and explicit techniques will be given. The proposed CFL extension using eigenvalue perturbation may be viewed as a continuation of previous explicit CFL extension methods. The described CFL extension techniques have been implemented as benchmarks for comparison with the proposed eigenvalue perturbation technique.
3.1.1 Existing Implicit CFL Extension Methods

Implicit methods for solving Maxwell’s equations utilize implicit time integration methods to achieve unconditional stability at any time-step. This comes at the expense of significantly increased computational complexity. The standard FDTD method utilizes explicit finite difference approximations of temporal and spatial derivatives, which results in the CFL limit. Contrary to the explicit FDTD case, implicit formulations allow for the update of all nodes within the simulation space at each time-step, thus removing any causality constraints. The most straightforward implicit formulation is the replacement of the explicit time integration with an implicit one while maintaining the spatial discretization arrangement. This formulation was first applied to the FDTD system in 1999 in [1] and applied to FDTD sub-gridding in [9]. Through applying only the finite difference approximation to the curl operator of Maxwell’s equation of (2.1), we obtain a system in the form

\[
\begin{bmatrix}
D_e & 0 \\
0 & D_\mu
\end{bmatrix}
\begin{bmatrix}
\frac{dE(t)}{dt} \\
\frac{dH(t)}{dt}
\end{bmatrix}
= -\begin{bmatrix}
D_{\sigma_e} & -K \\
K^T & D_{\sigma_m}
\end{bmatrix}
\begin{bmatrix}
E(t) \\
H(t)
\end{bmatrix}
\] (3.1)

where the $D_e$, $D_\mu$, $D_{\sigma_e}$, $D_{\sigma_m}$, $K$ matrices are the previously outlined system matrices of Section 2.1.1. Since Maxwell’s equations are hyperbolic in nature, (3.1) cannot be directly solved using a single forward-Euler time integration. The standard FDTD formulation overcomes this limitation through the temporal staggering of the electric and magnetic field update equations. Applying leap-frog explicit time integration to (3.1) will result in the standard FDTD equations. Alternatively, the trapezoidal rule integration method may be applied, resulting in a set of implicit FDTD equations that are stable for any time step. Casting the implicit system into the same form as the update system of (2.4), we arrive at the following discrete system first described in [1]

\[
\begin{bmatrix}
E|^{n+\frac{1}{2}} \\
H|^{n+\frac{1}{2}}
\end{bmatrix}
= \begin{bmatrix}
\frac{D_e}{\Delta T} + \frac{D_{\sigma_e}}{2} & \frac{K}{2} \\
-\frac{K^T}{2} & \frac{D_\mu}{\Delta T} + \frac{D_{\sigma_m}}{2}
\end{bmatrix}^{-1}
\begin{bmatrix}
\frac{D_e}{\Delta T} - \frac{D_{\sigma_e}}{2} & -\frac{K}{2} \\
\frac{K^T}{2} & \frac{D_\mu}{\Delta T} - \frac{D_{\sigma_m}}{2}
\end{bmatrix}
\begin{bmatrix}
E|^{n-\frac{1}{2}} \\
H|^{n-\frac{1}{2}}
\end{bmatrix}
\] (3.2)

where $A_I$ is the square update matrix generated using the trapezoidal rule method. Finding $A_I$ in (3.2) requires the inversion of a large $2 \times 2$ block matrix which may be prohibitive in practice. Due to the implicit time integration, the time staggering of electric and magnetic fields is no longer needed. The primary difference between the explicit and implicit discrete update system of (2.4) and (3.2) is the sparsity and complexity of applying the update matrix $A$ at each time-step. The difference between the
sparsity of the update matrix $A$ between the explicit and implicit cases may be seen in Figure 3.1. The change in sparsity changes the number of operations required at each time-step from $O(N)$ to $O(N^2)$, where $N$ is the size of the square $A$ and $A_I$ matrices.

The sparsity of the explicit $A$ matrix demonstrates the computational advantages of standard FDTD, but also leads to the CFL limitation. A physical explanation of the CFL limit is the causality condition for a travelling plane wave. At each time-step for standard FDTD, each simulation node is updated as a function of its immediate neighbours. This results in an efficient update scheme, but also limits the wave propagation to one spatial cell per time-step, hence leading to the CFL limit. At each time-step for the implicit case, the $A_I$ matrix couples the updates of each discrete node with all other nodes. Hence, a travelling plane wave may traverse any number of cells per time-step. Since the propagating wave is no longer restricted to a set distance per time-step, the causality condition and equivalent CFL constraint no longer apply.

An advancement of the direct implicit FDTD method is the Alternating-Direction-Implicit FDTD (ADI-FDTD) method [11, 25]. The 3D ADI-FDTD method was first proposed in 1999 by multiple groups in parallel and has generated significantly more interest from the research community. The main characteristic of the ADI-FDTD method is the splitting of the standard time-step into two half-steps. By performing alternating explicit and implicit half step updates at each time-step, the update system maintains unconditional stability. In addition, the matrix inversion required at each implicit half-step is reduced to the inversion of a tridiagonal matrix, significantly improving computational efficiency. Due to the length of the ADI-FDTD description, we would like to refer to the implementation details given in [11] and [25] for the 2D and 3D ADI-FDTD implementation. Over the past decade hundreds of publications have been made for the analysis and application of the ADI-FDTD method [17, 26], although these...
Chapter 3. Overcoming the CFL Limit of the FDTD Method

will not be covered within the scope of this thesis. The more recent Locally One-Dimensional FDTD (LOD-FDTD) method [12] may be viewed as a variation of the standard ADI-FDTD form utilizing the same time splitting procedure. The implementation used within the scope of this thesis is from the original 1999 publication for the basic 2D ADI-FDTD method [11].

3.1.2 Existing Explicit CFL Extension Methods

Explicit CFL extension techniques work on the principle of enforcing the stability of the FDTD simulation above the CFL limit. One of the first techniques for achieving this for FDTD simulations was spatial filtering [13], which was first proposed in 2011. In spatial filtering, the CFL conditions of (2.8) are revisited in the context of the FDTD dispersion relations of (2.10) and the effective propagating wavenumber \( \tilde{k}_{\text{max}} \). In the case of a \( \Delta t \) beyond the CFL limit, the actual angular frequency \( \omega \) of the dispersion equation becomes complex. It may be observed that as the CFL is exceeded, certain high frequency spatial harmonics of the simulation domain become unstable. By forcing \( \omega \) to remain real and assuming \( \Delta x = \Delta y = \Delta z = \Delta \), the CFL conditions for 1D, 2D, and 3D FDTD simulations may be revised as

\[
\Delta t \leq \frac{\Delta}{c \sin \frac{k_{\text{max}} \Delta}{2}},
\]

\[
\Delta t \leq \frac{\Delta}{\sqrt{2} c \sin \frac{k_{\text{max}} \Delta}{2\sqrt{2}}},
\]

\[
\Delta t \leq \frac{\Delta}{\sqrt{3} c \sin \frac{k_{\text{max}} \Delta}{2\sqrt{3}}}.
\]

Compared to the standard CFL equations, the \( \left( \sin \frac{k_{\text{max}} \Delta}{2\sqrt{D}} \right)^{-1} \) term of (3.3), where \( D \) is the dimension of the simulation, provides an additional parameter to control the CFL stability limit. As \( \Delta t \) is increased, the \( \left( \sin \frac{k_{\text{max}} \Delta}{2\sqrt{D}} \right) \) term may be decreased to uphold the inequality of (3.3) through limiting \( k_{\text{max}} \). The premise of limiting the maximum wavenumber \( k_{\text{max}} \) within the simulation mesh is equivalent to a low-pass filtering operation of the spatial harmonics. Low-pass filtering the spatial harmonics in frequency is equivalent to expanding the waveform in space. This results in the propagating waveform traversing more than one cell per time-step. The CFL equivalent causality condition is thus satisfied even for CFL values above 1. In [13] and [21] the low-pass filtering operation was performed using forward and inverse Fourier transformations of the spatial mesh combined with a low-pass filter. For a simulation with CFL
extension factor $CE$, the equation

$$CE = \frac{1}{\sin \frac{k_{max} \Delta}{2\sqrt{D}}}$$

must be solved for $\tilde{k}_{max}$, which can be used to derive the low-pass cut-off frequency. The low-pass filtering operation was found to preserve the harmonics within the frequency of interest provided that the CFL was not extended beyond a set limit. The most interesting aspect of this work with respect to the context of this thesis is that the CFL limit may be overcome through filtering out at each time-step the harmonics that would make the solution unstable.

More recently, a system level approach to the explicit CFL extension problem was presented in [14]. Although called unconditionally stable FDTD, the method stabilizes the unstable FDTD equations at time-steps above the CFL limit, achieving a similar result to spatial filtering. The method starts from the formulation (2.4) and derives the stability limit for a lossless FDTD simulation using the textbook approach of [5]. Using the system form of (2.4), a set of stability conditions has been derived based upon the $-M_{21}M_{12}$ matrix on the lower right corner of the $A$ matrix. The matrix $-M_{21}M_{12}$ is a positive definite matrix. Let us denote with $\lambda_{M,i}$ the eigenvalues of $-M_{21}M_{12}$. In the lossless case, if all these eigenvalues satisfy the condition

$$\lambda_{M,i} \leq 4 \text{ for } i = 1 \ldots N$$

(3.5)

then it can be shown that all eigenvalues of $A$ are within the unit circle.

Therefore, by identifying the eigenvalues $\lambda_{M,i}$ which violate (3.5), the update system (2.4) may be modified such that unstable eigenvalues are discarded. The lossless case of [14] was extended to the lossy case in [18]. A drawback of the stability condition (3.5) is its validity in the presence of losses. The introduction of loss into (2.6) will result in a decrease in the right side of (3.5). Although bypassed in [18], this behaviour is contradictory to the stability behaviour of standard FDTD, where the introduction of conductivities has no influence on the CFL limit. For a description of the implementation we refer the reader to the publications [14] and [18].

### 3.2 Extension of the CFL Limit Using Eigenvalue Perturbation

The test cases of this section will illustrate the impacts of the CFL extension process using eigenvalue perturbation. The test cases of this section will focus on the 2D PEC cavity case. PEC cavities offer simply analytical accuracy metrics in the form of resonant frequencies. The lossless nature of PEC cavities also allows for the straightforward verification of late time stability.
3.2.1 Eigenvalue Perturbation

Using (2.4) and the stability criteria (2.7), the stability enforcement of the FDTD equations may be easily performed. For a chosen time-step $\Delta t$ beyond the CFL limit, the update matrix $A$ will contain unstable eigenvalues. The stability enforcement process may be performed in three simple steps:

1. Perform the eigenvalue decomposition on $A$

   \[ A = U \Lambda U^{-1}. \]  

   The matrix $U$ contains the eigenvectors of $A$ while $\Lambda$ is a diagonal matrix whose entries are the eigenvalues $\lambda_i$ of $A$.

2. Perturb the unstable eigenvalues of $A$ that violate $|\lambda_i| \leq 1$

   \[ \hat{\lambda}_i = \gamma \frac{\lambda_i}{|\lambda_i|}, \]

   where $\gamma = 0.999$. In this way, the magnitude of the unstable eigenvalues is reduced below 1, enforcing their stability. The chosen value of $\gamma$ is slightly lower than 1 in order to avoid placing the perturbed eigenvalues right at the boundary between stability and instability. The stable and perturbed eigenvalues are collected to form a diagonal matrix $\hat{\Lambda}$.

3. Reconstruct a perturbed update matrix $\hat{A}$ from the perturbed eigenvalue matrix $\hat{\Lambda}$

   \[ \hat{A} = U \hat{\Lambda} U^{-1}. \]

   The perturbed matrix $\hat{A}$ is now stable for the time-step $\Delta t$ above the CFL limit.

This test cases of this section will demonstrate and justify the overall preservation of simulation accuracy for the explicit CFL extension case. In addition, the test cases will demonstrate that the unstable eigenvalues for modest CFL extension ratios are outside of the frequency of interest and have very little impact on the overall simulation results. The test cases performed in this Chapter are implemented in Matlab taking advantage of the included LAPACK library. The eigenvalue decomposition step is performed using the Matlab “eig” function. Since the eigenvalue decomposition has complexity greater than $O(N^3)$ and is severely memory limited, the test cases for this section are limited to less than 10 thousand states on a machine with 16 Gigabytes of memory. The introduction of model order reduction in Chapter 4 will overcome this limitation. The eigenvalue perturbation process may be used
3.2.2 Demonstration of FDTD Spatial Oversampling

Before introducing the proposed CFL extension method, we will show the oversampled nature of FDTD. The oversampling provides the theoretical justification for extending the CFL limit without compromising accuracy. This example will demonstrate the oversampled nature of standard FDTD using a 2D PEC cavity. The limitation to the 2D case is due to the complexity scaling of the eigenvalue decomposition algorithm.

A 2D PEC cavity of size $1 \times 1$ m is simulated in the transverse magnetic (TM) operating mode with $E_x$, $E_y$, and $H_z$ field nodes. The cavity is discretized with square cells of $\Delta x = \Delta y = \Delta = 0.05$ m. The mesh sizes for the $E_x$, $E_y$, and $H_z$ fields are 21 x 20, 20 x 21, and 20 x 20, resulting in a total of 1240 unknown states. A single ideal current source is placed on the $H_z$ node at (4,4), while a probe is placed on the $H_z$ node at (16,16). The current source is a Gaussian pulse of the form $e^{-\left(\frac{t-t_0}{T_s}\right)^2}$, where $T_s = \frac{1}{2f_{\text{max}}}$, $t_0 = 4T_s$, and $f_{\text{max}} = 0.5$ GHz. The frequency band of interest is equal to that of the input Gaussian pulse, from DC to 0.5 GHz. The resulting minimum $\frac{\lambda}{\Delta}$ ratio at 0.5 GHz is 12. The simulation was ran for 10,000 time-steps with a CFL of 1.

![System eigenvalues and Region of stability for standard FDTD and perturbed system](image.png)

**Figure 3.2**: Cavity of Section 3.2.2: Eigenvalues of the discrete update matrix $A$ for standard FDTD and perturbed system containing only the frequency band of interest for the 2D PEC cavity case at CFL = 1.

to perturb both stable and unstable eigenvalues.
For \( s = j2\pi f_{\text{max}} \) we may use the forward and backward transformations

\[
z = e^{sT} \quad \text{and} \quad s = \frac{1}{T} \ln(z)
\]

where \( T \) is the time-step \( \Delta t \) used. At CFL = 1, the time-step \( \Delta t \) is \( 1.1793 \times 10^{-10} \) seconds. The frequency band of interest (DC to 0.5 GHz) corresponds to the range of angles \([-0.3705, 0.3705]\) radians from the positive real axis. This range defines the angular sector shown in black in Figure 3.2b. The point \( z = -1 \), instead, corresponds to the spatial harmonics of 4.24 GHz. In Figure 3.2a, the full eigenvalues decomposition of the discrete update matrix \( A \) are plotted. Due to the lossless nature of the simulation, all eigenvalues have a magnitude of 1 and rest on the unit circle.

We now show the negligible role of the eigenvalues located beyond \( f_{\text{max}} \). All eigenvalues that fall outside of the angular sector related to the frequency range of interest are perturbed according to the process of Section 3.2.1 in order to move them inside the range. This process is shown in Figure 3.2a and 3.2b. Then, we ran the FDTD simulation using both the original and the perturbed update matrices \( A \). The time and frequency domain results at the \( H_z \) probe at (16,16), depicted in Figure 3.3, show the negligible role of the perturbed eigenvalues, and confirm the oversampled nature of FDTD. The relative error norms for the time and frequency domain results are 0.015\% and 0.000071\%. The relative error does not increase as the number of time-steps is increased. To further illustrate the convergence of the two test cases, Figure 3.4 plots the waveform across the \( H_z \) field nodes at 500 time-steps for the two test cases. It may be seen that the magnitude across all field nodes within the simulation domain are faithfully replicated. Noticeable errors in both time and frequencies may be observed if eigenvalues
This test case demonstrates two important observations that will become important to the scope of this thesis. The first is that for a given frequency band of interest, only the \( z \)-domain eigenvalues within the band are influential to the time and frequency output. Due to the oversampling of the FDTD simulation, a significant number of the system eigenvalues fall outside of the frequency band of interest. Such eigenvalues are precisely those that become unstable when a time-step above the CFL limit is used. Due to their small influence on the system response, they can be perturbed or removed to ensure late time stability without significantly affecting accuracy. The second observation is that there are 15 conjugate eigenvalue pairs contributing 7 resonate frequencies from DC to 0.5 GHz. Therefore, only a small portion of the system eigenvalues are needed in order to faithfully reproduce the simulation output. This observation is the main justification behind the model order reduction process of Chapter 4.

### 3.2.3 2D PEC Cavity CFL Extension Test Case

In this test case the 2D PEC cavity simulation of Section 3.2.2 is used to demonstrate the stability enforcement of the discrete FDTD system at a time-step beyond the CFL limit. All simulation settings remain the same as in Section 3.2.2 with the exception of the CFL limit. Although simple, the resonant PEC cavity simulations offers several insights into the accuracy and stability of the CFL extension technique. Due to the lossless nature, the simulation may be ran for a large number of time steps to
verify late time stability. The analytical resonant frequencies may be calculated through

\[
\frac{c}{2} \sqrt{\left( \frac{n_x}{L_x} \right)^2 + \left( \frac{n_y}{L_y} \right)^2}
\]

(3.10)

where \( c \) is the speed of light in the medium, \( n_x \) and \( n_y \) are the mode numbers, and \( L_x \) and \( L_y \) are the side lengths. Since (3.10) is only a function of the wave velocity and physical size, the error introduced due to numerical dispersion is directly proportional to the errors of the resonant frequencies.

For comparison purposes the implicit and explicit CFL extension methods of Section 3.1.1 and Section 3.1.2 have been implemented. The direct implicit method described in Section 3.1.1 as given in [1, 9] is implemented exactly as described. The implemented ADI-FDTD technique is the original 2D formulation presented by Namiki in 1999 [11]. The spatial filtering algorithm of [13] is implemented using the simplified form presented in [21], where only the \( H_z \) nodes are filtered at each time-step using the forward and inverse discrete cosine transforms. No timing information is collected; the purpose of this test case is to analyse the behaviour and accuracy of the different CFL extension techniques. Due to the relatively coarse cell size of \( \frac{\Delta x}{\Delta} = 12 \), modest CFL extension ratios of \( \text{CFL} = 2 \) and \( \text{CFL} = 3 \) will be used.

Figure 3.5 plots the eigenvalues of the discrete update matrix \( \mathbf{A} \) for the explicit FDTD system with \( \text{CFL} = 2 \). The stability condition \(|\lambda_i| \leq 1\) is violated by some eigenvalues. It has been observed that all unstable eigenvalues appear on the real-axis and are less than \( z = -1 \). Using the transformation (3.9) and the new time-step value \( \Delta t \), it can be found that the point \( z = -1 \) is now associated with the spatial harmonics of 2.12 GHz. The angle around the positive real axis containing the interested frequency
Chapter 3. Overcoming the CFL Limit of the FDTD Method

Figure 3.6: Cavity of Section 3.2.3: Eigenvalues of the update matrix for the proposed method and the implicit method [1] for the lossless 2D PEC cavity with CFL = 2.

The standard FDTD simulation was ran with CFL = 1 for 100,000 time-steps, while the CFL extension methods were ran for 50,000 and 33,333 time-steps for CFL = 2 and 3 due to the larger time-step. The CFL extension test cases are interpolated in time to obtain the same 100,000 length time-domain results as standard FDTD. Figure 3.6 plots the eigenvalues of the stability enforced explicit and implicit system update matrices $A$ and $A_I$ with CFL = 2. The stability enforcement step successfully perturbed all unstable eigenvalues into the stable region at the new maximum supported frequency of 2.12 GHz. There are a total of 83 conjugate pairs or 166 total eigenvalues within the stable region out of a total of 1240. Figure 3.7 plots the extracted frequency domain results of the cavity simulation with all CFL extension methods ran at CFL = 2.

The analytical resonant frequencies of the 2D PEC cavity simulation may be calculated from (3.10) and used as a metric of comparison to evaluate the accuracy of the tested CFL extension techniques. The first 6 resonant frequencies below 0.5 GHz for the analytical and simulation results have been collected in Table 3.1. The standard FDTD simulation was ran with CFL = 1, while all CFL extension
methods were ran with CFL = 2 and CFL = 3. The normalized relative error is the deviation of the extracted resonant frequency from the analytical results. A negative relative error denotes an extracted resonance lower than the analytical results and vice versa. Since the resonant frequency is a function of the effective wave velocity, the relative error of the resonance frequencies is directly related to the introduced numerical dispersion error. The magnitudes of the relative error are plotted in Figure 3.8. The increase in numerical dispersion errors is proportional to the increase in the CFL extension ratio. The implicit methods exhibit a negative normalized relative error, representing a slower wave velocity than the speed of light. This is consistent with the tests performed in [17, 26]. The opposite is true for explicit CFL extension methods, a conclusion consistent with the FDTD dispersion equations. Explicit CFL extension methods, including the proposed one, introduce smaller numerical dispersion compared to their implicit counterparts.

Table 3.1: Cavity of Section 3.2.3: Extracted resonant frequencies and normalized relative error for implicit and explicit CFL extension methods at CFL = 2 and CFL = 3.

<table>
<thead>
<tr>
<th>Resonant Modes</th>
<th>$TM_{0,1}$</th>
<th>$TM_{1,1}$</th>
<th>$TM_{2,0}$</th>
<th>$TM_{2,1}$</th>
<th>$TM_{2,2}$</th>
<th>$TM_{3,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical</td>
<td>0.149896</td>
<td>0.211985</td>
<td>0.299792</td>
<td>0.353178</td>
<td>0.423971</td>
<td>0.449689</td>
</tr>
<tr>
<td>FDTD (CFL=1)</td>
<td>0.149818</td>
<td>0.211985</td>
<td>0.299177</td>
<td>0.334867</td>
<td>0.423970</td>
<td>0.447588</td>
</tr>
<tr>
<td>Normalized Relative Error [%]</td>
<td>-0.052</td>
<td>0</td>
<td>-0.205</td>
<td>-0.093</td>
<td>0</td>
<td>-0.467</td>
</tr>
</tbody>
</table>

CFL Extension Ratio = 2

| Implicit [1] | 0.149131 | 0.210054 | 0.293829 | 0.327428 | 0.409020 | 0.430355 |
| Normalized Relative Error [%] | -0.510 | -0.910 | -1.989 | -2.312 | -3.526 | -4.299 |
| ADI-FDTD [11] | 0.149131 | 0.210691 | 0.293829 | 0.32897 | 0.413880 | 0.430335 |
| Normalized Relative Error [%] | -0.510 | -0.610 | -1.989 | -1.852 | -2.380 | -4.303 |
| Spatial Filtering [13] | 0.150051 | 0.212647 | 0.301051 | 0.337515 | 0.429440 | 0.458060 |
| Normalized Relative Error [%] | 0.103 | 0.312 | 0.420 | 0.697 | 1.289 | 1.861 |
| Proposed Method | 0.150051 | 0.212647 | 0.301051 | 0.337515 | 0.429440 | 0.458060 |
| Normalized Relative Error [%] | 0.103 | 0.312 | 0.420 | 0.697 | 1.289 | 1.861 |

CFL Extension Ratio = 3

| Implicit [1] | 0.148381 | 0.207881 | 0.288272 | 0.31982 | 0.39477 | 0.41369 |
| Normalized Relative Error [%] | -1.010 | -1.936 | -3.842 | -4.582 | -6.887 | -8.005 |
| ADI-FDTD [11] | 0.148381 | 0.209365 | 0.288272 | 0.323047 | 0.404129 | 0.430369 |
| Normalized Relative Error [%] | -1.010 | -1.235 | -3.842 | -3.619 | -4.860 | -8.005 |
| Spatial Filtering [13] | 0.150441 | 0.213774 | 0.304332 | 0.342199 | 0.439503 | 0.466116 |
| Normalized Relative Error [%] | 0.363 | 0.843 | 1.514 | 2.094 | 3.663 | 3.653 |
| Proposed Method | 0.150441 | 0.213774 | 0.304332 | 0.342199 | 0.439503 | 0.466116 |
| Normalized Relative Error [%] | 0.363 | 0.843 | 1.514 | 2.094 | 3.663 | 3.653 |

Figure 3.9 plots the 1-500 and 99,500-100,000 time-step time domain results for the tested methods. The numerical dispersion error introduces an accumulating error within the time domain results. For 1-500 time-steps, the explicit methods are able to capture the time domain waveform with relatively minor errors, while the implicit and ADI-FDTD methods fared worse. For CFL = 2, all waveforms of the CFL extension methods at 99,500-100,000 time-steps deviate from the standard FDTD results.
Based upon these observations, running the lossless case with different time-steps will eventually result in large deviations between any FDTD simulation due to the introduction of numerical dispersion errors. The numerical dispersion errors result in shifts in the frequency domain waveforms. Spatial filtering and the proposed method generated exactly the same results. Although theoretically stable, all test cases were ran to $10^7$ time-steps to confirm late time stability.

### 3.2.4 2D Dielectric Filled Cavity Test Case

The 2D PEC cavity test case of Section 3.2.3 compares the accuracy of explicit and implicit CFL extension techniques. The explicit spatial filtering and the proposed CFL extension techniques resulted in equivalent results for the lossless free space case. As illustrated in Section 3.1.2, the two methods are based upon similar principles, but utilize different methods to extend the CFL limit. This example will illustrate the difference in accuracy between the two methods when applied to an inhomogeneous system. This test case will reuse the previous 2D PEC cavity test case with the addition of a 0.5 m x 0.5 m magnetic slab with $\mu_r = 4$. Since our implementation of spatial filtering performs the filtering only on magnetic field nodes, a magnetic rather than dielectric material is used. The layout of this simple simulation case is shown in Figure 3.10.

The simulation has been ran with the spatial filtering and the proposed CFL extension method at CFL = 1 and CFL = 2. Due to the slowing of the propagating wave within the magnetic material, an increase in the number of stable eigenvalues from 166 to 322 can be observed with the addition of the magnetic material. Figure 3.11 plots the first 500 time-steps of the time domain results at the probe of the compared methods at CFL = 2. Figure 3.12 shows the extracted frequency domain results for the two compared methods. At CFL = 1, both methods maintain normalized frequency errors of less than $10^{-10}$ relative to standard FDTD results. At CFL = 2, the spatial filtering results exhibit increased errors both in terms of frequency and magnitude of the extracted resonant harmonics. The frequency domain filtering coupled with the forward and inverse transformations introduces additional errors in to the time domain results. In Figure 3.13 the relative errors of the spatial filtering and the proposed cases have been compared against the standard FDTD results, where both methods were ran at CFL = 2. In [21] it is noted that the specific spatial filtering errors may be removed by the splitting of the simulation domain along material boundaries, although this is not a trivial process and depends upon the simulation setup. The proposed method may be observed to be more applicable in simulations containing inhomogeneous materials compared to spatial filtering. In Chapters 4 and 5 it will be shown that the accuracy of the proposed method extends to discontinuous material and PEC structures.
Figure 3.7: Cavity of Section 3.2.3: Frequency domain results of implicit and explicit CFL extension methods for 2D PEC cavity test case with CFL = 2.
Figure 3.8: Cavity of Section 3.2.3: Relative error of extracted resonant frequencies for implicit and explicit CFL extension methods for 2D PEC cavity test case.
Figure 3.9: Cavity of Section 3.2.3: Early (1-500) and late time (99,500-100,000) time-step time domain results of implicit and explicit CFL extension methods for 2D PEC cavity test case with CFL = 2.
Figure 3.10: Cavity of Section 3.2.4: Simulation layout of 2D PEC cavity test case with magnetic material insert.

Figure 3.11: Cavity of Section 3.2.4: Time domain waveforms of spatial filtering and proposed CFL extension methods for magnetic material filled PEC cavity test case.
Figure 3.12: Cavity of Section 3.2.4: Comparison of frequency domain results of spatial filtering and proposed CFL extension methods for magnetic material filled PEC cavity test case at CFL = 2.

Figure 3.13: Cavity of Section 3.2.4: Normalized error of first 8 resonant frequencies of magnetic material filled PEC cavity test case for spatial filtering and system filtering CFL extension at CFL = 2.
3.3 Summary

This chapter introduces the eigenvalue perturbation based CFL extension technique using the notations of Chapter 2. The CFL limit may be extended using eigenvalue decomposition and perturbation using the discrete system stability criteria. The stability enforcement technique described was first presented in [15]. The implementation and theory behind existing implicit and explicit CFL extension techniques have also been briefly covered. Three test case have been ran using the 2D PEC cavity case to demonstrate key characteristics of eigenvalue perturbation based CFL extension. The first test case outlines the oversampled nature of standard FDTD with respect to the actual frequency band of interest. The second test case demonstrates the numerical dispersion characteristics of explicit CFL extension techniques relative to both standard FDTD and implicit CFL extension techniques. The third example demonstrates the superior accuracy of proposed method compared to previous spatial filtering CFL extension method when applied to discontinuous material boundaries. Although intuitive, the eigenvalue perturbation technique presented in this chapter cannot be applied to systems of over a few thousand nodes due to the complexity scaling of the eigenvalue decomposition function. Chapter 4 will introduce model order reduction to facilitate the application of the filtering process to a significantly reduced equivalent system, as well as an improved stability enforcement process.
Chapter 4

FDTD Equivalent System
Formulation and Model Order Reduction

Chapter 3 introduced the derivation and basis for overcoming the CFL limit through eigenvalue perturbation. Due to the complexity of the eigenvalue decomposition algorithm, the test cases were limited to 2D cases with a few thousand states. This chapter will introduce the model order reduction technique that is applied to a modified form of the discrete FDTD update system. The MOR technique used is the Krylov subspace projection method based upon moment matching. The MOR step projects the original state space into a significantly reduced state vector while capturing the most influential eigenvalues. The MOR step facilitates the use of the proposed stability enforcement beyond the CFL limit. The combination of these two independent methods form the proposed method for overcoming the CFL limit. The small 2D PEC cavity examples from Chapter 3 are expanded to significantly larger 2D and 3D test cases. The test cases serve to demonstrate the properties and accuracy of the MOR step, as well as the complexity of the proposed MOR and stability enforcement algorithm. The contents of this chapter was first presented in [16].
4.1 Stability-Preserving Model Order Reduction of FDTD Equations

4.1.1 Matrix Formulation of FDTD Equations

In Chapters 2 and 3 the discrete-time FDTD update equations were cast into a matrix form. While convenient from an analysis perspective, the system form of Chapters 3 (2.4) is difficult to reduce using existing model order reduction techniques. As performed in [15], the direct application of MOR to (2.4) does not preserve the stability of the original system. In this section, an improve formulation will be introduced that maintains the staggered leap-frog update format of standard FDTD. We start from the FDTD equations written in matrix form (2.3a) and (2.3b), which we repeat here for convenience

\[
\begin{align*}
\left( \frac{D_e}{\Delta t} + \frac{D_{\sigma_e}}{2} \right) E^{n+1} &= \left( \frac{D_e}{\Delta t} - \frac{D_{\sigma_e}}{2} \right) E^n - KH^{n+\frac{1}{2}} - J^{n+\frac{1}{2}} \quad (4.1a) \\
\left( \frac{D_\mu}{\Delta t} + \frac{D_{\sigma_m}}{2} \right) H^{n+\frac{3}{2}} &= \left( \frac{D_\mu}{\Delta t} - \frac{D_{\sigma_m}}{2} \right) H^n + KT E^{n+1} - M^{n+1}. \quad (4.1b)
\end{align*}
\]

where the \( D_e, D_{\sigma_e}, D_\mu, D_{\sigma_m}, \) and \( K \) matrices were previously defined in Chapter 2. To compact the notation, we rewrite (4.1) as [19]

\[
(R + F)x^{n+1} = (R - F)x^n + Bu^{n+1}, \quad (4.2)
\]

with

\[
R = \begin{bmatrix}
\frac{1}{\Delta t} D_e & -\frac{1}{2} K \\
-\frac{1}{2} K^T & \frac{1}{\Delta t} D_\mu
\end{bmatrix}, \quad F = \begin{bmatrix}
\frac{1}{2} D_{\sigma_e} & \frac{1}{2} K \\
-\frac{1}{2} K^T & \frac{1}{2} D_{\sigma_m}
\end{bmatrix}, \quad (4.3)
\]

and where

\[
x^n = \begin{bmatrix}
E^n \\
H^{n+\frac{1}{2}}
\end{bmatrix} \quad (4.4)
\]

is a vector of size \( N = N_e + N_h \), where \( N_e \) is the number of electric field unknowns, and \( N_h \) is the number of magnetic field unknowns.

4.1.2 Stability Conditions

The section will introduce the revised stability conditions for a discrete-dime FDTD system of form (4.2). Written in form (4.2), a system of FDTD equations can be interpreted as a discrete-time system with input \( u^{n+1} \) and state \( x^n \). Its solution will be stable if and only if all poles of (4.2) are inside the unit
circle in the complex plane or equivalently, if the following two conditions hold

\[
\begin{align*}
F^T + F &= \begin{bmatrix} D_\sigma & 0 \\ 0 & D_{\sigma_m} \end{bmatrix} \geq 0 \\
R &= \begin{bmatrix} \frac{1}{\Delta t} D_\epsilon - \frac{1}{2} K \\ -\frac{1}{2} K^T - \frac{1}{\Delta t} D_\mu \end{bmatrix} > 0
\end{align*}
\] (4.5)

where \( \geq 0 \) denotes a positive semidefinite matrix, and \( > 0 \) denotes a positive definite matrix\(^1\). Conditions (4.5) and (4.6) were proposed in [19] and have an intuitive physical explanation. Inequality (4.5) simply requires all conductivities to be positive. This is equivalent to the lossless or dissipative constraint on the FDTD simulation domain. Inequality (4.6) can be shown [19] to be equivalent to the CFL limit (2.8) and limits the maximum time-step \( \Delta t \) that can be used in a stable FDTD simulation.

Starting from inequality (4.6), the Schur complement conditions for positive definiteness states that \( R \) is positive definite if and only if

\[
\begin{align*}
\frac{1}{\Delta t} D_\mu &> 0 \tag{4.7a} \\
\frac{1}{\Delta t} D_\epsilon - \frac{\Delta t}{4} K D_\mu^{-1} K^T &> 0 \tag{4.7b}
\end{align*}
\]

Since \( D_\mu \) is a positive definite matrix, inequality (4.7a) always hold. The inequality (4.7b) can be rewritten in the form

\[
(D_\epsilon^{-\frac{1}{2}} K D_\mu^{-\frac{1}{2}})(D_\epsilon^{-\frac{1}{2}} K D_\mu^{-\frac{1}{2}})^T < \frac{4}{\Delta t^2} I.
\]

(4.8)

By denoting the singular values of \( D_\epsilon^{-\frac{1}{2}} K D_\mu^{-\frac{1}{2}} \) as \( \sigma_i \), it may be seen that (4.8) holds if and only if [19]

\[
\sigma_i < \frac{2}{\Delta t} \quad \forall \ i.
\]

(4.9)

The singular value of the \( D_\epsilon^{-\frac{1}{2}} K D_\mu^{-\frac{1}{2}} \) matrix is inversely proportional to the magnitude of the relative permittivity and permeability terms contained in \( D_\epsilon \) and \( D_\mu \). For free space the matrix \( D_\epsilon^{-\frac{1}{2}} K D_\mu^{-\frac{1}{2}} \) simplifies to \( cK \). From this relation we see that the singular values \( \sigma_i \) decrease with the increase of \( \epsilon_r \) and \( \mu_r \), thus allowing the use of a larger time-step \( \Delta t \). This is consistent with the expected increase in maximum time-step \( \Delta t \) from the CFL limit in dielectric and magnetic materials. In order to evaluate inequality (4.9), it is useful to further analyse the properties of the \( K \) matrix.

\(^1\)A symmetric matrix \( A \) is positive definite if for any vector \( x \neq 0 \) we have \( x^T A x > 0 \). It is positive semidefinite if \( x^T A x \geq 0 \).
The $K$ matrix is a structured matrix containing the centred difference approximation for the spatial derivative terms. A thorough analysis and derivation for the singular value of the $K$ matrix has been performed in [19]. A key result from [19] is that for a rectangular simulation domain with uniform cell size along each axis, the maximum singular value of the $K$ matrix is given by

$$\max(\text{svd}(K)) = \sqrt{\frac{4}{\Delta x^2} \cos^2 \left( \frac{\pi}{N_x} \right) + \frac{4}{\Delta y^2} \cos^2 \left( \frac{\pi}{N_y} \right) + \frac{4}{\Delta z^2} \cos^2 \left( \frac{\pi}{N_z} \right)}$$

(4.10)

where svd is the singular value decomposition function and $N_x$, $N_y$, $N_z$ are the cell numbers along each axis. The identity (4.10) can be extended to the 1D and 2D cases by replacing the right hand side with $\sqrt{\frac{4}{\Delta x^2} \cos^2 \left( \frac{\pi}{N_x} \right)}$ and $\sqrt{\frac{4}{\Delta x^2} \cos^2 \left( \frac{\pi}{N_x} \right) + \frac{4}{\Delta y^2} \cos^2 \left( \frac{\pi}{N_y} \right)}$ respectively. A minor observation is that the stability condition is not only a direct function of the cell size, but also weakly correlated to the number of cells along each axis. By plugging in (4.10) to the inequality (4.9) we have shown that a time-step less than or equal to the CFL limit will always satisfy the stability conditions of (4.5) and (4.6). It may be easily seen that as the time-step $\Delta t$ is increased in (4.9), the maximum singular value of the $K$ matrix must be decreased to maintain stability.

### 4.2 Krylov Subspace Projection Model Order Reduction

Model order reduction (MOR) is a well-studied field of system control theory that focuses on the reduction of large-scale systems. The examples of this thesis implemented the Krylov subspace projection based MOR technique generated via the Arnoldi iteration. The Arnoldi iterative algorithm may be directly applied to the discrete-time FDTD system of (4.2) to generate an orthonormal projection vector $V$. We now reduce FDTD equations (4.2) using the SPRIM model order reduction technique [23]. Firstly, from the matrices in (4.2), we generate a projection matrix

$$V = \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix}$$

(4.11)

Matrices $V_1$ and $V_2$ are orthonormal and of size $N_e \times \tilde{N}$ and $N_h \times \tilde{N}$, respectively, with $\tilde{N}$ much smaller than $N_e$ and $N_h$. Then, we approximate the full vector of unknowns $x^n$ with a reduced vector $\tilde{x}^n$ as

$$x^n \approx V \tilde{x}^n.$$  

(4.12)
The reduced states \( \tilde{x}|^n \) may be viewed as a compressed representation of the original states \( x|^n \), with each reduced state representing multiple states of the original system. This is equivalent to mapping a number of the original orthogonal FDTD nodes into a single "super" node. The model order reduction process is equivalent to keeping only the most influential spatial harmonics for a given FDTD simulation. The reduction process is equivalent to projecting the \( E|^n \) and \( H|^{n+\frac{1}{2}} \) state vectors as:

\[
E|^n \simeq V_1 \tilde{E}|^n \quad \text{and} \quad H|^{n+\frac{1}{2}} \simeq V_2 \tilde{H}|^{n+\frac{1}{2}}.
\]  

Substituting (4.12) into (4.2), and multiplying on the left by \( V^T \), we obtain:

\[
V^T(R + F)V \tilde{x}|^{n+1} = V^T(R - F)V \tilde{x}|^n + V^T Bu|^n
\]  

and, after carrying out matrix multiplications,

\[
(R + \tilde{F})\tilde{x}|^{n+1} = (R - \tilde{F})\tilde{x}|^n + \tilde{B}u|^n,
\]  

where \( \tilde{R} = V^T RV \), \( \tilde{F} = V^T FV \) and \( \tilde{B} = V^T B \) are “compressed” versions of \( R \), \( F \) and \( B \), respectively. The order of (4.15) is \( 2\tilde{N} \), which is much lower than then order \( N \) of the original system (4.2). The reduced model order and, consequently, its accuracy, can be controlled by choosing the number of columns \( \tilde{N} \) of the projection matrices \( V_1 \) and \( V_2 \) generated by the Arnoldi algorithm. Due to the small size, (4.15) can be solved very quickly to find the reduced unknowns \( \tilde{x}|^n \). Once \( \tilde{x}|^n \) is available, the fields at any point in the system are computed through (4.12).

Using (4.3) and (4.12), the matrices in (4.15) can be written as:

\[
\tilde{R} = \begin{bmatrix}
\frac{1}{\Delta t} \tilde{D}_\epsilon & -\frac{1}{2} \tilde{K} \\
-\frac{1}{2} \tilde{K}^T & \frac{1}{\Delta t} \tilde{D}_n
\end{bmatrix}, \quad
\tilde{F} = \begin{bmatrix}
\frac{1}{2} \tilde{D}_{\sigma_e} & \frac{1}{2} \tilde{K} \\
-\frac{1}{2} \tilde{K}^T & \frac{1}{2} \tilde{D}_{\sigma_m}
\end{bmatrix},
\]  

where

\[
\tilde{D}_\epsilon = V_1^T D_\epsilon V_1, \quad \tilde{D}_\mu = V_2^T D_\mu V_2
\]
\[
\tilde{D}_{\sigma_e} = V_1^T D_{\sigma_e} V_1, \quad \tilde{D}_{\sigma_m} = V_2^T D_{\sigma_m} V_2
\]
\[
\tilde{K} = V_1^T KV_2
\]

Owing to the block-diagonal nature of the projection matrix (4.11) used in SPRIM [23], the reduced
matrices (4.16) have exactly the same block structure of the original FDTD matrices (4.3). Blocks (4.17)-(4.19) are compressed counterparts of the original permittivity, permeability, conductivity and “curl” matrices. Although, after the reduction process these blocks are full, they can be easily diagonalized, owing to their small size $\tilde{N}$. Therefore, the reduction process preserved the structure of the original FDTD equations (4.2), which is a novel result. Being in the same form as FDTD equations, the solution of (4.15) can be computed in a leap-frog manner, for increased efficiency.

### 4.2.1 Stability Preservation Below the CFL Limit

We now discuss the stability of the reduced model (4.15). First, we consider the case when $\Delta t$ is below the CFL limit of the original FDTD equations, showing that the obtained reduced model is stable by construction. Since we have preserved the structure of the FDTD equations, stability conditions (4.5) and (4.6) can be also applied to the reduced model

\begin{align*}
\tilde{F}^T + \tilde{F} & \geq 0 \\
\tilde{R} & > 0
\end{align*}

(4.20)

(4.21)

The first condition can be rewritten as

\[
\tilde{F}^T + \tilde{F} = \begin{bmatrix}
V_1 & 0 \\
0 & V_2
\end{bmatrix}^T (\tilde{F}^T + \tilde{F}) \begin{bmatrix}
V_1 & 0 \\
0 & V_2
\end{bmatrix} \geq 0.
\]

(4.22)

Since the original model (4.2) satisfies (4.5), the last expression in (4.22) is positive semidefinite by construction, as it is the congruence of a positive semidefinite matrix [27]. Similarly, since $R > 0$ because of (4.6), and $V$ is full rank, we have

\[
\tilde{R} = \begin{bmatrix}
V_1 & 0 \\
0 & V_2
\end{bmatrix}^T R \begin{bmatrix}
V_1 & 0 \\
0 & V_2
\end{bmatrix} > 0
\]

(4.23)

Therefore, the proposed approach preserves stability by construction, avoiding the need for an additional post-processing step to enforce its stability as in [15].
4.3 Stability Enforcement Above the CFL Limit

4.3.1 Singular Value Perturbation

If the chosen \( \Delta t \) is beyond the CFL limit of the original FDTD equations, conditions (4.5) and (4.6) will be violated and reduced model (4.15) may contain unstable eigenvalues. However, due to its small size, its stability can be easily enforced, effectively breaking the CFL barrier.

From stability criteria (4.5) and (4.6), we see that changing \( \Delta t \) will only affect the second condition, since the first one does not depend on \( \Delta t \). In order to make the reduced model stable, we need to enforce

\[
\tilde{R} = \begin{bmatrix}
\frac{1}{\Delta t} \tilde{D}_e & -\frac{1}{2} \tilde{K} \\
-\frac{1}{2} \tilde{K}^T & \frac{1}{\Delta t} \tilde{D}_\mu
\end{bmatrix} > 0,
\]

which can be achieved by perturbing \( \tilde{K} \) as follows. As shown in Section (4.1.2), the condition above is equivalent to

\[
\tilde{\sigma}_i < \frac{2}{\Delta t} \text{ for } i = 1, \ldots, \tilde{N}.
\]

where \( \tilde{\sigma}_i \) are the singular values of \( \tilde{D}_e^{-\frac{1}{2}} \tilde{K} \tilde{D}_\mu^{-\frac{1}{2}} \). As the CFL limit is exceeded, singular values of the \( \tilde{D}_e^{-\frac{1}{2}} \tilde{K} \tilde{D}_\mu^{-\frac{1}{2}} \) matrix will violate the stability limit of (4.9), thus resulting in instability of the simulation.

The following steps can be applied to enforce the stability of the reduced system

1. Compute the singular value decomposition [27]

\[
\tilde{D}_e^{-\frac{1}{2}} \tilde{K} \tilde{D}_\mu^{-\frac{1}{2}} = USW^T,
\]

Matrix \( S \) is a diagonal matrix containing the singular values \( \tilde{\sigma}_i \).

2. Perturb the singular values \( \tilde{\sigma}_i \) that violate \( \tilde{\sigma}_i < \frac{2}{\Delta t} \)

\[
\tilde{\sigma}_i' = \begin{cases} 
\tilde{\sigma}_i & \text{if } \tilde{\sigma}_i < \frac{2}{\Delta t} \\
\gamma \frac{2}{\Delta t} & \text{otherwise}
\end{cases}
\]

where \( \gamma \) is to mitigate any numerical errors affecting stability and is chosen to be slightly less than 1. In the test cases we set \( \gamma = 0.999 \). Construct a new matrix \( S' \) containing the stable and perturbed singular values \( \tilde{\sigma}_i' \).
3. Obtain the perturbed $\tilde{K}'$ matrix

$$\tilde{K}' = \tilde{D}_1 \tilde{D}_2^T \tilde{U} \tilde{S}' \tilde{W}^T \tilde{D}_2^\dagger \tilde{D}_1^\dagger.$$  \hspace{1cm} (4.28)

Using $\tilde{K}'$, the perturbed reduced system satisfies (4.5) by construction and has been stabilized to satisfy (4.6). Therefore, the reduced system is stable for the time-step $\Delta t$ above the CFL limit. This is the stability enforcement method that we proposed in [16].

### 4.4 Optimizations and Practical Implementation

#### 4.4.1 Frequency Shifting

All order reduction methods based on moment matching generate reduced models accurate near a given expansion point in the complex frequency plane. As the order of the reduced model is increased through $\tilde{N}$, the bandwidth of validity of the reduced model around the expansion point grows. In terms of eigenvalues, as $\tilde{N}$ increases, more and more eigenvalues of the original system will be matched by the reduced model eigenvalues, starting from those closer to the expansion point. The default expansion point is the origin on the real-imaginary plane. By choosing the position of the expansion point, one can thus optimize the accuracy of the reduced model, and guide its convergence towards the most relevant eigenvalues of the system. Typical choices of expansion points include DC and the maximum frequency of interest $f_{\text{max}}$. For a sufficiently large $\tilde{N}$, the reduced model will capture the wideband response of the original system.

In order to improve the efficiency of the reduced model over a large bandwidth, the Complex Frequency Hopping (CFH) [28] technique may be used. Multiple expansion points with a smaller number of moments matched are distributed within the frequency band of interest. The cumulative results from all expansion points will often result in a more accurate wideband system, although with some difference in computational costs. In this thesis both single and CFH expansion point distributions are used. Based upon the $z$-domain properties of Chapter 3, the distribution of multiple expansion points are made according to

$$z_l = Me^{-j2\pi L f_{\text{max}} \Delta t},$$  \hspace{1cm} (4.29)

for $l = -L, \ldots, 0, \ldots, L$. This formula places $2L + 1$ expansion points along a circular arc of radius $M$ centered at the origin of the complex plane. Although the interested eigenvalues lie between $\pm f_{\text{max}}$, only the expansion points along the positive imaginary axis are used, exploiting properties of conjugate
4.4.2 Linear System Solution

A set of linear systems must be solved for each new moment generated with the Arnoldi process used to generate $V$. Recall that the $V$ is split into two sets represented the real and imaginary components, and split again with the application of the SPRIM algorithm. For a reduced system of size $2\tilde{N}$, $\frac{N}{2}$ linear system solutions are required to generate the original $V$ projection vector. The system is in the form

$$
\begin{equation}
[(R - F) + z_l(R + F)] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}
\end{equation}
$$

(4.30)
where \( z_l \) is the current expansion point. When \( z_l = 0 \), since \((R - F)\) is upper triangular, the system can be solved very efficiently. However, an expansion point at the original will first capture the most heavily damped and uninfluential eigenvalues, therefore resulting in poor overall accuracy. For \( z_l \neq 0 \), the system can be solved with one LU decomposition [29] in 2D and small 3D cases, similarly to what done in [9] and [10]. Once a LU decomposition has been performed, each linear solution becomes a forward and backward substitution operation which in the unoptimized case has complexity \( O(N^2) \). The LU decomposition is prohibitive for large simulation sizes has complexity \( \leq O(N^3) \). For large 3D cases, iterative methods must be used, and we adopted the conjugate gradient squared method [30] available in Matlab. The conjugate gradient method iteratively solved for the linear system solution until the normalized errors of the residue is below a set limit. It may be noted that the selection of the expansion point magnitude \( M \) has a severe impact on the convergence rate of the iterative solver. An expansion point with \( M \) much larger than 1 will result in faster iterative solver convergence, at the cost of decreased moment matching accuracy. This characteristic results in an additional tradeoff between computational cost and accuracy for large 3D simulations. In this thesis the \( M \) is often chosen to be approximately 1.1-1.2 with a normalized residue limit of \( 10^{-3} \).

In solving (4.30), we also exploit the 2x2 block structure of \( R \) and \( F \). Let us denote the four blocks of the system matrix as

\[
(R - F) + z_l(R + F) = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}
\]  

(4.31)

where \( A_{11} \) and \( A_{22} \) are diagonal matrices. Using the Schur complement [31], we first solve for \( x_1 \) in (4.30)

\[
(A_{11} - A_{12}A_{22}^{-1}A_{21})x_1 = b_1 - A_{12}A_{22}^{-1}b_2
\]

(4.32)

and then solve for \( x_2 \)

\[
x_2 = A_{22}^{-1}(b_2 - A_{21}x_1)
\]

(4.33)

which can be done very quickly since \( A_{22} \) is diagonal. With the implementation discussed in this section, we were able to apply the proposed method to 3D simulations of practical relevance, with more than one million unknowns.
4.4.3 Computational Complexity

This section will give a short description of the individual steps of the proposed method and of their approximate computational complexity. We will define a variable TS that denotes the number of time-steps that the simulation is run. The complexity of standard FDTD is \( TS \cdot O(N) \). The proposed method may be divided into the following steps:

- **Model order reduction**: this process includes the Arnoldi iteration, orthogonalization, and projection steps that make up the MOR algorithm. The complexity of this process will be covered below for the direct and iterative linear system solvers.

- **Stability enforcement**: this process includes the singular value decomposition and stability enforcement of the reduced system and has a complexity of \( O(\tilde{N}^3) \).

- **Run time**: this process includes the time-step iterations of the reduced stability enforced system. The reduced system matrices are full due to the reduction process, leading to a complexity of \( (TS \cdot O(\tilde{N}^2)) \).

- **Overhead**: this process forms the original \( N \) sized system matrices and includes all single matrix operations used into the proposed method. These small overhead computations have complexity \( O(N) \).

When a direct solver is used inside the MOR algorithm, its computational complexity can be divided as follows:

- **LU decomposition**: the LU decomposition algorithm is used to decompose the solution matrix into lower and upper triangular matrices. There are a number of optimization of the standard LU decomposition, with the basic method having complexity \( O(N^3) \).

- **Linear system solution**: for each Arnoldi iteration, a set of linear systems must be solved to generate a new projection vector of \( \mathbf{V} \). Due to the LU decomposition, each linear system can be solved using forward and backward substitution at a complexity of \( (\tilde{N} \cdot O(N^2)) \).

- **Gram-Schmidt orthogonalization**: this step is used to orthogonalize each new projection vector of \( \mathbf{V} \) generated through the linear system solution. This operations has a total complexity of \( O(N^2) \).

We now discuss the case where an iterative solver is used to solve the linear systems required to compute the reduced model. We first define a variable CR to represent the average number of iterations for
convergence for the iterative solution solver. The cost of the model order reduction step can be thus divided into two parts:

- **Iterative linear system solution**: for each Arnoldi iteration, an iterative solver is used to generate each new projection vector. The computational cost of this process is directly related to the number of iterations required for convergence. The total complexity of this operation is \((CR \cdot \tilde{N} \cdot O(N))\).

- **Gram-Schmidt orthogonalization**: as previously mentioned, this operation has a complexity of \((O(N^2))\).

The main memory consumption of the proposed method is the storage of the \(V_1\) and \(V_2\) matrices. These two matrices are full and of combined size \(N \times \tilde{N}\) for a reduced system of size \(2\tilde{N}\).

### 4.5 Verification Test Cases

This section will demonstrate the combination of model order reduction and CFL extension through singular value perturbation. The combination of these two processes form the proposed method. Similar to Chapter 3, the test cases of this section will focus on 2D and 3D PEC cavities. PEC cavities offer simply analytical accuracy metrics in the form of resonant frequencies. The lossless nature of PEC cavities also allows for the straightforward verification of late time stability.

#### 4.5.1 2D Lossless PEC Case

This test is aimed at evaluating the impact of the model order reduction process on the accuracy and eigenvalues of the FDTD simulations. This will be evaluated using an expanded 2D PEC cavity case similar to that used in Chapter 3. This test case will also investigate the scaling of total runtime of the proposed method with respect to the reduced model size \(2\tilde{N}\) and the CFL number. Direct linear system solution using LU decomposition is used. The 1 m \(\times\) 1 m 2D cavity operates in the TM mode and is discretized into a 100 \(\times\) 100 mesh with \(\Delta x = \Delta y = \Delta = 1\) cm. A Gaussian current source with bandwidth 0.5 GHz is placed at \((x=5, y=5)\), while a probe on the \(H_z\) node is placed at \((x=95, y=95)\). The maximum \(\frac{\Delta}{\Delta}\) at 0.5 GHz is 60. The size of the full system \(N\) is 30,200 and the simulation was ran for 10,000 time-steps.

The test case was first run for various reduced order sizes to evaluate the accuracy and efficiency of the MOR process. Yee’s FDTD and the reduction algorithm at various reduced system sizes were both ran at CFL = 1. Reduced model sizes ranging from 20 to 400 were tested. Two expansion distributions
are tested: a single expansion point at $f_{\text{max}} = 0.5$ GHz and the CFH expansion of (4.29) with $L = 5$. In both cases the magnitude of the expansion $M$ is 1.1. The metric used for evaluation of accuracy is the average normalized error across all $H_z$ nodes verses standard FDTD results per time-step. Assuming that output $y_{i,j}$ and $\tilde{y}_{i,j}$ are the values of the $H_z$ nodes for the standard FDTD and reduced systems at $(x = i, y = j)$, the normalized average error across the entire domain is given by

$$E_{\text{norm}} = \frac{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} |y_{i,j} - \tilde{y}_{i,j}|}{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} |y_{i,j}|} \cdot 100\%.$$  

(4.34)

This definition evaluates the reduced system’s ability to accurately capture all simulation nodes as opposed to only the source to probe response. Figure 4.2 plots the $E_{\text{norm}}$ results as a function of time-steps ran for reduced model sizes of 20, 40, 60, 80, and 100. An accuracy bound of less than 1% normalized error across all nodes is used. It is clear that a reduced system size of 80 is necessary to accurately capture the time domain waveforms of the full simulations. For a reduced system size of 80, the maximum normalized error is less than 0.2% across all $H_z$ nodes. The reduction of the average normalized error from $2\tilde{N} = 20$ to $2\tilde{N} = 80$ is dramatic, while the accuracy appears to plateau as $2\tilde{N}$ is increased further. No accumulative time domain error is introduced due to the reduction algorithm. As the size of the reduced system is reduced, the CFH case results in superior accuracy compared to the single expansion case, although both appear to have similar accuracy at $\tilde{N} = 40$ or reduced model size 80. The runtime breakdown for the proposed algorithm from $2\tilde{N} = 80$ to $2\tilde{N} = 400$ in increments of 80 is presented in Table 4.1, while the breakdown for the stages of the MOR process is presented in Table 4.2. The $O(\tilde{N}^2)$ run time and Gram-Schmidt algorithms begin to dominate the run time of the proposed method as $\tilde{N}$ is increased. The proposed algorithm no longer has any runtime benefits over standard FDTD at $2\tilde{N} = 400$, although this is a function of the number of time-steps run. At $\tilde{N} = 40$ the runtime of the reduced model is speed-up by 69.55X from the standard FDTD results. The overall runtime of the proposed method with the MOR and stability enforcement included is still 9.64X of the FDTD runtime.

Now, we repeat the test using a time-step $\Delta t$ above the CFL limit. We use a reduced model order of 80, and consider CFL extension factors of 5, 10 and 15. The reduction process shrinks the size of the FDTD equations from $N = 30200$ to $2\tilde{N} = 80$, which is less then the 0.27% of the original size. The extraction of the 6 non-zero TM modes along with normalized error comparisons to the analytical results is presented in Table 4.3. Through performing an eigenvalue decomposition on the reduced system, 8
Figure 4.2: 2D cavity of Section 4.5.1: normalized time domain error $E_{\text{norm}}$ across all $H_z$ nodes for single and CFH expansion point case for reduced model size 20, 40, 60, 80, and 100.

Table 4.1: 2D cavity of Section 4.5.1: run time breakdown of proposed method simulation using single expansion point for reduced model size 20, 40, 60, 80, and 100 at CFL = 1. All times are in seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Reduced Size (2N)</th>
<th>Model Order Reduction</th>
<th>Stability Enforcement</th>
<th>Overhead</th>
<th>Run Time (Speed-up)</th>
<th>Total (Speed-up)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D FDTD</td>
<td></td>
<td></td>
<td></td>
<td>0.008</td>
<td>5.147</td>
<td>5.155</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>80</td>
<td>0.332</td>
<td>0.002</td>
<td>0.121</td>
<td>0.074 (69.55X)</td>
<td>0.529 (9.74X)</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>160</td>
<td>0.828</td>
<td>0.007</td>
<td>0.273</td>
<td>0.123 (41.84X)</td>
<td>1.231 (4.17X)</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>240</td>
<td>1.594</td>
<td>0.012</td>
<td>0.541</td>
<td>0.316 (16.28X)</td>
<td>2.463 (2.09X)</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>320</td>
<td>2.609</td>
<td>0.020</td>
<td>0.589</td>
<td>0.660 (7.79X)</td>
<td>3.878 (1.33X)</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>400</td>
<td>3.871</td>
<td>0.049</td>
<td>0.721</td>
<td>1.568 (3.28X)</td>
<td>6.209 (0.83X)</td>
</tr>
</tbody>
</table>

Table 4.2: 2D cavity of Section 4.5.1: run time breakdown of MOR process using direct linear solution method for reduced model size 20, 40, 60, 80, and 100. All times are in seconds.

<table>
<thead>
<tr>
<th>MOR Breakdown</th>
<th>Reduced Size (2N)</th>
<th>LU Decomposition</th>
<th>Gram Schmidt</th>
<th>Linear System Solution</th>
<th>MOR total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed (CFL=1)</td>
<td>80</td>
<td>0.115</td>
<td>0.140</td>
<td>0.077</td>
<td>0.332</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>160</td>
<td>0.115</td>
<td>0.560</td>
<td>0.153</td>
<td>0.828</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>240</td>
<td>0.115</td>
<td>1.251</td>
<td>0.228</td>
<td>1.594</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>320</td>
<td>0.115</td>
<td>2.189</td>
<td>0.305</td>
<td>2.609</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>400</td>
<td>0.115</td>
<td>3.380</td>
<td>0.376</td>
<td>3.871</td>
</tr>
</tbody>
</table>
Table 4.3: 2D cavity of Section 4.5.1: extracted resonant frequencies and normalized relative error compared to analytical values of proposed method with CFL = 1, 5, 10, 15.

<table>
<thead>
<tr>
<th>Resonant Modes</th>
<th>$TM_{0,1}$</th>
<th>$TM_{1,1}$</th>
<th>$TM_{2,0}$</th>
<th>$TM_{2,1}$</th>
<th>$TM_{2,2}$</th>
<th>$TM_{3,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Analytical</strong></td>
<td>0.149896</td>
<td>0.211985</td>
<td>0.299792</td>
<td>0.335178</td>
<td>0.423971</td>
<td>0.449689</td>
</tr>
<tr>
<td><strong>FDTD (CFL=1)</strong></td>
<td>0.149895</td>
<td>0.211985</td>
<td>0.299768</td>
<td>0.335159</td>
<td>0.423971</td>
<td>0.449611</td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>-0.0007 0</td>
<td>-0.0080 -0.0057 0</td>
<td>-0.0173</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CFL Extension Ratio = 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Proposed Method</strong></td>
<td>0.149895</td>
<td>0.211985</td>
<td>0.299768</td>
<td>0.335159</td>
<td>0.423971</td>
<td>0.449611</td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>-0.0007 0</td>
<td>-0.0080 -0.0057 0</td>
<td>-0.0173</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CFL Extension Ratio = 5</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Proposed Method</strong></td>
<td>0.149969</td>
<td>0.212197</td>
<td>0.300362</td>
<td>0.335997</td>
<td>0.425667</td>
<td>0.451624</td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>0.0487 0.0000</td>
<td>0.1901 0.2443 0.4000</td>
<td>0.4303</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CFL Extension Ratio = 10</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Proposed Method</strong></td>
<td>0.150202</td>
<td>0.212865</td>
<td>0.302270</td>
<td>0.338668</td>
<td>0.431200</td>
<td>0.458291</td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>0.2041 0.4151</td>
<td>0.8266 1.0412 1.7051</td>
<td>1.9129</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CFL Extension Ratio = 15</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Proposed Method</strong></td>
<td>0.150594</td>
<td>0.213988</td>
<td>0.305587</td>
<td>0.343401</td>
<td>0.441407</td>
<td>0.470703</td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>0.4657 0.9449</td>
<td>1.9330 2.4533 4.1125</td>
<td>4.6730</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Conjugate pairs are found to be below $f_{max}$. The values of these eigenvalues are outlined in Table 4.4 for various CFL values. In addition to the first 6 non-zero TM modes, the $TM_{0,0} = 0$ GHz and $TM_{3,1} = 0.47395$ GHz harmonics have also been captured. The data of Table 4.4 shows that each eigenvalue of the reduced model corresponds to a resonance frequency of the cavity. The resonance frequencies extracted from the simulation results match accurately the exact value calculated from the analytical formula for any CFL value. These results may be viewed as a testament to the accuracy of the proposed reduction and CFL extension method. The run time breakdown for the proposed method at CFL = 1, 5, 10, and 15 is presented in Table 4.5. Due to the CFL extension, a fraction of the reduced system size 2$\tilde{N}$ will be perturbed during the stability enforcement process. The reduced system size is given as a fraction of the stable singular values identified by the MOR algorithm over the total reduced system size. The final reduced system size remains 2$\tilde{N} = 80$. As the time-step is increased from CFL = 1 to 15, the speed-up of the reduced model improved from 69.55X to 1029.40X, roughly proportional to the increase in CFL. Taking into account the total runtime of the reduction and stability enforcement process, the overall speed-up increases from 9.74X to 11.23X. The frequency domain waveform and normalized error of the extracted resonant frequencies compared to analytical values has been included in Figure 4.3 and Figure 4.4. Compared to the 2D cavity test case of Chapter 3, equal increases in the CFL extension ratio results in a lower introduced numerical dispersion error. This may be attributed to the 5X increase in the $\frac{\lambda}{\Delta}$ ratio.
Table 4.4: 2D cavity of Section 4.5.1: the 8 eigenvalues from DC to $f_{max} = 0.5 \ GHz$ of the reduced system mapped to physical frequencies and compared with extracted simulations results at CFL = 1, 5, 10, 15.

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Analytical Frequency</th>
<th>Simulation</th>
<th>Eigenvalue</th>
<th>Analytical Frequency</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00000+j0.00000</td>
<td>0</td>
<td>-</td>
<td>1.00000+j0.00000</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>0.9975+j0.02221</td>
<td>0.14989</td>
<td>0.14990</td>
<td>0.99383+j0.11090</td>
<td>0.14997</td>
<td>0.14997</td>
</tr>
<tr>
<td>0.9951+j0.03141</td>
<td>0.21199</td>
<td>0.21199</td>
<td>0.98766+j0.15659</td>
<td>0.21220</td>
<td>0.21220</td>
</tr>
<tr>
<td>0.99901+j0.04441</td>
<td>0.29977</td>
<td>0.29977</td>
<td>0.97533+j0.22073</td>
<td>0.30036</td>
<td>0.30036</td>
</tr>
<tr>
<td>0.9987+j0.04965</td>
<td>0.33517</td>
<td>0.33516</td>
<td>0.96917+j0.24641</td>
<td>0.33600</td>
<td>0.33600</td>
</tr>
<tr>
<td>0.99803+j0.06279</td>
<td>0.42397</td>
<td>0.42397</td>
<td>0.95067+j0.31021</td>
<td>0.42566</td>
<td>0.42567</td>
</tr>
<tr>
<td>0.99778+j0.06658</td>
<td>0.44961</td>
<td>0.44961</td>
<td>0.94452+j0.32844</td>
<td>0.45163</td>
<td>0.45162</td>
</tr>
<tr>
<td>0.99753+j0.07018</td>
<td>0.47395</td>
<td>-</td>
<td>0.93836+j0.34567</td>
<td>0.47632</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4.5: 2D cavity of Section 4.5.1: run time breakdown of proposed method simulation with reduced model size 80 and CFL = 1, 5, 10, 15. All times are in seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Stable/Reduced Size ($2N$)</th>
<th>Model Order Reduction</th>
<th>Stability Enforcement</th>
<th>Overhead</th>
<th>Run Time (Speed-up)</th>
<th>Total (Speed-up)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D FDTD</td>
<td>0.008</td>
<td>5.147</td>
<td>5.155</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Proposed</td>
<td>80/80</td>
<td>0.332</td>
<td>0.002</td>
<td>0.121</td>
<td>0.074 (69.55X)</td>
<td>0.529 (9.74X)</td>
</tr>
<tr>
<td>(CFL=1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Proposed</td>
<td>66/80</td>
<td>0.332</td>
<td>0.002</td>
<td>0.121</td>
<td>0.015 (343.13X)</td>
<td>0.470 (10.96X)</td>
</tr>
<tr>
<td>(CFL=5)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Proposed</td>
<td>52/80</td>
<td>0.332</td>
<td>0.002</td>
<td>0.121</td>
<td>0.007 (725.38X)</td>
<td>0.462 (11.16X)</td>
</tr>
<tr>
<td>(CFL=10)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Proposed</td>
<td>36/80</td>
<td>0.332</td>
<td>0.002</td>
<td>0.121</td>
<td>0.005 (1029.40X)</td>
<td>0.459 (11.23X)</td>
</tr>
<tr>
<td>(CFL=15)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.3: 2D cavity of Section 4.5.1: frequency domain waveform for reduced model size 80 at CFL = 1, 5, 10, 15.

Figure 4.4: 2D cavity of Section 4.5.1: normalized error of extracted resonant frequencies for reduced model size 80 at CFL = 1, 5, 10, 15.
4.5.2 3D Lossless PEC Case

In this section, we consider a 3D cavity. This test case will illustrate the runtime characteristics of the proposed algorithm when an iterative solver is applied instead of the LU decomposition. The simulation domain is an empty $1 \text{m} \times 1 \text{m} \times 1 \text{m}$ cavity terminated on all sides with PEC walls. The cavity is discretized into a $100 \times 100 \times 100$ mesh with $\Delta x = \Delta y = \Delta z = \Delta = 1 \text{cm}$, resulting in a full system size $N$ of 6,120,600. A Gaussian voltage source with bandwidth $0.5 \text{GHz}$ is placed at $(x=5, y=5, z=5)$, while a probe on the $E_z$ node is placed at $(x=95, y=95, z=95)$. The maximum $\lambda/\Delta$ at 0.5 GHz is 60. Five expansion points are distributed using (4.29) using $M = 1.1$ and $L = 5$. A reduced system size $2\tilde{N}$ of 120 is used. Recall that it takes $\frac{\tilde{N}}{2}$ linear system solutions of size $N$ to generate a final reduced system of size $2\tilde{N}$. The memory consumption of storing the $V$ projection vector is $N \times \tilde{N}$. Assuming 8 bytes per matrix entry, the peak memory consumption of storing the $V$ projection matrix is approximately 2.736 gigabytes. When combined with additional requirements from smaller matrices and additional external program overheads, the memory requirements of this test case is near the maximum allowed for a modern work station. The simulation was ran for 10,000 time-steps at CFL = 1, 5, 10, and 15. The residue limit for the iterative conjugate gradient solver is $10^{-3}$.

The resonant frequency accuracy metric is again used, where the resonant frequencies for a 3D PEC cavity are given by

$$f_{n_x,n_y,n_z} = \frac{c}{2} \sqrt{\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2 + \left(\frac{n_z}{L_z}\right)^2}$$  (4.35)

where $n_x, n_y, n_z$ are the resonant modes and $L_x, L_y, L_z$ are the side lengths of the cavity which are all 1 m. The lowest resonance frequencies are $f_{1,1,0} = 0.21199$, $f_{1,1,1} = 0.25963$, $f_{2,1,0} = 0.33518$, $f_{2,1,1} = 0.36717$, $f_{2,2,0} = 0.42397$, and $f_{2,2,1} = 0.44969 \text{GHz}$. The extracted frequency domain results and normalized resonant frequency errors are presented in Figure 4.5. The proposed method at CFL = 1 accurately converges to the standard FDTD results at the same time-step. The proposed method for CFL = 5, 10, and 15 are slightly offset from the standard FDTD results due to the introduction of numerical dispersion errors. It may be noted from Figure 4.3 and Figure 4.4 that the numerical dispersion errors of the 3D cavity case is less than that of the 2D case using the same spatial discretization and CFL ratio. This is consistent with the observations on the numerical dispersion behaviour in Section 2.3.

The run time breakdown for the proposed method at CFL = 1, 5, 10, and 15 is presented in Table 4.6. Similar to the previous example, the reduced system size is given as a fraction of stable and total reduced system size, with the final stable system having size $2\tilde{N} = 120$ in all cases. The breakdown for the MOR process is outlined in Table 4.7. The reduced system has been reduced to less than 0.002% of the original simulation size. Due to the dramatic reduction ratio, the runtime of the reduced model...
is completely negligible compared to the run time of the overall proposed method and standard FDTD. The runtime of the reduced model has an overall speed-up of 14218X at CFL = 1 and increases 210428X at CFL = 15. When taking into account the total proposed algorithm runtime, the very impressive numbers fall to a more modest but still useful speed-up of approximately 4.28X. The extension of the CFL limit on the reduced model has very little impact on overall runtime. It may be seen from the breakdown of the MOR process that the majority of the total runtime is taken by the iterative linear solution solver.
Table 4.7: 3D cavity of Section 4.5.2: execution time breakdown for model order reduction process. All times are in seconds.

<table>
<thead>
<tr>
<th>MOR Breakdown</th>
<th>Average Iterations to Converge</th>
<th>Gram Schmidt linear system solution</th>
<th>MOR total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed (All CFL)</td>
<td>42.65</td>
<td>687.599</td>
<td>716.18</td>
</tr>
</tbody>
</table>

4.6 Summary

This Chapter introduces the application of model order reduction and system level CFL extension on the explicit FDTD equations, something not achieved in the existing literature. The main contributions include the casting of FDTD equations into a form compatible with the Krylov subspace projection method and the deriving of a set of stability enforcement procedures. This chapter also outlines the accuracy and implementation optimizations to the Arnoldi subspace generation process when applied to the discrete FDTD system. Using the SPRIM technique, the reduction process maintains the structure and the reciprocity of the FDTD equations. For a time-step below the CFL limit, the reduction process preserves the stability of the full model by construction, which is a novel theoretical result. For unstable CFL values, stability may be enforced through limiting the singular values of the spatial difference matrix. The combination of model order reduction and stability enforcement forms the proposed CFL extension technique. The proposed method has been applied to 2D and 3D PEC cavity test cases to evaluated accuracy and runtime characteristics. The original simulation may be reduced to < 1% of the original system size without sacrificing accuracy across all simulation nodes. The run-time of the reduced system is accelerated by over 1000X compared to standard FDTD, although this is somewhat offset by the runtime of the reduction algorithm. The late time stability of the reduced system has been verified. The key theoretical contribution of this chapter is that FDTD simulation may be reduced to a fraction of their full system size with minimum impacts on overall accuracy. The introduced model order reduction algorithm is simply one of many possible choices. The reduced model may be efficiently perturbed to enforce stability at unstable CFL values. Chapter 5 will apply the proposed reduction and stability enforcement method to more practical FDTD simulations.
Chapter 5

Proposed CFL Extension Technique: Test Cases

Chapter 3 and Chapter 4 have focused on the impact of the MOR and stability enforcement process on overall accuracy, as well as the runtime characteristics of the proposed method. As a result, the main utilized test cases were 2D and 3D lossless PEC cavities. The lossless PEC test case allows for the demonstration of late time stability and allows the use of analytical resonances as a metric of accuracy. This Chapter will focus on the application of the proposed method to practical 2D and 3D FDTD simulations. The test cases will demonstrate the utility of the proposed method in the extraction of time domain waveform shapes and frequency domain scattering parameters.

5.1 2D Test Case: Waveguide Structure with PEC Irises

The first example is a 2D waveguide filter operating in the TM mode. This test case is used to demonstrate the proposed method’s efficiency in reducing high Q resonating structures containing inhomogeneous lossy materials. The main accuracy metric is the extracted transmission coefficient of the waveguide structure. In addition, this test case will introduce simulation domain termination using matched conductivities. This waveguide test case represents a common passband filter structure.

The waveguide is of size 5 cm × 50 cm and is discretized into a 40 × 400 mesh with Δx = Δy = ∆ = 1.25 mm. The layout of the waveguide is shown in Fig. 5.1. A Gaussian current line source with bandwidth of 3 GHz is placed at one end of the waveguide at y = 1 cm, while a line probe is placed on the other end at y = 4 cm. The waveguide is filled with a dielectric material with ε_r = 2. Five
irises (length: 1.25 cm, aperture size: 1 cm, separation: 5 cm) are evenly placed within the waveguide. The waveguide is terminated at both ends on a 4th-order matched absorber with thickness of 5 cells. A matched absorber utilizes graded conductivity values to minimize reflections at an interface, effectively giving the effect of infinite propagation. For a 5 cell matched absorber, the electric conductivity values used are

\[
\sigma_{e_i} = -\frac{(m+1) \ln[R]}{2} \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{L \Delta x} \left( \frac{i}{L} \right)^m \quad \text{for} \quad m = 4, \quad R = e^{-8}, \quad L = 5, \quad \text{and} \quad i = 1 \ldots L \quad (5.1)
\]

where \(m\) is the order of the absorber, \(R\) is the reflection coefficient, and \(L\) is the length of the absorber. The magnetic conductivity values also utilize a similar form with a factor of \(\frac{\mu}{\varepsilon}\). A matched absorber is easily implemented by stamping the conductivity values in to the matrices \(D_{\sigma_e}\) and \(D_{\sigma_m}\) of (2.3). The main drawback of a matched absorber is the increase in reflections at non-normal incidence, which is resolved in the uni-axial perfectly matched layer (UPML) case. UPMLs are the standard termination method for FDTD simulations. UPMLs were not implemented due to the requirement of introducing auxiliary dispersion equations, an extension not covered in this thesis. For a maximum frequency of interest of 3 GHz and \(\Delta = 1.25\) mm, the resulting minimum \(\frac{\lambda}{\Delta}\) ratio is 80. The original system size is \(N = 48,440\), and the size of the reduced model generated with the proposed algorithm is \(2\tilde{N} = 200\). A single expansion point of magnitude \(M = 1.1\) is placed at \(z = 1.1\). FDTD and the proposed technique were ran for 20,000 timesteps, in order to allow for the majority of the input power to dissipate in the structure. LU decomposition was used to solve the linear systems necessary to compute the reduced model. The proposed method was ran with CFL = 1, 3, 6, and 9.

Figure 5.2 shows the simulation results for both standard FDTD and the proposed method were ran at and above the CFL limit. Excellent convergence in the time and frequency results may be observed. The reduction algorithm accurately captures the high Q resonating structure and matched absorber termination. The impact of the accumulating time domain numerical dispersion error is mitigated.
5.2 3D Test Case: Slots on a PEC Screen

The proposed method is applied to the focusing PEC screen structure first proposed in [32] and subsequently investigated using FDTD in [33]. Both single and three slit structures were investigated in [33]. It was found in the three slit case that a spatial resolution of less than 0.1 mm around each slit is required to accurately replicate the three slot focusing phenomenon. The previous 3D cavity example from Chapter 4 demonstrated the current maximum problem size of the proposed method. Due to the current memory limitations of the proposed algorithm, only the single slit case has been implemented.
Table 5.1: Waveguide of Section 5.1: execution time breakdown for Yee’s FDTD and the proposed method at refined CFL numbers. All times are in seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Stable/Reduced Size (2N)</th>
<th>Model Order Reduction</th>
<th>Stability Enforcement</th>
<th>Overhead</th>
<th>Run Time (Speed-up)</th>
<th>Total (Speed-up)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D FDTD</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.012</td>
<td>34.531</td>
<td>34.543</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>200/200</td>
<td>1.734</td>
<td>0.008</td>
<td>0.726</td>
<td>0.399 (84X)</td>
<td>2.867 (12.05X)</td>
</tr>
<tr>
<td>Proposed (CFL=3)</td>
<td>186/200</td>
<td>1.734</td>
<td>0.008</td>
<td>0.732</td>
<td>0.130 (265X)</td>
<td>2.598 (13.29X)</td>
</tr>
<tr>
<td>Proposed (CFL=6)</td>
<td>164/200</td>
<td>1.734</td>
<td>0.008</td>
<td>0.730</td>
<td>0.064 (539X)</td>
<td>2.532 (13.64X)</td>
</tr>
<tr>
<td>Proposed (CFL=9)</td>
<td>144/200</td>
<td>1.734</td>
<td>0.008</td>
<td>0.721</td>
<td>0.047 (734X)</td>
<td>2.515 (13.73X)</td>
</tr>
</tbody>
</table>

Table 5.2: Waveguide of Section 5.1: execution time breakdown for model order reduction process. All times are in seconds.

<table>
<thead>
<tr>
<th>MOR Breakdown</th>
<th>LU Decomposition</th>
<th>Gram Schmidt</th>
<th>Linear System Solution</th>
<th>MOR total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed (All CFL)</td>
<td>0.150</td>
<td>1.276</td>
<td>0.308</td>
<td>1.734</td>
</tr>
</tbody>
</table>

Figure 5.3 shows the physical layout of the single slit focusing structure. This test case involves the transmission of a plane wave through a metallic screen with a central slot for focusing onto an image plane. The 3D simulation domain is of size $60 \times 60 \times 60$ with $\Delta x = \Delta y = \Delta z = 0.3 \text{ mm}$, and is terminated on all sides with 4th-order, 5-cell matched absorbers. A plane of uniform sinusoidal sources at 10 GHz is placed on one side of the PEC screen at a distance of $0.15\lambda$ ($z = 15$) to replicate an incident plane wave. The sinusoidal sources are placed on the $E_y$ nodes of a region outside the matched absorber. The region of the sources is 50 x 50 cells wide. The PEC screen lies on the $x$-$y$ axis at $z = 30$ and is 1 cell thick. The PEC condition is imposed on the $E_x$ and $E_y$ nodes at $z = 30$. The PEC screen extends into the matched absorber region. The screen has a single focusing slot of size $13.2 \text{ mm} \times 1.2 \text{ mm}$. Probes are placed on the $E_y$ at other side of the screen along the centre axis of the image plane, at a distance of $0.15\lambda$ from the screen ($x = 30, z = 45$). A very high $\frac{\lambda}{\Delta}$ ratio of 100 is required due to the resonating nature of the structure and the required spatial resolution to capture all fringing fields around the PEC slot. The fine mesh makes the size of the original FDTD equations quite high ($N = 1,361,886$). Due to the single-frequency excitation, a single expansion point is used, given by

$$z_0 = Me^{-j2\pi f_{max} \Delta t},$$

with $M = 1.2$ and $f_{max} = 10 \text{ GHz}$. The proposed method was used to generate a reduced model of order 40 and simulations were ran for 10,000 time-steps until a steady state was reached on the image.
Chapter 5. Proposed CFL Extension Technique: Test Cases

Figure 5.3: Focusing PEC screen of Section 5.2: simulation layout

plane. The absolute values of the $E_y$ nodes on the image plane at ($z=45$) are averaged from 5,000 to 10,000 time-steps. The averaged magnitudes at each $E_y$ node form the steady state waveform at the image plane. Due to the large problem size, the MOR process utilizes the iterative CGS linear system solver with residue limit $10^{-3}$. The proposed method was ran with CFL = 1, 3 and 5.

Fig. 5.4 compares the electric field on the image plane calculated with the proposed method and Yee’s FDTD. Using interpolation in space, Yee’s FDTD and the proposed method at all CFL values generated a half-beamwidth width of approximately 8.96 mm. Table 5.3 shows the simulation time breakdown for standard FDTD and the proposed method, while the timing results for the MOR step is shown in Table 5.4. The reduction process reduces the simulation run time to less than 0.1% of Yee’s FDTD. The overall speed-ups of the proposed method range between 7.54X-7.56X for the tested CFL values. The run time of the MOR process occupies over 90% of the proposed method, while the iterative conjugate gradient squared (CGS) solutions took up over 96% of the MOR process runtime with an average of 32.1 iterations to convergence. In this case, the extension of the CFL limit has a small influence on the total solution time for the proposed method, since the reduction step dominates the solution of the reduced model due to the fairly large size of the problem. However, the acceleration of the runtimes are proportional to the CFL extension ratio from 2226X to 11131X.
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Figure 5.4: Focusing PEC screen of Section 5.2: averaged time domain $E_y$ electric field nodes at image plane $0.15\lambda \ (x=30, \ z=45)$ from focusing PEC screen for Yee’s FDTD at CFL = 1 and proposed method with CFL = 1, 3, and 5.

Table 5.3: Focusing PEC screen of Section 5.2: execution time breakdown for Yee’s FDTD and the proposed method at refined CFL numbers. All times are in seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Stable/Reduced Size ($2N$)</th>
<th>Model Order Reduction</th>
<th>Stability Enforcement</th>
<th>Overhead</th>
<th>Run Time (Speed-up)</th>
<th>Total (Speed-up)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D FDTD</td>
<td></td>
<td></td>
<td></td>
<td>3.244</td>
<td>545.453</td>
<td>548.697</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>80/80</td>
<td>67.765</td>
<td>0.003</td>
<td>4.720</td>
<td>0.245 (2226X)</td>
<td>72.733 (7.54X)</td>
</tr>
<tr>
<td>Proposed (CFL=3)</td>
<td>72/80</td>
<td>67.765</td>
<td>0.003</td>
<td>4.720</td>
<td>0.082 (6651X)</td>
<td>72.570 (7.56X)</td>
</tr>
<tr>
<td>Proposed (CFL=5)</td>
<td>64/80</td>
<td>67.765</td>
<td>0.003</td>
<td>4.720</td>
<td>0.049 (11131X)</td>
<td>72.537 (7.56X)</td>
</tr>
</tbody>
</table>

Table 5.4: Focusing PEC screen of Section 5.2: execution time breakdown for model order reduction process. All times are in seconds.

<table>
<thead>
<tr>
<th>MOR Breakdown</th>
<th>Average Iterations to Converge</th>
<th>Gram Schmidt</th>
<th>Linear System Solution</th>
<th>MOR total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed (All CFL)</td>
<td>32.1</td>
<td>2.114</td>
<td>65.651</td>
<td>67.765</td>
</tr>
</tbody>
</table>
5.3 3D Test Case: Microstrip Filter Structure

The proposed method is applied to a 3D multi-port microstrip filter from [34]. This test case demonstrates the proposed method’s accuracy for 3D multi-port structures in both time frequency. In addition to port to port responses, all nodes within the simulation domain may be accurately captured using a significantly reduced model. Figure 5.5 shows the physical layout of the microstrip filter structure. The simulation domain is of size $80 \times 90 \times 14$ cells, with $\Delta x = \Delta y = 0.4\text{ mm}$ and $\Delta z = 0.2\text{ mm}$, and is terminated on 5 sides with 4th-order, 5-cell matched absorbers. The 6th side is the PEC ground plane of the microstrip. A PEC microstrip rests on a dielectric substrate with $\epsilon_r = 2$ and thickness of 3 cells. The PEC microstrip lies on the $x$-$y$ plane at $z = 3$ and is 7-cells wide (2.8 mm) and 1 cell (0.2 mm) thick. Both the PEC microstrip and dielectric slab extends into the matched absorber. The physical structure and dielectric material properties determine the reflection and transmission coefficients of the filter. A line probe and source are placed at the two ends of the microstrip on the $E_z$ nodes. A Gaussian pulse of $f_{\text{max}} = 20$ GHz bandwidth is used as excitation to extract the $S_{21}$ and $S_{11}$ parameters, resulting in a $\frac{\lambda}{\Delta}$ ratio of 26.49. A single FDTD simulation with a straight microstrip line was first run to extract the transmitted waveform. The size of the original FDTD equations is $N = 619,164$. A reduced model of order 100 was generated using 5 expansion points evenly distributed from DC to 20 GHz with $M = 1.2$. Simulations were ran for 5,000 timesteps, when most of the input power was dissipated. Similar to the previous example, the MOR process utilizes the iterative CGS linear system solver with residue limit $10^{-3}$. The proposed method was ran with CFL = 1, 3 and 5.

Figure 5.6 depicts the time domain reflected and transmitted waveforms, while Figure 5.7 plots the $S_{11}$ and $S_{21}$ parameters extracted from the time domain analysis. For all CFL cases the time and frequency domain results of the proposed method converge to those of Yee’s FDTD at CFL = 1. These results further demonstrate the excellent accuracy of the proposed technique and its stable behavior even at time-steps significantly higher than the CFL limit. Table 5.5 shows the simulation time breakdown for standard FDTD and the proposed method, while the timing results for the MOR step is shown in Table 5.6. A speed-up of 2.334X over standard FDTD may be observed. A similar conclusion as from Section 5.2 may be drawn, where the proposed trades a large MOR runtime for negligible actual simulation runtime. The iterative CGS solution took up over 83% of the MOR process runtime with an average of 24.16 iterations to convergence. Figure 5.8 shows a snapshot of the $E_z$ nodes on the microstrip ($z = 4$) at 500 and 1000 time-steps for Yee’s FDTD and the proposed method at CFL = 1. The propagation of the incident wave on the PEC microstrip is clearly visible in both cases, while the attenuation within the matched absorber is also accurately captured. This example demonstrates that
Table 5.5: Microstrip filter of Section 5.3: execution time breakdown for Yee’s FDTD and the proposed method at refined CFL numbers. All times are in seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Stable/Reduced Size ($2N$)</th>
<th>Model Order Reduction</th>
<th>Stability Enforcement</th>
<th>Overhead</th>
<th>Run Time (Speed-up)</th>
<th>Total (Speed-up)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D FDTD</td>
<td></td>
<td></td>
<td></td>
<td>1.947</td>
<td>139.747</td>
<td>141.694</td>
</tr>
<tr>
<td>Proposed (CFL=1)</td>
<td>100/100</td>
<td>57.45</td>
<td>0.005</td>
<td>0.893</td>
<td>0.303 (461X)</td>
<td>60.701 (2.334X)</td>
</tr>
<tr>
<td>Proposed (CFL=3)</td>
<td>84/100</td>
<td>57.45</td>
<td>0.005</td>
<td>0.893</td>
<td>0.100 (1397X)</td>
<td>60.498 (2.342X)</td>
</tr>
<tr>
<td>Proposed (CFL=5)</td>
<td>72/100</td>
<td>57.45</td>
<td>0.005</td>
<td>0.893</td>
<td>0.062 (2253X)</td>
<td>60.460 (2.343X)</td>
</tr>
</tbody>
</table>

the reduced model of less than 0.02% of the full system size is able to accurately capture the information across all nodes of the simulation domain, as opposed to only the port to port responses. The average error across all $E_z$ nodes between standard FDTD and the reduced model in Figure 5.8 is less than 0.3%.
Figure 5.6: Microstrip filter of Section 5.3: transmitted and reflected waveforms on $E_z$ probes for Yee’s FDTD at CFL = 1 and proposed method at CFL = 1, 3, and 5.

Table 5.6: Microstrip filter of Section 5.3: execution time breakdown for model order reduction process. All times are in seconds.

<table>
<thead>
<tr>
<th>MOR Breakdown</th>
<th>Average Iterations to Converge</th>
<th>Gram Schmidt</th>
<th>Linear System Solution</th>
<th>MOR total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed (All CFL)</td>
<td>24.16</td>
<td>7.787</td>
<td>47.929</td>
<td>57.45</td>
</tr>
</tbody>
</table>
Figure 5.8: Microstrip filter of Section 5.3: waveform across $E_z$ nodes on microstrip $x$-$y$ plane ($z = 4$) at 500 and 1000 time-steps for Yee’s FDTD and proposed method at CFL = 1.
5.4 Summary

This chapter presented 3 test cases that demonstrate the proposed method’s accuracy when applied to practical FDTD simulation cases. The reduction algorithm is able to accurately capture the time and frequency domain responses of resonating and lossy structures. In addition to the source to probe responses, the proposed method is also able to accurately capture the shapes of the propagating waveform across all simulation nodes. A reduction in size to less than 0.2% of the full system size has been achieved in the 3D test cases. When combined with CFL extension, the runtime of the reduced models present a speed-up factor of over 1000X with respect to original FDTD. However, the inclusion of the reduction and stability enforcement process lowers the speed-up factor to a more modest 3X-5X. Chapter 6 will introduce the FDTD sub-gridding technique for local mesh refinement. In this application the reduction and stability enforcement process is applied to only a fine mesh region of the overall simulation.
Chapter 6

Proposed CFL Extension Technique: Application to FDTD Sub-gridding

In this chapter the proposed method is combined with the FDTD sub-gridding technique. The FDTD sub-gridding method utilizes different cell sizes across the simulation domain to increase the spatial resolution where required. Typically, one has fine grids in selected portions of the simulation domain where small geometrical details are present, and a coarse grid elsewhere. Unfortunately, the CFL limit of the entire simulation is the CFL limit of the finest mesh, which is the most constraining. This issue can severely limit the computational efficiency of FDTD sub-gridding, unless different time steps are used in the different meshes. However, using multiple time-steps require the introduction of time interpolation at different mesh interfaces. This leads to additional implementation steps while introducing small time interpolation errors. In this Chapter, we show how the proposed method for extending the CFL limit can be used to circumvent this issue. Our main idea is the following: prior to running the entire simulation, the FDTD equations for each fine grid are processed with the method of Chapter 4 in order to extend their CFL limit. Then, the reduced models for the fine grids are instantiated into the main simulation. Having extended the CFL limit for the fine grids, the whole simulation will not be constrained by the CFL limit of the fine grids, as in standard sub-gridding. For comparison purposes the proposed method will be benchmarked against standard FDTD with uniform fine cell size, the standard FDTD sub-gridding technique, and an implicit CFL extension sub-gridding method. The contents of this chapter is an extension of the work published in [16] and consist mainly of the preliminary results of ongoing research. Due to time constraints, only the two dimensional case will be considered. The current obstacles and limitations of the current formulation will be discussed in detail. The proposed CFL extension method
provides improved computational speed-ups over the examples of Chapter 4 due to the unique CFL and memory constraints of the FDTD sub-gridding technique.

6.1 The FDTD Sub-gridding Technique

The standard FDTD techniques utilizes a uniform rectangular spatial mesh for the full simulation domain. This discretization results in a uniform CFL limit for all simulation cells, allowing for the use of a uniform CFL ratio of throughout. The CFL = 1 ratio minimizes the numerical dispersion errors throughout the simulation domain according to (2.10). In order to increase spatial resolution, it is necessary to decrease the spatial discretization size across the full simulation domain. This has significant negative consequences for both computational cost and memory requirements. The finite spatial resolution results in a tradeoff between spatial approximation errors and computation costs.

Methods of locally increasing spatial resolution while minimizing computation impacts include the non-uniform and sub-gridding mesh refinement methods. Non-uniform and sub-gridding methods maintain the rectangular mesh structure of standard FDTD while splitting the simulation domain into coarse and fine cell regions. In this chapter we define a grid refinement variable GR that specifies the ratio between fine and coarse mesh sizes. For a full domain simulation, the per time-step memory and computation cost scale by $O(GR^2)$ and $O(GR^3)$ for 2D and 3D mesh refinement, while the maximum stable time-step $\Delta t$ scales by $\frac{1}{GR}$. In Figure 6.1 a sample layout for a uniform mesh, a non-uniform mesh, and a mesh with sub-gridding is illustrated. The sub-gridding mesh diagram of Figure 6.1 has a grid refinement of GR = 2. Both methods utilize local fine cell sizes where required while maintaining a coarse mesh in most of the simulation domain, in order to reduce memory usage and CPU time.

Both methods attempt to alleviate the per time-step memory and computational cost increases of full domain mesh refinement. In both cases the maximum stable time-step is constrained by the finest cell size. Non-uniform mesh refinement utilizes a gradual and often logarithmic decrease of cell sizes across the simulation domain. The use of a non-uniform meshing disturbs the accuracy of the centred finite difference approximation. FDTD sub-gridding utilizes discontinuous cell sizes for coarse and fine simulation domains. The domains are connected using interpolation and extrapolation in space. When running at the fine mesh CFL limit, the fine cell regions will be run with CFL = 1 and maintain minimum numerical dispersion errors. The coarse cells will be run with CFL = $\frac{1}{GR}$ and introduce additional numerical dispersion errors as per (2.10). In general, the FDTD sub-gridding method achieves superior accuracy and memory efficiency to the non-uniform mesh refinement method. It must be noted however, that the non-uniform mesh is much easier to implement than the sub-gridding case, requiring only a
change of the $\Delta x$, $\Delta y$, and $\Delta z$ values across the domain.

There have been numerous previous publications investigating the accuracy and stability of the FDTD sub-gridding technique [7, 8, 35, 36]. A well known stability criteria is that the FDTD sub-gridding scheme is stable if and only if

1. the updates of the fine and coarse mesh nodes at the boundary is reciprocal [35],

2. the time-step satisfies the CFL limit of the fine mesh [7].

The examples of this thesis will focus on the 2D transverse magnetic FDTD sub-gridding simulation setup as illustrated in [35]. Although there are numerous valid connection schemes, this chapter will utilize the coarse electric and fine magnetic connection scheme as illustrated in Figure 6.2 [35]. At each time-step the electric field on the boundary nodes of the coarse cell are extrapolated to update the magnetic nodes in the fine grid. At the alternate half-step the magnetic field on the boundary nodes of the fine cell are interpolated to update the electric nodes in the coarse grid. The connection between coarse and fine mesh regions will be covered in more detail in Section 6.2.1. This implementation utilizes a simple linear interpolation scheme and represent the “stable and accurate” connection scheme proposed in [35]. The boundary connection utilizes the magnetic nodes in the fine cell at the same assumed position as coarse cell magnetic node locations. A visual representation is presented in Figure 6.2. The boundaries of the fine mesh simulation domain are terminated using PEC walls according to the FDTD sub-gridding scheme presented in [7, 8, 35]. This implementation allows for the straightforward and reciprocal connection of coarse and fine mesh regions. For a sub-grid of $N_x$ and $N_y$ coarse cells along each axis, the number of electric and magnetic nodes in the fine mesh for any grid refinement ratio $GR$ is given in Table 6.1. For simplicity, only odd $GR$ values are implemented within the test cases.

The sources and probes of the simulation may be applied in both coarse and fine mesh regions. The
Figure 6.2: Connection scheme at straight and corner boundary between coarse and fine meshes. Solid arrows indicate simulation node locations. Dashed arrows indicate the reciprocal interpolation and extraction procedure. The coloured regions indicate the fine mesh $H_z$ nodes used for the update of coarse mesh $E_x$ and $E_y$ nodes.
Table 6.1: Size of $E_x$, $E_y$, and $H_z$ fine cell sub-grid mesh sizes as a function of $N_x$ and $N_y$ coarse cell sizes and grid refinement ratio $GR$.

<table>
<thead>
<tr>
<th>Node Type</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_x$</td>
<td>$(N_x \times GR) \times (N_y \times GR - 1)$</td>
</tr>
<tr>
<td>$E_y$</td>
<td>$(N_x \times GR - 1) \times (N_y \times GR)$</td>
</tr>
<tr>
<td>$H_z$</td>
<td>$(N_x \times GR) \times (N_y \times GR)$</td>
</tr>
</tbody>
</table>

operations associated with the sources and probes are performed during the updates of the associated nodes. We provide here a short summary of the per time-step operations for the FDTD sub-grid:

At time-step $n$:

- Update the coarse mesh electric field nodes as in standard FDTD using coarse mesh magnetic field nodes. Update the coarse mesh $E_x$ and $E_y$ nodes at the boundary using extrapolation from the fine mesh $H_z$ nodes according to Figure 6.2.

- Update the fine mesh electric field nodes as in standard FDTD using fine mesh magnetic field nodes. No interfacing with coarse mesh boundary cells are required.

- Apply coarse and fine mesh electric field sources and probes.

At time-step $n + \frac{1}{2}$:

- Update the coarse mesh magnetic field nodes as in standard FDTD using coarse mesh electric field nodes. No interfacing with fine mesh boundary cells are required.

- Update the fine mesh magnetic field nodes as in standard FDTD using fine mesh electric field nodes. Update the fine mesh $H_z$ nodes at the boundary using interpolation from the coarse mesh $E_x$ and $E_y$ nodes according to Figure 6.2.

- Apply coarse and fine mesh magnetic field sources and probes.

It must be noted that the operations for fine and coarse mesh updates at each half-step are not dependent upon each other and may be performed in an arbitrary order. The leap-frog update scheme of standard FDTD is preserved. The interpolation and extrapolation schemes must be reciprocal to maintain overall stability [7, 8].

While more computationally efficient than using an uniform fine mesh simulation, sub-gridding has also some drawbacks in terms of efficiency and accuracy. The FDTD sub-gridding techniques introduce two factors impacting overall computational speed when compared to a uniform coarse mesh simulation. The first is the reduction of the maximum allowed time-step for the whole simulation to the CFL limit of the fine grid. Relative to the time-step of the coarse grid, the time-step is reduced by $GR$,
Chapter 6. Proposed CFL Extension Technique: Application to FDTD Sub-gridding

The grid refinement ratio. The second factor is the increase in number of unknowns due to the grid refinement. Although the increase is moderate, since refinement is only applied locally, it still leads to an increased computational cost per time-step. In addition to computational impacts, additional numerical dispersion errors are also introduced due to the use of a fine time-step. Recall from the numerical dispersion characteristics of (2.10) and Figure 2.1 that numerical dispersion errors are minimized at CFL = 1 for any mesh size. The reduced time-step results in an effective CFL of \( \frac{1}{GR} \) in the coarse mesh, resulting in additional numerical dispersion errors when compared to an unrefined simulation. Finally, the interpolation/extrapolation operations performed at the interface between fine and coarse mesh also introduce additional errors.

6.2 Extending the CFL Limit of FDTD Sub-gridding

The standard FDTD sub-gridding technique alleviates some of the memory and computational requirements for increased spatial resolution. However, the need to use a fine time-step still leads to long simulation times. Overcoming the fine mesh CFL constraint has been subject of intense research. Almost all implicit and explicit CFL extension methods discussed in Chapter 3 have been applied to the FDTD sub-gridding application, often with mixed results. The direct implicit methods discussed in Section 3.1.1 have been applied to the sub-gridding application in [9] and [10]. If the CFL limit of the fine grid is extended to the limit of the coarse grid, one would expect to be able to run the entire simulation at the time-step of the coarse grid. Unfortunately, this is not the case for the method of [9] and [10]. While these methods extend the CFL limit in the fine mesh domain, they do not guarantee the overall stability of the simulation at the full coarse mesh CFL limit. Moreover, the maximum time step that ensures stable results has to be determined experimentally. The ADI-FDTD method has been applied to the fine cell mesh in [20]. The paper presents a GR ratio of 2 and does not demonstrate overall stability at the coarse mesh CFL limit for higher GR values. The spatial filtering techniques have been applied to the sub-gridding application in [21]. In this case the stability at the coarse mesh CFL limit at any GR ratio is demonstrated in free space using the analytical cutoff frequency. In the case of sub-grid meshes containing inhomogeneous materials, a reduction of the cutoff frequency must be made to preserve overall stability. This section will describe the application of the CFL extension method of Chapter 4 to FDTD sub-gridding.

The proposed method of MOR and CFL extension may be used to alleviate the two main issues of FDTD sub-gridding. Through local CFL extension of the fine mesh, the coarse mesh CFL limit may be achieved. For the same simulation time duration, the number of time-steps required when compared
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The proposed method therefore resolves both computational issues of local mesh refinement. It should be noted that the proposed method may be easily applied using the same principles to the non-uniform FDTD mesh to improve the overall CFL limit. This section will outline the theory and implementation of the proposed method to FDTD sub-gridding. Section 6.3 will then present numerical results.

6.2.1 System Formulation

In Chapters 3 and 4, we discussed how the FDTD equations for a uniform mesh can be cast into matrix form (2.3). Five sub-matrices, namely $D_\epsilon$, $D_\mu$, $D_\sigma_e$, $D_\sigma_m$, and $K$, were sufficient to completely characterize a FDTD system. We will reuse this representation in the sub-gridding case for representing the FDTD equations of the coarse and fine grids. All quantities related to the fine grid will be denoted with a $F$ subscript, as in $x_F$. Quantities related to the coarse grid will be denoted with a $C$ subscript, as in $x_C$. The number of ports of the sub-grid system is $2N_x + 2N_y$ and will be denoted $N_B$, where $N_x$ and $N_y$ are the size of the sub-grid in coarse cells. The physical interpretation of $N_B$ is the number of $E_x$ and $E_y$ nodes that border the sub-grid region. The FDTD sub-gridding update equations may be written:

At a time-step $n$:

$$
\begin{align*}
\left( \frac{D_{\epsilon,C}}{\Delta t} + \frac{D_{\sigma_e,C}}{2} \right) E_C^{n+1} &= \left( \frac{D_{\epsilon,C}}{\Delta t} - \frac{D_{\sigma_e,C}}{2} \right) E_C^n - K_C H_C^{n+\frac{1}{2}} - TH_F^{n+\frac{1}{2}} - J^{n+\frac{1}{2}} \\
\left( \frac{D_{\epsilon,F}}{\Delta t} + \frac{D_{\sigma_e,F}}{2} \right) E_F^{n+1} &= \left( \frac{D_{\epsilon,F}}{\Delta t} - \frac{D_{\sigma_e,F}}{2} \right) E_F^n - K_F H_F^{n+\frac{1}{2}}.
\end{align*}
$$

(6.1)

At a time-step $n + \frac{1}{2}$:

$$
\begin{align*}
\left( \frac{D_{\mu,C}}{\Delta t} + \frac{D_{\sigma_m,C}}{2} \right) H_C^{n+\frac{1}{2}} - K_C^T E_C^{n+1} &= \left( \frac{D_{\mu,C}}{\Delta t} - \frac{D_{\sigma_m,C}}{2} \right) H_C^{n+\frac{1}{2}} - M^{n+1}.
\end{align*}

(6.2)

where $E_C^n$ and $H_C^{n+\frac{1}{2}}$ are the state vectors of the coarse mesh and $E_F^n$ and $H_F^{n+\frac{1}{2}}$ are the state vectors of the fine mesh. The state vector size of the coarse and fine mesh electric and magnetic field nodes will be denoted as $(N_{e,C}, N_{m,C})$ and $(N_{e,F}, N_{m,F})$. The equations (6.1) and (6.2) are of the same form as the single domain equation of (2.3). The $J$ and $M$ are external electric and magnetic field excitations, that for simplicity we assume are located in the coarse mesh. The matrix $T$ is the transition
matrix that performs the connection between the different mesh domains and requires special attention.

In order to derive the transition matrix $T$, we must first define the four matrices:

- A coarse to boundary node matrix ($M_{CB}$) of size $N_B \times N_{e,C}$. This matrix extracts the coarse $E_x$ and $E_y$ nodes into a vector of size $N_B$ for the update of the fine mesh $H_z$ nodes. This matrix contains only 1’s as coupling terms.

- A fine to boundary node matrix ($M_{FB}$) of size $N_B \times N_{m,F}$. This matrix extracts the fine $H_z$ nodes into a vector of size $N_B$ for the update of the coarse mesh $E_x$ and $E_y$ nodes. This matrix contains only 1’s as coupling terms.

- Update matrix for coarse mesh ($M_{BC}$) of size $N_{e,C} \times N_B$. This matrix performs extrapolation of the fine mesh $H_z$ nodes into the update equations of the coarse $E_x$ and $E_y$ nodes. This matrix contains the terms $\left(\pm \frac{1}{\Delta x}, \pm \frac{1}{\Delta y}\right)$.

- Update matrix for fine mesh ($M_{BF}$) of size $N_{m,F} \times N_B$. This matrix performs interpolation of the coarse mesh $E_x$ and $E_y$ boundary nodes into the update equations of the fine $H_z$ nodes. The interpolation terms have values of $\left(\frac{1}{GR}\right)$ while the fine update terms have values of $\left(\pm \frac{GR}{\Delta x}, \pm \frac{GR}{\Delta y}\right)$. This matrix therefore contains the terms $\left(\pm \frac{1}{\Delta x}, \pm \frac{1}{\Delta y}\right)$.

The matrices ($M_{BF}M_{CB}$) and ($M_{BC}M_{FB}$) are of size $(N_{m,F} \times N_{e,C})$ and $(N_{e,C} \times N_{m,F})$ respectively and represent the coupling between coarse and fine mesh boundary nodes. Due to the reciprocal interface between coarse and fine meshes, the relation $(M_{BC}M_{FB}) = -(M_{BF}M_{CB})^T$ always holds. We will declare a transition matrix $T = \left(M_{BC}M_{FB}\right)$ that will be used for the interfaces between the coarse and fine boundary nodes.

By combining (6.1) and (6.2) in a unique system, we arrive at

\[
\begin{bmatrix}
\frac{D_{e,C}}{\Delta t} + \frac{D_{\sigma_{e,C}}}{2} & 0 & 0 & 0 \\
0 & \frac{D_{e,F}}{\Delta t} + \frac{D_{\sigma_{e,F}}}{2} & 0 & 0 \\
-\mathbf{K}_C^T & 0 & \frac{D_{\mu,C}}{\Delta t} + \frac{D_{\sigma_{m,C}}}{2} & 0 \\
-\mathbf{T} & -\mathbf{K}_F^T & 0 & \frac{D_{\mu,F}}{\Delta t} + \frac{D_{\sigma_{m,F}}}{2}
\end{bmatrix}
\begin{bmatrix}
\mathbf{E}_C|^{n+1} \\
\mathbf{E}_F|^{n+1} \\
\mathbf{H}_C|^{n+\frac{1}{2}} \\
\mathbf{H}_F|^{n+\frac{1}{2}}
\end{bmatrix} = \begin{bmatrix}
\mathbf{E}_C|^{n} \\
\mathbf{E}_F|^{n} \\
\mathbf{H}_C|^{n+\frac{1}{2}} \\
\mathbf{H}_F|^{n+\frac{1}{2}}
\end{bmatrix}
\]

(6.3)
This system of equations describes the entire simulation domain, comprising of both coarse and fine grids. We note that (6.3) is in the same form as in the uniform grid case (4.2). Therefore, it can be written as

\[(R + F)x^{n+1} = (R - F)x^n + Bu^{n+1}.\]  

(6.4)

where

\[R = \begin{bmatrix} \frac{1}{\Delta t}D_\epsilon & -\frac{1}{2}K \\ -\frac{1}{2}K^T & \frac{1}{\Delta t}D_\mu \end{bmatrix}, \quad F = \begin{bmatrix} \frac{1}{2}D_{\sigma_e} & \frac{1}{2}K \\ -\frac{1}{2}K^T & \frac{1}{2}D_{\sigma_m} \end{bmatrix},\]  

(6.5)

The state space vectors are

\[E^n | E_C^{n+1} \begin{bmatrix} E_F^{n+1} \end{bmatrix} \quad H^{n+\frac{1}{2}} | H_C^{n+\frac{1}{2}} \begin{bmatrix} H_F^{n+\frac{1}{2}} \end{bmatrix} \quad x^n | E^n \begin{bmatrix} E^n \end{bmatrix} \]  

(6.6)

The five system matrices \(D_\epsilon, D_\mu, D_{\sigma_e}, D_{\sigma_m},\) and \(K\) are

\[K = \begin{bmatrix} K_C & 0 \\ 0 & K_F \end{bmatrix}, \quad D_\epsilon = \begin{bmatrix} D_{\epsilon,C} & 0 \\ 0 & D_{\epsilon,F} \end{bmatrix}, \quad D_\mu = \begin{bmatrix} D_{\mu,C} & 0 \\ 0 & D_{\mu,F} \end{bmatrix}, \]  

\[D_{\sigma_e} = \begin{bmatrix} D_{\sigma_e,C} & 0 \\ 0 & D_{\sigma_e,F} \end{bmatrix}, \quad D_{\sigma_m} = \begin{bmatrix} D_{\sigma_m,C} & 0 \\ 0 & D_{\sigma_m,F} \end{bmatrix} \]  

(6.7)

The full domain FDTD sub-grid system containing coarse, fine, and boundary cells is fully described by the five matrices in (6.7) using the state space representation of (6.6). Although, for simplicity, we have assumed only one fine region, the theory that we present can be easily extended to account for multiple refinement regions.

### 6.2.2 Stability Criterion for a Mesh with Sub-gridding

The equations for a FDTD system with sub-gridding (6.4) are in the same form as the equations for a standard FDTD that were used in Chapter 4. Therefore, all results we derived in Chapter 4 (stability conditions, stability enforcement, MOR process) can be directly applied to the FDTD sub-gridded system (6.4). The stability conditions imposed on \(R\) and \(F\) are stated in (4.5) and (4.6), and are repeated here for convenience. Since the conductivities in the coarse and fine meshes are positive, it can be easily shown that the condition (4.5) will be always satisfied. The stability of the FDTD sub-gridding
simulation is determined by the inequality

\[
\text{singular values of } \left( D_e^{-\frac{1}{2}} K D_{\mu}^{-\frac{1}{2}} \right) \leq \frac{2}{\Delta t}.
\] (6.8)

The matrix \( D_e^{-\frac{1}{2}} K D_{\mu}^{-\frac{1}{2}} \), using (6.7), can be written as

\[
\text{singular values of } \begin{bmatrix}
D_{\epsilon,C}^{-\frac{1}{2}} K C D_{\mu,C}^{-\frac{1}{2}} & D_{\epsilon,C}^{-\frac{1}{2}} T D_{\mu,F}^{-\frac{1}{2}} \\
0 & D_{\epsilon,F}^{-\frac{1}{2}} K F D_{\mu,F}^{-\frac{1}{2}}
\end{bmatrix} \leq \frac{2}{\Delta t}.
\] (6.9)

We see that, as expected, the stability of the sub-gridded system will depend on both the coarse and fine mesh stability conditions, as well as the coupling matrix \( T \). The diagonal block matrices of (6.8) are the matrices that control the stability of the coarse and fine grids taken individually. A well known characteristics of (6.8) is that the inequality is always satisfied at the fine mesh CFL time-step. While (6.8) may be easily enforced based upon the process presented in previous chapters through the perturbation of the full \( K \) matrix, we opt for a better approach. Rather than forming and perturbing the \( K \) matrix for the whole system, which can be huge, we will extend the CFL limit by manipulating the equations of the fine grid only. The ultimate goal of sub-gridding CFL extension is the automatic generation of a blackbox fine mesh system that can be run with the full coarse mesh CFL limit without stability issues. To date, this has not yet been achieved.

6.2.3 Proposed Method to Extend the CFL in FDTD Sub-gridding

As discussed in the previous section, we want to extend the CFL limit in FDTD sub-gridding by acting only on the equations of the fine mesh. By extracting the equations in (6.1) and (6.2) that correspond to the fine mesh, we can write the following system description for the fine mesh

\[
\begin{align*}
\left( \frac{D_{e,F}}{\Delta t} + \frac{D_{\sigma_e,F}}{2} \right) E_F^{n+1} &= \left( \frac{D_{\epsilon,F}}{\Delta t} - \frac{D_{\sigma_e,F}}{2} \right) E_F^{n} - K_F H_F^{n+\frac{1}{2}} \\
\left( \frac{D_{\mu,F}}{\Delta t} + \frac{D_{\sigma_m,F}}{2} \right) H_F^{n+\frac{3}{2}} - K_F T E_F^{n+1} &= \left( \frac{D_{\mu,F}}{\Delta t} - \frac{D_{\sigma_m,F}}{2} \right) H_F^{n+\frac{1}{2}} + M_{BF} (M_{CB} E_C^{n+1}) \\
y &= M_{FB} H_F^{n+\frac{1}{2}}
\end{align*}
\] (6.10)

where the first equations updated the \( E_F^n \) nodes of the fine grid, and the second equations updates the \( H_F^{n+\frac{1}{2}} \) nodes. The \( T \) matrix has been decomposed into its basic matrix components \( M_{BF} \) and \( M_{CB} \). In the second equation, the term \( M_{CB} E_C^{n+1} \) can be seen as the input for this system. Indeed, it is the information provided by the coarse mesh to the fine mesh. The last equation, instead, can be
interpreted as an output equation. It extracts, from the magnetic field vector $\mathbf{H}_F |_{n+\frac{3}{2}}$, those values $y$ that need to be passed to the coarse mesh. For a sub-grid region with height and width $N_x$ and $N_y$ in coarse cells, the system of (6.10) has $2N_x + 2N_y$ ports. Using the same notations as Chapters 3 and 4, the matrix boundary to fine mesh matrix $\mathbf{M}_{BF}$ may be interpreted as the $\mathbf{B}$ matrix while the fine mesh to boundary matrix $\mathbf{M}_{FB}$ may be interpreted as the $\mathbf{L}^T$ matrix. The Krylov subspace projection base model order reduction algorithm introduced in Chapter 4 is applied to (6.10) in order to reduce its size and ease stability enforcement. Through applying the SPRIM [23] algorithm we arrive at two projections vectors $\mathbf{V}_1$ and $\mathbf{V}_2$ and the reduced system matrices

$$
\begin{align*}
\tilde{\mathbf{D}}_{e,F} &= \mathbf{V}_1^T \mathbf{D}_{e,F} \mathbf{V}_1 \\
\tilde{\mathbf{D}}_{\mu,F} &= \mathbf{V}_2^T \mathbf{D}_{\mu,F} \mathbf{V}_2 \\
\tilde{\mathbf{D}}_{\sigma,e,F} &= \mathbf{V}_1^T \mathbf{D}_{\sigma,e,F} \mathbf{V}_1 \\
\tilde{\mathbf{D}}_{\sigma,m,F} &= \mathbf{V}_2^T \mathbf{D}_{\sigma,m,F} \mathbf{V}_2 \\
\tilde{\mathbf{K}}_F &= \mathbf{V}_1^T \mathbf{K}_F \mathbf{V}_2.
\end{align*}
$$

(6.11)

This is accompanied by the reduced $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{L}}$ matrices

$$
\begin{align*}
\tilde{\mathbf{B}} &= \mathbf{V}_2^T \mathbf{B} = \mathbf{V}_2^T \mathbf{M}_{BF} \\
\tilde{\mathbf{L}}^T &= \mathbf{L}^T \mathbf{V}_2 = \mathbf{M}_{FB} \mathbf{V}_2.
\end{align*}
$$

(6.12)

It can be seen from (6.12) that the reciprocity of the reduced transition matrix

$$
\tilde{\mathbf{T}} = (\mathbf{M}_{BC} \mathbf{M}_{FB}) \mathbf{V}_2 = - (\mathbf{M}_{BF} \mathbf{M}_{CB})^T \mathbf{V}_2
$$

(6.13)

is still satisfied.

Now, we perturb the reduced matrices of the fine grid in order to extend the CFL limit. Our core idea is to limit the singular values of the matrix which controls the stability of the fine grid. This can be achieved with the following steps:

1. Compute the singular value decomposition [27]

$$
\tilde{\mathbf{D}}_{e,F}^{-\frac{1}{2}} \tilde{\mathbf{K}}_F \tilde{\mathbf{D}}_{\mu,F}^{-\frac{1}{2}} = \mathbf{U} \mathbf{S} \mathbf{W}^T,
$$

(6.14)

2. Iterative through the singular values $\sigma_i$. For each singular value that satisfy $\sigma_i < \beta \frac{2}{\Delta t}$, append the associated column from $\mathbf{U}$ and $\mathbf{W}$ associated with the stable $\sigma_i$ into new matrices $\mathbf{U}'$ and $\mathbf{W}'$. After completion, the $\mathbf{U}'$ and $\mathbf{W}'$ matrices will contains a set of orthonormal projection vectors associated only with the stable singular values. The $\beta$ variable is used to enforce the stability condition (6.9) and set to be 0.9. The maximum $\beta$ for stability is a function of the grid refinement.
Chapter 6. Proposed CFL Extension Technique: Application to FDTD Sub-gridding

ratio GR, although $\beta = 0.9$ is sufficient to satisfy all test cases of this chapter.

3. Obtain a subset of the reduced system that spans only the stable singular values using $U'$ and $W'$

$$
\bar{D}_{e,F} = (U')^T \bar{D}_{e,F} U' \quad \bar{D}_{\mu,F} = (W')^T \bar{D}_{\mu,F} W' \quad (6.15)
$$

$$
\bar{D}_{\sigma,v,F} = (U')^T \bar{D}_{\sigma,v,F} U' \quad \bar{D}_{\sigma,m,F} = (W')^T \bar{D}_{\sigma,m,F} W' \quad (6.16)
$$

$$
\bar{K}_F = (U')^T \bar{K}_F W' \quad (6.17)
$$

Similarly, the matrices $\bar{B}$, $\bar{L}$ matrices are further reduced into $\bar{B}'$ and $\bar{L}'$ through

$$
\bar{B}' = (W')^T \bar{B} \quad \bar{L}' = (\bar{L})^T W' \quad (6.18)
$$

The key limitation of the current stability enforcement process is the selection of the $\beta$ variable. It is previous established in (6.8) that the stability of the fine mesh alone at the coarse grid CFL limit is not sufficient alone to ensure the stability of the overall simulation. The inclusion of the $\beta$ factor is our first attempt to achieve stable simulations. However, an analytical criterion to determine an optimal $\beta$ is currently unavailable. Apart from this issue, that future work will hopefully address, numerical examples will demonstrate that the proposed method can extend the CFL limit of FDTD simulations with sub-gridding, and lead to substantial speed-ups. The singular value removal process may be applied to the single domain test cases of Chapters 4 and 5 with very little difference in accuracy. In addition, the removal of unstable singular values will further reduce the reduced system size. Overall it may be said that singular value removal is a superior stability enforcement process to singular value perturbation. The introduction and usage of singular value perturbation in Chapters 4 and 5 was for consistency with existing publications [15, 16]. Singular value perturbation also offers a simpler numerical explanation. All test cases of this Chapter will utilize singular value removal.

6.3 Test Cases

This section will apply the proposed CFL extension algorithm to two 2D FDTD sub-gridding test cases, consisting of a PEC cavity and a waveguide with two irises. The test cases will compare the following algorithms:

- **FDTD**: this is the standard FDTD method with a uniform *coarse* mesh over the entire domain.

The simulation will be run at the coarse mesh CFL limit.
• **Full refinement:** this is the standard FDTD method with a uniform and fine mesh across the entire domain. For comparison purposes, this method will be considered the gold standard. The simulation will be run at the fine mesh CFL time-step.

• **Sub-gridding:** this is the standard FDTD sub-gridding technique with local mesh refinement with linear spatial interpolation and extrapolation [35]. The simulation will be run at the fine mesh CFL time-step.

• **Sub-gridding with MOR:** in this method, we will apply the MOR process to the fine FDTD mesh using the procedures of Section 6.2. This is equivalent to the proposed method with only the model order reduction step applied. The purpose of this simulation is to verify the accuracy of the MOR process. The results of this method should converge to the standard FDTD sub-gridding results. The CFL limitations of the fine mesh region remain, thus the simulation will be run at the fine mesh CFL time-step.

• **Implicit with MOR:** this method applies the direct implicit CFL extension technique to the fine mesh regions as described in [9]. The reduced and CFL extended implicit system is then connected to the coarse mesh. Due to the unconditional stability of the implicit fine mesh, the coarse mesh CFL time-step may be used throughout the full simulation.

• **Proposed Method:** this is the method proposed in Section 6.2. It first reduces the fine grid equations, and then extends their stability limit with the perturbation process of Section 6.2.3. The CFL extension step enforces the stability of the fine mesh region at the coarse mesh CFL limit. This allows the use of the coarse mesh CFL time-step throughout the full simulation.

6.3.1 Empty PEC Cavity

This test case utilizes the 2D PEC cavity of size 1 m × 1 m first shown in Chapters 3 and 4. The PEC cavity test case will again be used to verify the late time stability of the overall simulation. The 2D cavity operates in the TM mode and is discretized into a 20 × 20 mesh with Δx = Δy = Δ = 5 cm. A Gaussian current source with bandwidth 0.5 GHz is placed at (x=3, y=3), while a probe on the H_z node is placed at (x=17, y=17). A fine mesh is used in the region 6 ≤ x, y ≤ 15. The simulation mesh for the square cavity with mesh refinement ratio GR = 3 is shown in Figure 6.3. The sub-gridding interface is implemented as described in Section 6.2. Grid refinement ratios ranging from GR = 1 to 9 have been tested in increments of 2. All methods were run at the maximum allowable time-step of CFL = 1 or CFL = \( \frac{1}{GR} \) depending upon their respective stability limits. At the interface between coarse
and fine meshes, 40 “ports” are identified, which correspond to the field values exchanged back and forth between the fine and coarse meshes. The proposed mesh was run with a single expansion point at $f_{\text{max}} = 0.5 \text{ GHz}$ and $M = 1.1$. The linear system solution for the reduction process is performed using direct LU decomposition. The number of moments matched before the application of SPRIM splitting is 3 for all CFL values. With SPRIM splitting [23] of the projection vectors, this results in a reduced system sizes of 480 before the stability enforcement process. The 5 benchmark methods outlined at the beginning of Section 6.3 have been implemented for comparison. The simulation was ran for 10,000 time steps. The full refinement and standard sub-gridding test cases are restricted to run at the fine time-step for stability reasons. Therefore, they were ran at the maximum time-step $\frac{1}{GR}$ of the coarse mesh CFL limit. The dictates an increased number of time-steps to run at the fine time-step for stability reasons. Therefore, they were ran for $10,000 \cdot GR$ to cover the same time window as other methods.

The normalized errors compared to analytical results of the extracted first 6 non-zero TM modes are presented in Table 6.2 for all tested methods. The sub-gridding scheme using implicit CFL extension of the fine mesh becomes unstable for $GR > 3$. Therefore the results for the implicit case are only presented for $GR = 3$. This is consistent with the conclusions of [9], where the combination of stable implicit and explicit domains do not guarantee overall stability at high grid refinement ratios. Due to the difficulty of analysing the combination of explicit and implicit systems, the source of this instability is not very well understood. It can be seen that the sub-gridding with MOR method has the same results as the standard sub-gridding method for $GR = 3$. It may therefore be concluded that the reduced system size of 480 fully captures the behaviour of the fine mesh domain. Based upon the conclusions of Chapters 3 and 4, any error observed for the proposed method is due to the extension of the CFL limit. The full refinement FDTD case has superior accuracy to all tested sub-gridding methods and has less than 0.005\% normalized relative errors across all resonant frequencies with $GR = 9$. Figure 6.4 plots the normalized relative errors of the extracted resonant frequencies for standard sub-gridding and the proposed method at various grid refinement values. It is observed that the errors in the two plots are similar in magnitude, and they do not increase as the grid refinement ratio is increased. As $GR$ increases, there are indeed two opposite trends that partially compensate each other. On the one hand, as $GR$ increases, the fine grid becomes finer, increasing spatial resolution and decreasing numerical dispersion errors. On the other hand, as $GR$ grows, the CFL has to be extended farther, and more dispersion is introduced. Overall the accuracy of the proposed sub-gridding method with explicit CFL extension is competitive with that of the standard FDTD sub-gridding technique.

\[1\] Having established the accuracy of the reduced model size, the MOR sub-gridding results are not presented for $GR = 5, 7, \text{ and } 9$ since they converged to the standard sub-gridding results.
Figure 6.3: 2D Cavity of Section 6.3.1: simulation mesh with grid refinement ratio GR = 3.
Table 6.2: 2D Cavity of Section 6.3.1: Extracted resonant frequencies and normalized relative error for various FDTD sub-gridding methods with and without CFL extension for GR = 3-9.

<table>
<thead>
<tr>
<th>Resonant Modes</th>
<th>$TM_{0,1}$</th>
<th>$TM_{1,1}$</th>
<th>$TM_{2,0}$</th>
<th>$TM_{2,1}$</th>
<th>$TM_{2,2}$</th>
<th>$TM_{3,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Analytical</strong></td>
<td>0.149896</td>
<td>0.211985</td>
<td>0.299792</td>
<td>0.335178</td>
<td>0.423971</td>
<td>0.449689</td>
</tr>
<tr>
<td><strong>FDTD (CFL=1)</strong></td>
<td>0.149818</td>
<td>0.211977</td>
<td>0.334867</td>
<td>0.423970</td>
<td>0.44758</td>
<td></td>
</tr>
<tr>
<td><strong>Normalized Relative Error [%]</strong></td>
<td>-0.0520</td>
<td>-0.0000</td>
<td>-0.2051</td>
<td>-0.0928</td>
<td>-0.0002</td>
<td>-0.4672</td>
</tr>
</tbody>
</table>

Grid Refinement Ratio = 3

| Full refinement | 0.149800 | 0.211992 | 0.299735 | 0.335155 | 0.423986 | 0.449496 |
| **Normalized Relative Error [%]** | -0.0040 | 0.0033 | -0.0190 | -0.0009 | 0.0035 | -0.0429 |

**FDTD sub-gridding**

| Normalized Relative Error [%] | -0.0294 | -0.0241 | -0.3232 | -0.2742 | -0.3312 | -0.8268 |

**MOR sub-gridding**

| Normalized Relative Error [%] | -0.0294 | -0.0241 | -0.3232 | -0.2742 | -0.3312 | -0.8268 |

**Implicit method**

| Normalized Relative Error [%] | 0.149829 | 0.212030 | 0.298988 | 0.334670 | 0.423097 | 0.446660 |

**Proposed method**

| Normalized Relative Error [%] | 0.149852 | 0.211934 | 0.298823 | 0.334259 | 0.422601 | 0.445971 |

Grid Refinement Ratio = 5

| Full refinement | 0.149899 | 0.211994 | 0.299779 | 0.335191 | 0.423986 | 0.449623 |
| **Normalized Relative Error [%]** | 0.0020 | 0.0043 | 0.0039 | 0.0035 | -0.0147 |

**FDTD sub-gridding**

| Normalized Relative Error [%] | -0.0287 | -0.0241 | -0.3232 | -0.2742 | -0.3312 | -0.8268 |

**Proposed method**

| Normalized Relative Error [%] | 0.150225 | 0.212284 | 0.300587 | 0.335596 | 0.425938 | 0.448695 |
| Normalized Relative Error [%] | 0.2195 | 0.1410 | 0.2652 | 0.1247 | 0.4639 | -0.2210 |

Grid Refinement Ratio = 7

| Full refinement | 0.149901 | 0.211994 | 0.299798 | 0.335186 | 0.423988 | 0.449689 |
| **Normalized Relative Error [%]** | 0.0033 | 0.0042 | 0.0007 | 0.0021 | 0.0040 | -0.0033 |

**FDTD sub-gridding**

| Normalized Relative Error [%] | -0.0247 | -0.0259 | -0.3359 | -0.2900 | -0.3566 | -0.8626 |

**Proposed method**

| Normalized Relative Error [%] | 0.150266 | 0.212314 | 0.300712 | 0.335619 | 0.426122 | 0.448820 |
| Normalized Relative Error [%] | 0.2468 | 0.1519 | 0.2962 | 0.1274 | 0.4974 | -0.1995 |

Grid Refinement Ratio = 9

| Full refinement | 0.149895 | 0.211985 | 0.299768 | 0.335159 | 0.423971 | 0.449611 |
| **Normalized Relative Error [%]** | 0.0033 | 0.0042 | 0.0020 | 0.0024 | 0.0040 | -0.0000 |

**FDTD sub-gridding**

| Normalized Relative Error [%] | -0.0247 | -0.0259 | -0.3356 | -0.2927 | -0.3606 | -0.8659 |

**Proposed method**

| Normalized Relative Error [%] | 0.150268 | 0.212316 | 0.300724 | 0.335624 | 0.426137 | 0.448828 |
| Normalized Relative Error [%] | 0.2482 | 0.1561 | 0.3109 | 0.1331 | 0.5109 | -0.1915 |
Figure 6.4: 2D Cavity of Section 6.3.1: Relative error of extracted resonant frequencies for standard coarse mesh FDTD, sub-gridding, and proposed method for 2D PEC cavity test case at GR = 3-9.

Table 6.3 plots the runtime breakdown for full mesh refinement, standard sub-gridding, and sub-gridding with the proposed CFL extension methods for grid refinement ratios ranging from 3 to 9. In the uniform coarse mesh FDTD simulation, the number of unknowns in the coarse region is 960. In the region that will be refined, the number of unknowns is 280. The size of the fine mesh state size rapidly increases to 24,120 at GR = 9. In the proposed method, the rapid increase in size is mitigated both by the reduction process and by the enforcement procedure. Since “unstable” singular values are eliminated, the size of the obtained model is further reduced. In this specific example, the original size of 24,120 is reduced to 126 for GR = 3 and 124 for GR = 5, 7 and 9 out of the full reduced system size of 480. An interesting observation is that the size of the stability enforced model remains constant as the effective CFL extension and GR ratios are increased. In order to achieve the same local spatial resolution, the proposed sub-gridding method with MOR and CFL extension out performs the two benchmark methods in terms of total runtime by several magnitudes. Finally, the CPU times reported in the last column on Table 6.3 demonstrate the speed-ups that can be obtained with the proposed method. For a grid refinement ratio of 3, the proposed method ensures a speed up of 4X with respect to the standard FDTD sub-gridding algorithm. Speed up increases to 12.7X, 26.3X and 37X for refinement ratios of 5, 7, and 9, respectively. This outcome shows how model order reduction and CFL-extension can significantly improve the cost of an FDTD analysis in presence of sub-gridding. While the generation of the reduced model is somewhat expensive, the final system has significant computation and memory benefits. The stability of the model generated by the proposed technique has been verified by checking that conditions for stability (6.8) hold for the coarse time step.
### Table 6.3: 2D Cavity of Section 6.3.1: Runtime breakdown of various FDTD sub-gridding methods with and without CFL extension for GR = 3-9.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fine Mesh Size (Stable/Total)</th>
<th>Model Order Reduction</th>
<th>Overhead</th>
<th>Run Time</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid Refinement Ratio = 1 (Coarse mesh size = 960, Coarse mesh size of sub-grid region = 280)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2D FDTD</td>
<td></td>
<td></td>
<td></td>
<td>1.515</td>
<td>1.522</td>
</tr>
<tr>
<td>Grid Refinement Ratio = 3 (Coarse mesh size = 960, Fine mesh sub-grid size = 2640)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Full Refinement</td>
<td>10920</td>
<td>0.015</td>
<td>18.783</td>
<td>18.798</td>
<td></td>
</tr>
<tr>
<td>Sub-gridding</td>
<td>2640</td>
<td>0.019</td>
<td>5.714</td>
<td>5.735</td>
<td></td>
</tr>
<tr>
<td>Proposed Method</td>
<td>126</td>
<td>0.298</td>
<td>0.117</td>
<td>1.007</td>
<td>1.442</td>
</tr>
<tr>
<td>Grid Refinement Ratio = 5 (Coarse mesh size = 960, Fine mesh sub-grid size = 7400)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Full Refinement</td>
<td>30200</td>
<td>0.011</td>
<td>63.454</td>
<td>63.465</td>
<td></td>
</tr>
<tr>
<td>Sub-gridding</td>
<td>7400</td>
<td>0.016</td>
<td>20.147</td>
<td>20.163</td>
<td></td>
</tr>
<tr>
<td>Proposed Method</td>
<td>124</td>
<td>0.499</td>
<td>0.114</td>
<td>0.964</td>
<td>1.577</td>
</tr>
<tr>
<td>Grid Refinement Ratio = 7 (Coarse mesh size = 960, Fine mesh sub-grid size = 14560)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Full Refinement</td>
<td>59080</td>
<td>0.011</td>
<td>119.447</td>
<td>119.458</td>
<td></td>
</tr>
<tr>
<td>Sub-gridding</td>
<td>14560</td>
<td>0.017</td>
<td>52.525</td>
<td>52.542</td>
<td></td>
</tr>
<tr>
<td>Proposed Method</td>
<td>124</td>
<td>0.915</td>
<td>0.110</td>
<td>0.965</td>
<td>1.990</td>
</tr>
<tr>
<td>Grid Refinement Ratio = 9 (Coarse mesh size = 960, Fine mesh sub-grid size = 24120)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Full Refinement</td>
<td>97560</td>
<td>0.015</td>
<td>242.718</td>
<td>242.733</td>
<td></td>
</tr>
<tr>
<td>Sub-gridding</td>
<td>24120</td>
<td>0.020</td>
<td>105.733</td>
<td>105.753</td>
<td></td>
</tr>
<tr>
<td>Proposed Method</td>
<td>124</td>
<td>1.757</td>
<td>0.114</td>
<td>0.963</td>
<td>2.854</td>
</tr>
</tbody>
</table>
6.3.2 Waveguide with PEC Irises

This test case utilizes a 2D waveguide operating in the TM mode with two PEC irises. For this test case we will assume that the two irises to be infinitesimally thin. The minimum thickness of a resolvable PEC sheet is limited by the minimum spatial discretization size of the FDTD mesh. Hence, the accuracy of the FDTD simulation is directly related to the spatial discretization size around the two irises. This test case will illustrate the improved accuracy of local mesh refinement techniques in resolving the infinitesimally thin PEC irises when compared to a uniform coarse mesh. In addition, this test case will demonstrate the superior computational efficiency of the proposed method compared with existing local mesh refinement techniques.

The waveguide is of size $0.7 \text{ m} \times 4 \text{ m}$ and is discretized into a $14 \times 80$ mesh with $\Delta x = \Delta y = \Delta = 5 \text{ cm}$. Two PEC irises of aperture size $0.2 \text{ m}$ are placed along the waveguide 1 m apart. Two local high resolution sub-grids of size $0.5 \text{ m} \times 0.5 \text{ m}$ are placed around the two PEC irises. The layout of the waveguide with the fine mesh regions is shown in Figure 6.5. The PEC wall of the iris is imposed on the $E_x$ nodes at $(y=30)$ and $(y=50)$. The iris thickness of 1 cell is kept constant for all grid refinement ratios. Based upon this implementation, the thickness of the PEC iris wall is dependent upon the spatial discretization size. The implementation of the PEC iris across the coarse and fine mesh regions for GR = 5 is illustrated in Figure 6.6. The waveguide is terminated at both ends on a 4th-order matched absorber with a thickness of 10 cells. A line source and probe are placed at $(y=18)$ and $(y=62)$. The waveguide is excited with a Gaussian pulse with maximum frequency $f_{\text{max}} = 0.4 \text{ GHz}$. The minimum $\lambda/\Delta$ for the coarse mesh at 0.4 GHz is 15. There are a total of 40 ports in the interface between coarse and fine meshes. The proposed mesh was again ran with a single expansion point at $f_{\text{max}} = 0.4 \text{ GHz}$ with magnitude $M = 1.1$. The linear system solution for the reduction process is performed using direct LU decomposition. The simulation was ran for 10,000 time steps. A preliminary simulation with an empty waveguide was used to extract the incident waveform.

The waveguide simulation was first ran at grid refinement ratios GR = 1, 9, and 15 for the following methods: full mesh refinement, sub-gridding, sub-gridding with MOR, and the proposed method. Three moments per port are used in the generation of the reduced fine mesh model, resulting in a reduced system size of 480. The full mesh refinement simulation is taken as the gold standard for all comparisons. Figure 6.7 plots the time and extracted frequency domain results at GR = 3. We observe that the proposed method, as well as the other sub-gridding methods match very well the results obtained with a refinement of the entire domain. In the frequency-domain plot, a small deviation can be observed between the results obtained with a coarse and a refined grid. This confirms that, for this problem,
Figure 6.5: Waveguide of Section 6.3.2: layout

refinement is beneficial and not superfluous. Figure 6.8 is a zoomed view of the frequency domain results from 0.208 GHz to 0.2145 GHz for the various grid refinement ratios. Both the standard FDTD sub-gridding and the proposed sub-gridding methods introduce some errors compared to the full mesh refinement case, although a good match may still be observed. The shifting in frequency domain results is a sign of numerical dispersion errors. The results of Figure 6.8 demonstrate that both the standard and proposed sub-grid example offer good approximations of a full mesh refinement simulation. The standard FDTD sub-grid and the proposed method offer comparable accuracy based upon the deviation of frequency domain peaks from the full mesh refinement results.

Table 6.4 presents the runtime breakdowns for full mesh refinement, standard sub-gridding, sub-gridding with MOR, and the proposed sub-gridding method for grid refinement ratios GR = 1, 9, and 15. At GR = 15, the model order reduction algorithm reduces the fine mesh system of size 67200 to 480. The convergence between the standard sub-gridding and sub-gridding with MOR case demonstrates that the fine mesh system is fully characterized using the 480 reduced model size. The proposed sub-gridding method demonstrates significant runtime improvements over all benchmarked methods. The CFL extension step plays a key role in allowing the use of a large time step for the full simulation, thus further reducing the overall system runtime.
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\[ \square = \text{PEC Region} \]
\[ \downarrow = \text{PEC Iris } E_y \text{ Node} \]

Figure 6.6: Waveguide of Section 6.3.2: Standard FDTD and refined sub-grid mesh around PEC iris region with GR = 5.
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Figure 6.7: Waveguide of Section 6.3.2: time and frequency domain results of various FDTD sub-gridding methods for GR = 3.

Figure 6.8: Waveguide of Section 6.3.2: zoomed frequency domain results of various FDTD sub-gridding methods from 0.208 GHz to 0.2145 GHz at GR = 3-15.
Table 6.4: Waveguide of Section 6.3.2: Runtime breakdown of various FDTD sub-gridding methods with and without CFL extension for GR = 3-15.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fine Mesh Size (Stable/Total)</th>
<th>Model Order Reduction</th>
<th>Overhead</th>
<th>Run Time</th>
<th>Total</th>
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<tr>
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<td>1.515</td>
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<td>109.573</td>
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6.4 Summary

In this chapter, after reviewing the standard approach to sub-gridding in FDTD, we have proposed a new method to accelerate simulations involving sub-gridding. The proposed method combines the reduction process presented in the previous chapters with a perturbation approach to extend the CFL limit of simulations with sub-gridding. The proposed sub-gridding method with CFL extension has been benchmarked against existing methods of local mesh refinement. The test cases used include 2D cavities and a waveguide with iris structures. In all test cases, the proposed method outperformed the benchmarked methods in terms of total runtime. The accuracy of the proposed method does not degrade as the grid refinement ratio is increased. The accuracy of the proposed method is competitive with the standard FDTD sub-gridding technique while being much faster. The stability of the proposed algorithm has been tested to very high grid refinement ratios of up to 15. Although the proposed method is still experimental, and deserves further studies, it definitively shows a large potential. In particular, the idea of combining the CFL-extension approach devised in this thesis with sub-gridding seems to be highly promising.
Chapter 7

Conclusion

7.1 Summary

FDTD simulations can be time-consuming in presence of small geometrical features, and in general for structures involving multiple geometrical scales. When a fine mesh is used to capture such features, the well-known CFL limit imposes a very small time step in order to ensure stability. This issue may dramatically increase the computational cost and memory consumption of a multi-scale FDTD analysis. In this thesis, we proposed a new way to significantly increase FDTD efficiency for multiscale simulations based upon two core ideas: CFL limit extension and model order reduction.

Our approach to extend the CFL limit was presented in Chapters 2 and 3. FDTD equations are seen as a discrete-time linear system that, when the CFL limit is exceeded, will have some unstable eigenvalues. By perturbing such eigenvalues, we show that late time stability can be rigorously enforced at time-steps larger than the CFL limit, and simulation speed-ups can be obtained. Numerical tests were presented to show that the CFL extension can be achieved without sacrificing accuracy. Differently from previous works, this approach does not require filtering operations performed at runtime that may reduce computational efficiency. Also, the devised method is easier to implement when discontinuous materials are present. Since finding eigenvalues is an expensive operation, the proposed CFL extension method works best when combined with model order reduction.

In Chapter 4, we presented an innovative method for the model order reduction of FDTD equations. By reducing the number of unknowns, we obtain a first source of speed-up. In addition, we allow for the application of the CFL extension method from the previous chapter to larger systems, which further accelerates the simulation. In the proposed reduction process, there are several new contributions with
Chapter 7. Conclusion

respect to the state of the art:

1. the reduction process preserves the structure of the FDTD equations, which improves efficiency and makes the obtained reduced models easy to integrate in an existing FDTD code;

2. below the CFL limit, the reduced model is guaranteed to be stable by construction;

3. above the CFL limit, the preservation of the structure of the FDTD equations enables a direct application of the CFL extension method presented in Chapter 4;

4. the reduction process can handle 3D problems with more than 1 million unknowns, thanks to the optimized implementation devised in this thesis. Previous works on the same problem were not applied to cases with more than 1 million unknowns.

The proposed reduction and CFL-extension methods were applied to microstrip circuits, waveguides and resonant cavities. Speed-ups of up to 10000X were comparing the run-time of the reduced model and standard FDTD, while more modest speed-ups of 5X to 10X were obtained when taking into account the MOR and stability enforcement process. Examples also demonstrated the accuracy of the proposed method, which always resulted in average errors lower than 0.2% in the time-domain with respect to FDTD.

Finally, in Chapter 6, the proposed ideas were combined with FDTD sub-gridding, a common procedure to locally refine a FDTD mesh. While useful from an accuracy standpoint, refining a FDTD grid has two drawbacks: it increases the number of unknowns and makes the CFL limit tighter. Using the reduction and CFL-extension methods presented in this thesis, we demonstrated that such issues can be mitigated. The FDTD equations for the refined grid are first reduced with the reduction method presented in Chapter 4. Then, their stability limit is extended using a modified version of the stability enforcement algorithm presented in Chapter 4. Finally, the obtained model is instantiated into the original simulation, where it is coupled to surrounding coarse grid. Numerical tests showed that this approach allows to run the overall simulation at the large time step supported by the coarse grid, with substantial CPU time savings with respect to standard sub-gridding. Speed-ups up to 30X were demonstrated compared to the standard sub-gridding implementation. Although not complete, the work in this final chapter demonstrates the great potential of the ideas developed throughout the thesis in accelerating multiscale FDTD simulations.
7.2 Contributions

There are two key contributions in this thesis: the CFL extension method, and the new model order reduction method for FDTD systems. The detailed derivation and verification process are described in Chapters 2-5. The research performed has results in the following publications:


The following publication has been submitted and is currently under review:

1. X. Li, C. D. Sarris, and P. Triverio, “Structure-Preserving Reduction of Finite-Difference Time-Domain Equations with Controllable Stability Beyond the CFL Limit,” *IEEE Transactions on Microwave Theory and Techniques*

The contents of Chapter 6 is the progress of ongoing work on the application of the proposed method to the FDTD sub-gridding technique. Although not complete, the work has demonstrated very promising results.

7.3 Future Work

There are a number of potential future research topics associated with the proposed method and the FDTD sub-gridding application:

- All CFL extension techniques demonstrate increased numerical dispersion errors when run above the CFL limit. The magnitude of the numerical dispersion errors introduced by the proposed method may be approximated using the FDTD numerical dispersion equations from Chapter 2. The numerical dispersion errors of the reduced models may be compensated for through eigen-value perturbation. We have performed this experiment with some success for cavity test cases, although at the cost of introducing magnitude errors. This topic is worth investigating to reduce the introduced numerical dispersions errors.
• The test cases of Chapter 4 demonstrated that unstable eigenvalues lie outside of the frequency of interest for modest CFL extension ratios. For the 2D cavity case, it was found that only 16 of the 80 reduced system eigenvalues are within the frequency band of interest. As the CFL ratio is increased, these 64 superfluous eigenvalues are into the first to enter the unstable region. A connection between these two results indicates that the MOR process may be further optimized. In the ideal case, the MOR process would only capture the eigenvalues within the frequency band of interest. This would render the stability enforcement process unnecessary for modest CFL extension ratios since the reduced system can be guaranteed to have no eigenvalues in the unstable region.

• The iterative conjugate gradient solver used in Chapter 4 and 5 is a basic implementation using the Matlab libraries. The conjugate gradient squared algorithm in general may be optimized through the use of pre-conditioners and internal optimizations to improve the convergence rate [37, 38]. These optimizations are worth investigating since the CGS iterative solver takes up the majority of the runtime for the proposed method.

• The sub-gridding method presented in Section 6 requires the empirical estimation of the coefficient $\beta$ that will guarantee the stability of the overall simulation. The key challenge in this derivation is that one wants to avoid the need to assemble the equations for the coarse grid which surrounds the fine mesh. We are confident that a rigorous result can be found, leading to an optimal way to extend the CFL limit of a mesh with sub-gridding to the limit of the coarse grid.

• The axillary equation method is widely used for including dispersive materials in FDTD simulations, including meta-materials. We believe that it is possible to extend the methods in this thesis to such case, which has interesting practical applications.
Bibliography


