EFFICIENT TIME-DOMAIN MODELING OF PERIODIC-STRUCTURE-BASED MICROWAVE AND OPTICAL GEOMETRIES

by

Dongying Li

A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy
Graduate Department of Edward St. Rogers Sr. Department of Electrical and Computer Engineering
University of Toronto

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Abstract

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2011

A set of tools are proposed for the efficient modeling of several classes of problems related to periodic structures in microwave and optical regimes with Finite-Difference Time-Domain method. The first category of problems under study is the interaction of non-periodic sources and printed elements with infinitely periodic structures. Such problems would typically require a time-consuming simulation of a finite number of unit cells of the periodic structures, chosen to be large enough to achieve convergence. To alleviate computational cost, the sine-cosine method for the Finite-Difference Time-Domain based dispersion analysis of periodic structures is extended to incorporate the presence of non-periodic, wideband sources, enabling the fast modeling of driven periodic structures via a small number of low cost simulations. The proposed method is then modified for the accelerated simulation of microwave circuit geometries printed on periodic substrates. The scheme employs periodic boundary conditions applied at the substrate, to dramatically reduce the computational domain and hence, the cost of such simulations. Emphasis is also given on radiation pattern calculation, and the consequences of the truncated computational domain of the proposed method on the computation of the electric and magnetic surface currents invoked in the near-to-far-field transformation. It has been further demonstrated that from the mesh truncation point of view, the scheme, which has a
unified form regardless dispersion and conductivity, serves as a much simpler but equally
effective alternative to the Perfectly Matched Layer provided that the simulated domain
is periodic in the direction of termination. The second category of problems focuses on
the efficient characterization of nonlinear periodic structures. In Finite-Difference Time-
Domain, the simulation of these problems is typically hindered by the fine spatial and
time gridding. Originally proposed for linear structures, the Alternating-Direction Im-
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are extended to incorporate nonlinear media. Both methods are able to use time-step
sizes beyond the conventional stability limit, offering significant savings in simulation
time.
Acknowledgements

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<tr>
<td>ε</td>
<td>Permittivity</td>
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<tr>
<td>ε₀</td>
<td>Free-Space Permittivity</td>
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<tr>
<td>εᵣ</td>
<td>Relative Permittivity</td>
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<tr>
<td>η</td>
<td>Characteristic Wave Impedance</td>
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<tr>
<td>η₀</td>
<td>Free-Space Characteristic Wave Impedance</td>
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<tr>
<td>λ</td>
<td>Wavelength</td>
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<tr>
<td>µ</td>
<td>Permeability</td>
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<td>µ₀</td>
<td>Free-Space Permeability</td>
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<tr>
<td>µᵣ</td>
<td>Relative Permeability</td>
</tr>
<tr>
<td>σ</td>
<td>Electric Conductivity</td>
</tr>
<tr>
<td>vₚ</td>
<td>Phase Velocity</td>
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<tr>
<td>χ</td>
<td>Electric Susceptibility</td>
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<tr>
<td>χ⁽¹⁾</td>
<td>First-Order Susceptibility</td>
</tr>
<tr>
<td>χ⁽³⁾</td>
<td>Third-Order Susceptibility</td>
</tr>
<tr>
<td>ω</td>
<td>Angular Frequency</td>
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<tr>
<td>B</td>
<td>Magnetic Flux Density</td>
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<tr>
<td>D</td>
<td>Electric Flux Density</td>
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<tr>
<td>E</td>
<td>Electric Field</td>
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<tr>
<td>H</td>
<td>Magnetic Field</td>
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<tr>
<td>Symbol</td>
<td>Description</td>
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<td>------------------------------</td>
</tr>
<tr>
<td>$P$</td>
<td>Polarization</td>
</tr>
<tr>
<td>$\vec{k}$</td>
<td>Wavevector</td>
</tr>
<tr>
<td>$\vec{k}_p$</td>
<td>Floquet Wavevector</td>
</tr>
<tr>
<td>1D</td>
<td>One-Dimensional</td>
</tr>
<tr>
<td>2D</td>
<td>Two-Dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three-Dimensional</td>
</tr>
<tr>
<td>ADI</td>
<td>Alternating-Direction Implicit</td>
</tr>
<tr>
<td>BPM</td>
<td>Beam Propagation Method</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy (limit)</td>
</tr>
<tr>
<td>CL</td>
<td>Complex-Looped</td>
</tr>
<tr>
<td>DFT</td>
<td>Discrete Fourier Transform</td>
</tr>
<tr>
<td>EBG</td>
<td>Electromagnetic Bandgap</td>
</tr>
<tr>
<td>FDTD</td>
<td>Finite-Difference Time-Domain</td>
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<tr>
<td>GHz</td>
<td>Gigahertz ($10^9$ Hz)</td>
</tr>
<tr>
<td>HFSS</td>
<td>High-Frequency Structure Simulator (Ansoft)</td>
</tr>
<tr>
<td>IDFT</td>
<td>Inverse Discrete Fourier Transform</td>
</tr>
<tr>
<td>MHz</td>
<td>Megahertz ($10^6$ Hz)</td>
</tr>
<tr>
<td>MoM</td>
<td>Method of Moment</td>
</tr>
<tr>
<td>NRI</td>
<td>Negative-Refractive Index</td>
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<tr>
<td>NRI-TL</td>
<td>Negative-Refractive Index Transmission Line</td>
</tr>
<tr>
<td>PBC</td>
<td>Periodic Boundary Condition</td>
</tr>
<tr>
<td>PML</td>
<td>Perfectly Matched Layer</td>
</tr>
<tr>
<td>PRI</td>
<td>Positive-Refractive Index</td>
</tr>
<tr>
<td>PRI-TL</td>
<td>Positive-Refractive Index Transmission Line</td>
</tr>
<tr>
<td>RL</td>
<td>Real-Looped</td>
</tr>
<tr>
<td>THz</td>
<td>Terahertz ($10^{12}$ Hz)</td>
</tr>
<tr>
<td>TLM</td>
<td>Transmission Line Matrix</td>
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TM  Transverse-Magnetic
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Chapter 1

Introduction

Numerical modeling of periodic structures in the time domain is conventionally based on terminating one unit cell with periodic boundary conditions (PBCs). The scheme is widely adopted to obtain dispersion properties of periodic structures. By scanning the irreducible Brillouin zone, the modal frequencies corresponding to a single wavenumber inside an infinitely periodic structure is obtained during each simulation.

Although such a scheme efficiently characterizes the dispersion property of infinitely periodic structures, the ample information contained in the periodic analysis is yet to be directly exploited in the simulations of practical periodic-structure-related problems. The direct application of the PBC in these problems is prevented by: 1) The spatial finiteness of excitations inside periodic structures; 2) the combination of periodic structures with non-periodic elements, such as printed circuits or antennas; 3) the finiteness of periodic structures themselves; and finally 4) the dependence of material properties on the local field intensity due to nonlinearity, which breaks the spatial periodicity. Figure 2.1 shows two periodic-structure-related problems, including a free-space transmission-line super-lens excited by a point source, and a microstrip line on a substrate with a patterned ground. Typically, information from dispersion analysis, such as the Bloch impedance of the unit cell, serves as design guidelines. However, to obtain the response of the device,
1.1 Background and Motivation

The interest in the modeling of periodic structures stems from the many applications they can support. The research of periodic structures, which can be traced back to 1950s and 1960s, leads towards the development of several categories of applications, including frequency selective surfaces [3], photonic and electromagnetic band-gap (EBG) crystals [4, 5], superlattices [6], or artificial dielectrics [7], varying in the electric sizes of the unit cell and design purposes. In nonlinear optics, optical superlattices and photonic crystals [4] with nonlinearity have been adopted for various applications, such as optical switching [8, 9] and frequency conversion [10].

From the last decade, the interest in artificial dielectrics has been enhanced by the experimental verification [11] of the negative-refractive-index (NRI) media proposed by the theoretical work of Veselago and Pendry [12, 13]. Since then, extensive research
activities have been aimed at synthesizing media with unusual macroscopic properties (metamaterials [14–16]). Along with this trend, numerical tools that can capture unconventional wave effects observed in metamaterial geometries such as the growth of evanescent waves, negative refraction, or negative group velocity, and illuminate the underlying physics have been proposed. To this end, time-domain techniques, such as the Finite-Difference Time-Domain (FDTD) [17], are particularly useful, because they effectively model the rich transients involved in the evolution of these effects. The potential of FDTD to significantly contribute to understanding the nature of wave propagation in synthesized media has been demonstrated in several papers. In [18–20], the causal evolution of backward waves in NRI media was illustrated numerically via FDTD. Moreover, sub-wavelength focusing enabled by NRI slabs was demonstrated using FDTD [21] and Transmission-Line Matrix (TLM) method [22]. In [23], the transient and steady state time-domain field inside NRI media were simulated using the extended FDTD method incorporating lumped elements [24].

To simulate linear periodic structures in FDTD, PBCs are developed to terminate the computational domain with a single unit cell. These PBCs are based on the time-domain translation of the Floquet’s theorem, including the direct field methods such as the angled update method [25], the spatially-looped method [26], the sine-cosine method [27] and the spectral FDTD [28], as well as the field-transformation method such as the multi-spatial grid method [29] or the split-field method [30, 31]. Conventionally, PBCs can only extract fields corresponding to one Floquet wavevector per simulation. Thus, they have been widely adopted in practical applications for the purpose of dispersion analysis. In [32], the sine-cosine method [27] was employed to analyze a two-dimensional NRI transmission-line (NRI-TL) structure [33]. In [34], this method was extended to account for leaky-wave radiation from the same structure, indicating an efficient FDTD based methodology for the concurrent computation of attenuation and phase constants of fast-waves in periodic geometries. Moreover, in an effort to investigate the possibility of
transferring the concepts of NRI-TL from the microwave to the optical regime (along the lines of [35]), a conformal periodic FDTD analysis of plasmonic nano-particle arrays in a triangular mesh was presented in [36].

More recently, the problem of efficiently modeling driven periodic structures by means of PBCs was investigated. Since the presence of a non-periodic source is not compatible with the use of PBCs, this problem would be typical handled by simulating a finite version of the periodic structure, up to the number of cells necessary to achieve the convergence of the solution. Evidently, the efficiency of this approach largely depends on the nature of the problem at hand and may be quite costly in terms of execution time and computer memory. In the frequency domain, the similar problem was addressed in [37] in the context of the Method of Moments (MoM) by invoking the array-scanning method of [38], to model the interaction of a printed microstrip line with an EBG substrate. The efficiency of the algorithm was further enhanced by the application of Kummer’s transformation [39]. In [40], the combination of FDTD and the array-scanning method was introduced, and in parallel with this work, the same problem was independently considered by Qiang et al. in [41,42], from the viewpoint of a spectral FDTD method [28].

For nonlinear periodic structures, PBCs are not applicable, since the material properties depend on the spatial field intensity, thus interrupting the spatial periodicity. However, attempts can still be made to improve the efficiency of the time-domain modeling of general nonlinear structures. In optical applications, the Beam-Propagation Method (BPM) [43,44] is widely used as an efficient numerical tool for time-domain simulations. Based on a simplified form of the Helmholtz equation, BPM offers a fast means to calculate time-domain optical beams in inhomogeneous media. However, due to the fact that BPM automatically neglects backward propagation modes, its accuracy is compromised when dealing with media with strong nonlinearity or high permittivity contrast along the direction of propagation. Recently, efforts have been made to accelerate FDTD simulations with nonlinear media. In [45], the well-know unconditionally stable Alternating-
Direction Implicit FDTD (ADI-FDTD) was extended to simulate nonlinear media via a
z-transform method, allowing time step sizes beyond the stability limit in FDTD.

1.2 Objectives

The objectives of this thesis work include the following aspects: (1) the development
of an efficient scheme for FDTD modeling of the interaction between broadband, non-
periodic sources and periodic structures through a small number of low-cost simulations
with only one unit cell; (2) the efficient FDTD modeling of the interaction between non-
periodic microstrip lines/antennas and periodic substrates via PBCs; (3) the validation
of efficiency and accuracy of the above algorithms as a unified FDTD mesh truncation
method; and (4) the fast characterization of finite nonlinear periodic stacks via FDTD.

1.3 Outline

Chapter 2 states the problem of a periodic structure driven by a non-periodic source and
the reason why it is not directly solvable via conventional PBC-based methods. A brief
introduction is given on different categories of PBCs in FDTD. A rigorous derivation of
the sine-cosine method is formulated, showing that it can be applied for the broadband
characterization of periodic structures. The sine-cosine method is then combined with
the time-domain form of the array-scanning method to offer an efficient solution to driven
periodic structures. In Chapter 3, the methodology proposed in Chapter 2 is validated
by a transmission-line metamaterial “perfect lens” example. The efficiency and accuracy
of the method is discussed in detail. The scheme is then further extended to model
non-periodic metallic objects such as microstrip lines and antennas, by introducing a
combined PBC/absorber termination. The far-field radiation pattern calculation and
the antenna feed modeling under the proposed scheme are also discussed. Chapter 4
revisits the sine-cosine array-scanning FDTD in a mesh-truncation point of view and
compares its performance with conventional mesh termination method such as Perfectly Matched Layer (PML) absorbers. It is proved that the method offers a unified treatment for mesh truncation regardless the dispersion and conductivity of the media, and is able to deliver comparable, and potentially better, performance with PMLs. Lastly, Chapter 5 offers two efficient alternatives to accelerate nonlinear FDTD, both aiming to extend the time step size in FDTD beyond conventional stability limit. The two methods are applied to efficiently simulate a finite nonlinear periodic stack in the optical regime.
Chapter 2

Formulation of a Sine-Cosine Array-Scanning FDTD Method

A methodology to efficiently model the interaction between a non-periodic source and an infinitely periodic structure in the time domain is discussed in this chapter. The theory of time-domain periodic boundaries is briefly introduced. Among different boundary conditions, the sine-cosine method is discussed in detail, with emphasis on its broadband characteristic. The sine-cosine boundary is then further combined with a time-domain version of the array-scanning method to offer a fast and accurate solution for the problem at hand based on a number of small and low-cost simulations.

2.1 Problem Statement

Figure 2.1 depicts a broadband, non-periodic source interacting with an infinitely periodic geometry, which is frequently encountered in periodic structure related problems, such as electromagnetic bandgap (EBG) structures and artificial dielectrics. For simplicity, the geometry is assumed to be two-dimensional (2D). Due to the presence of a non-periodic source, this problem would be conventionally handled by simulating a finite version of the periodic structure, up to the number of cells necessary to achieve the convergence of
Figure 2.1: Geometry of the problem under consideration: a non-periodic source exciting a 2D, infinite periodic structure of spatial period $d_x$ and $d_y$ along the $x$- and $y$-axis.

the solution. Evidently, the efficiency of this approach largely depends on the nature of the problem at hand and may be quite costly in terms of execution time and computer memory.

Instead of approximating the infinite periodic structure by a truncated version of it, the proposed solution in this work is based on the computational domain of Fig. 2.2(a), where periodic boundary conditions (PBCs) are applied to the electric field phasors (denoted by $\tilde{\cdot}$) at the boundaries along the two directions of periodicity:

$$\tilde{E}(\tau + \vec{p}) = \tilde{E}(\tau) \exp (-j\vec{k}_p \cdot \vec{p})$$  \hspace{1cm} (2.1a)

$$\tilde{H}(\tau + \vec{p}) = \tilde{H}(\tau) \exp (-j\vec{k}_p \cdot \vec{p})$$  \hspace{1cm} (2.1b)

where $\vec{p} = \hat{x}d_x + \hat{y}d_y$ is the lattice vector of the periodic structure and $\vec{k}_p = \hat{x}k_x + \hat{y}k_y$ is a Floquet wavevector.

However, several problems arise from the proposed computational domain. First, a suitable PBC is required to terminate the problem of Fig. 2.2(b). The PBC applied must admit broadband incident waves, while at the same time being able to stably scan the complete irreducible Brillouin zone. Second, and most importantly, the proposed
Figure 2.2: a) Proposed computational domain for the problem in Fig. 2.1. b) Problem corresponding to the computational domain shown above. ©(2008)IEEE.

The computational domain leads to the solution of the problem shown in Fig. 2.2(b), where the response of the structure to an array, consisting of phase-shifted, periodic replicas of the original source is determined. (In Fig. 2.2(b), $\phi_x = k_x d_x$, $\phi_y = k_y d_y$.)

The purpose of this chapter is thus two-fold. First, it is rigorously shown that the sine-cosine method of [27] can be applied for the broadband characterization of periodic structures, although it had been originally suggested that its applicability was limited to monochromatic simulations [17]. On the contrary, a new formulation of the method offers new insights to its broadband character and the sources necessary to excite Floquet modes in a sine-cosine based Finite-Difference Time-Domain (FDTD) mesh. This paves
the way for the coupling of the sine-cosine method with the array-scanning technique, which results in an efficient modeling tool for the interaction of broadband, non-periodic sources with periodic geometries, based on a small number of low-cost simulations.

2.2 Time-Domain Periodic Boundary Conditions

To efficiently characterize periodic structures, periodic boundaries are applied in FDTD to limit the computational domain to a single unit cell. Such boundaries are based on Floquet’s theorem, i.e. applying a time-domain interpretation of (2.1a) and (2.1b) to update field components on periodic boundaries. Such an update usually consists of a spatially-looped two-stage process. Figure 2.3 shows the example of field components at periodic boundaries, within an FDTD lattice of Yee cells, assuming TM polarization. The black squares/dots denote field components available from FDTD updates, and the white ones denote unknown components that require updates using (2.1a) and (2.1b). In the first stage, the magnetic field value at the boundary \( y = d_y + \Delta y/2 \) is calculated using (2.1b); in the second stage, the Electric field at \( y = d_y \) is obtained from FDTD update, and the field value at \( y = 0 \) can thus be computed from (2.1a).

In FDTD, a time-domain version of the Floquet’s theorem to calculated these unknown field components on periodic boundaries in Fig. 2.3 can be obtained by performing an inverse Fourier transform on (2.1a) and (2.1b):

\[
E_z(x, 0, t) = E_z(x, d_y, t + \frac{k_y d_y}{\omega_0}) \quad (2.2a)
\]

\[
H_x(x, dy + \Delta y/2, t) = H_x(x, \Delta y/2, t - \frac{k_y d_y}{\omega_0}) \quad (2.2b)
\]

with each modal frequency \( \omega_0 \). For normal incidence where \( k_y = 0 \), (2.2a) and (2.2b) can be computed concurrently in the same time step in FDTD. However, for \( k_y > 0 \), (2.2a) requires future values of \( E_z \), which is not available in a time-stepping scheme. The same situation applies to (2.2b) when \( k_y < 0 \).
To resolve this problem, two general categories of PBCs have been developed under the FDTD scheme. The first category, i.e. the direct-field methods, directly deals with the original electric and magnetic field. Among these methods, the spatially-looped FDTD [26], the spectral FDTD [28], and the sine-cosine method [27] work directly with the complex field components to avoid the requirement of time-advance data, and the real and imaginary part of the fields are coupled at the periodic boundary through update equations. On the contrary, the angled update method [25] uses an artificial “slant” domain to introduce a numerical time gradient between periodic boundaries, which offsets the time gradient of the Floquet modes. For all the direct-field methods, additional auxiliary domains are needed, i.e. the “slant” domain for the angled update method, and computational domain for the update of the imaginary part of the field for the rest of the methods.

The field transformation methods, on the other hand, work on auxiliary field quantities $\tilde{P} = \tilde{E} \exp(-j\vec{k}_p \cdot \tau)$ and $\tilde{Q} = \tilde{H} \exp(-j\vec{k}_p \cdot \tau)$. Since the time gradient is absorbed in the expression of $\tilde{P}$ and $\tilde{Q}$, no time-advance data are needed. Such methods include
the multi-spatial grid method [29] and the split-field method [30, 31]. The field transformation methods do not need additional memory space for auxiliary computational domains. However, this advantage is accompanied by increased complexity of the update scheme.

The numerical stability is a crucial issue for most PBCs. For field transformation methods such as the split-field method and the multi-spatial grid method, the stability is largely associated with the Floquet wave vector associated with the boundary. When $\mathbf{k} \cdot \mathbf{d}$ approaching $\pm \pi$, the maximum time step size to guarantee a stable simulation tends to zero, making these methods impractical for dispersion analyses, where $\mathbf{k}$ varies within the complete irreducible Brillouin zone, i.e. $-\pi \leq \mathbf{k} \cdot \mathbf{d} \leq \pi$. For direct-field methods, the stability of the real-looped (RL) version of the spatially-looped FDTD is also limited by the incident wave angle, while a maximum time step number is applied on the angled update method to guarantee its stability. On the contrary, the complex-looped (CL) version of the spatially-looped FDTD, the sine cosine method, and the spectral FDTD are always stable regardless of the Floquet wavevector of the PBC.

2.2.1 The Sine-Cosine Method: a Rigorous Derivation

In a periodic structure with lattice vector $\mathbf{\bar{p}}$, the frequency domain field component can be decomposed into a number of Floquet modes

$$E(\mathbf{r}, \omega) = \sum_p E(\mathbf{k}_p, \mathbf{\tau}, \omega) e^{-j\mathbf{k}_p \cdot \mathbf{r}}$$

(2.3)

where $\mathbf{k}_p$ is the Floquet vectors associated with the $p$–th Floquet mode under frequency $\omega$, and $\mathbf{\tau}$ is an observation point inside the periodic structure. To this end, a field expansion of the time-domain field in terms of Floquet modes can be obtained by performing
an inverse Fourier transform on (2.3) and rearranging the terms:

\[
E(r, t) = \text{Re} \left\{ \sum_p E(k_p, r, \omega) e^{-j k_p \cdot r} \right\} e^{j \omega t} d\omega
\]

\[
= \text{Re} \sum_p e^{-j k_p \cdot r} \frac{1}{2\pi} \int_{\omega(k_p)} E(k_p, t) e^{j \omega t} d\omega
\]

\[
= \text{Re} \sum_p e^{-j k_p \cdot r} E(k_p, r, t)
\]

\[
= \text{Re} \sum_p \left\{ E^p_c(r, t) - j E^p_s(r, t) \right\}
\]

(2.4)

where \(\omega(k_p)\) is an either discrete or continuous spectrum of frequencies corresponding to the Floquet wavevector \(k_p\) and:

\[
E^p_c(r, t) = \cos (k_p \cdot r) E(k_p, t)
\]

(2.5a)

\[
E^p_s(r, t) = \sin (k_p \cdot r) E(k_p, t).
\]

(2.5b)

Note that these two waves have identical frequency spectra (as they share a common temporal dependence). Moreover,

\[
E^p_c(r + p, t) = \cos (k_p \cdot r + k_p \cdot p) E(k_p, t)
\]

\[
= \cos (k_p \cdot p) \cos (k_p \cdot r) E(k_p, t) - \sin (k_p \cdot p) \sin (k_p \cdot r) E(k_p, t)
\]

\[
= \cos (k_p \cdot p) E^p_c(r, t) - \sin (k_p \cdot p) E^p_s(r, t).
\]

(2.6)

Similarly,

\[
E^p_s(r + p, t) = \sin (k_p \cdot p) E^p_c(r, t) + \cos (k_p \cdot p) E^p_s(r, t).
\]

(2.7)

It is now clear the (2.6) and (2.7) can be exploited to update field components at the boundary of a periodic unit cell, and it is the exact formulation mentioned in [27]. To apply this method, two identical computational domains are set up and excited with identical sources, each representing the field component \(E_c\) and \(E_s\). The unknown electric field along the periodic boundary is computed from (2.6) and (2.7), and the magnetic field can be computed following the same way. For example, in Fig. 2.3, the unknown
field component can be updated by:

\[ H_{xc}(x, d_y + \Delta y/2, t) = \cos (k_y d_y) H_{xc}(x, \Delta y/2, t) - \sin (k_y d_y) H_{xs}(x, \Delta y/2, t) \] (2.8a)

\[ H_{xs}(x, d_y + \Delta y/2, t) = \sin (k_y d_y) H_{xc}(x, \Delta y/2, t) + \cos (k_y d_y) H_{xs}(x, \Delta y/2, t) \] (2.8b)

\[ E_{zc}(x, 0, t) = \cos (k_y d_y) E_{zc}(x, d_y, t) + \sin (k_y d_y) E_{zs}(x, d_y, t) \] (2.8c)

\[ E_{zs}(x, 0, t) = - \sin (k_y d_y) E_{zc}(x, d_y, t) + \cos (k_y d_y) E_{zs}(x, d_y, t). \] (2.8d)

These formulations offer new insights into the sine-cosine method. Clearly, the two waves in (2.6) and (2.7) are neither monochromatic nor at phase quadrature in time. In fact, the sine/cosine waves are distinguished based on their spatial rather than temporal dependence. Therefore, they can be excited by identical broadband sources (instead of sine/cosine modulated ones), provided that the frequency spectrum of such sources includes \( \omega(k_p) \). With \( E_p^C(r, t) \), \( E_p^S(r, t) \) being excited (in their respective meshes), their spectral analysis yields all frequencies \( \omega(k_p) \) at once. This is demonstrated through the numerical results of the following section.

### 2.2.2 Numerical Validation

The broadband validity of the sine-cosine method is verified through the dispersion analysis of a negative-refractive-index transmission-line (NRI-TL) structure. Consider the unit cell of the 2D NRI-TL structure that was originally presented in [33], shown in Fig. 2.4(a). The corresponding positive-refractive index transmission-line (PRI-TL) unit cell is also appended in Fig. 2.4(b).

This unit cell resides on a substrate of thickness 1.52 mm and relative permittivity \( \varepsilon_r = 3 \). The spatial periods \( d_x \) and \( d_y \) (indicated in Fig. 2.4) are both equal to 8.4 mm. The width \( w \) of the microstrip lines is 0.75 mm. In the FDTD mesh, the NRI unit cell is discretized by \( 22 \times 22 \times 16 \) Yee cells. Three of the sixteen cells in the \( z \)-direction model the substrate. The open boundary in the vertical direction is simulated by a uniaxial Perfectly Matched Layer absorber [17]. This absorber consists of ten cells with
a fourth-order polynomial conductivity grading. The maximum conductivity value is $\sigma_{\text{max}} = 0.01194/\Delta$, with $\Delta$ being the Yee cell size in the direction of mesh truncation (hence, in this case that the open boundary is parallel to the $x-y$ plane, $\Delta = \Delta_z$).

Moreover, the serial capacitor and the shunt inductor, shown in Fig. 2.4(a), are chosen to be $C = 3.34$ pF and $L = 16.02$ nH. The two sine-cosine grids are excited by a 0.5-3 GHz Gabor pulse:

$$\exp\left(\frac{t - t_0}{t_w}\right)^2 \sin (2\pi f_c t)$$

applied to the $E_z$ components in cells (6,11,1), (6,11,2), (6,11,3) inside the substrate. The Gabor pulse parameters are $t_w = 624$ ps and $t_0 = 3t_w$. The time step is set to 0.723 ps and 60,000 time steps are performed for three cases of $k_x d_x = 0.0833\pi$, 0.167\pi.
and 0.333\pi, while \( k_y = 0 \). Hence, all three points are along the \( \Gamma - X \) portion of the Brillouin diagram of the structure that is occupied by three TM waves, as shown in previous studies as well [32]: a backward, a forward and a surface wave. In Figs. 2.5, 2.6 and 2.7, the \( \Gamma - X \) part of the Brillouin diagram for the NRI-TL unit cell, independently determined by Ansoft’s HFSS, is shown along with the magnitude of the Fourier transform (normalized to its maximum) of a vertical electric field component \( E_z \) determined by the sine-cosine FDTD method and sampled within the substrate, from 0-5 GHz. For each case of \( k_x d_x \), the FDTD-calculated field presents multiple resonances, which correspond to the frequencies \( \omega(k_x d_x) \), given by the intersections of the diagram with the constant \( k_x d_x \) lines. Hence, the FDTD and HFSS calculated resonant frequencies are in excellent agreement. Moreover, it is clearly shown that a single run of the sine-cosine FDTD, with the same excitation for each grid, is sufficient to determine all resonant frequencies at
Figure 2.6: On the left: magnitude of the Fourier transform (normalized to its maximum) of a vertical electric field component $E_z$ within the substrate of the NRI-TL unit cell of Fig. 2.4(a), determined by the sine-cosine FDTD for $k_x d_x = 0.167 \pi$. On the right: Dispersion diagram ($\Gamma - X$) for the unit cell of Fig. 2.4(a), determined by Ansoft HFSS.

Note that the boundary conditions (2.6), (2.7) enforce the Floquet wavevector, while they are independent of frequency, thus setting up an eigenvalue problem in the time-domain, where only the modes with that given wavevector are excited. This is analogous to the way FDTD can be used to characterize cavity resonances or waveguide dispersion [46] over a broad-bandwidth.

2.3 The Sine-Cosine Array-Scanning FDTD

The combination of PBCs with a broadband source leads to the solution of the problem shown in Fig. 2.2(b), where the response of the structure to an array, consisting of phase-shifted, periodic repetitions of the original source, is determined. It is the purpose of the array-scanning technique to isolate the effect of the original source, as described below.
Figure 2.7: On the left: magnitude of the Fourier transform (normalized to its maximum) of a vertical electric field component $E_z$ within the substrate of the NRI-TL unit cell of Fig. 2.4(a), determined by the sine-cosine FDTD for $k_x d_x = 0.33 \pi$. On the right: Dispersion diagram ($\Gamma$ – $X$) for the unit cell of Fig. 2.4(a), determined by Ansoft HFSS.

The array-scanning method is first proposed in [38], as a means to characterize the mutual impedance between a single element inside an infinite array and an exterior element. Given the total vector potential of the array $\vec{A}_{array}(\vec{k})$, where $\vec{k} = k_x \hat{x} + k_y \hat{y}$ is the propagation constant of an incident plane wave, the vector potential of the center element of the array can be isolated through an integration of plane wave expansion

$$A_0 = \int_{-\pi/d_x}^{\pi/d_x} \int_{-\pi/d_y}^{\pi/d_y} \vec{A}_{array} dk_x dk_y.$$  \hspace{1cm} (2.10)

Here $d_x$ and $d_y$ are the periodicities of the array in the $x$– and the $y$–directions. This method can be easily generalized to calculate any field components.

By generalizing the original expression of the array-scanning method and transferring it into the time-domain expression, the method is combined with the sine-cosine boundary condition to solve the problem of Fig. 2.1(a). Let $\vec{E}_{array}(\vec{r}_0, \vec{k}_p, t)$ be the electric field determined by the sine-cosine method, at a point $\vec{r}_0$ within the unit cell, for a Floquet
wavevector \( \vec{k}_p = \hat{x}k_x + \hat{y}k_y \) within the Brillouin zone of the structure (hence, \(-\pi/d_x \leq k_x \leq \pi/d_x \) and \(-\pi/d_y \leq k_y \leq \pi/d_y \)). The electric field \( \vec{E}_0 \) at this point that is only due to the original source can be found by integrating over \( k_x, k_y \):

\[
\vec{E}_0(\tau_0, t) = \frac{d_x d_y}{4\pi^2} \int_{-\pi/d_x}^{\pi/d_x} \int_{-\pi/d_y}^{\pi/d_y} \vec{E}_{\text{array}}(\tau_0, \vec{k}_p, t) \, dk_x dk_y. \tag{2.11}
\]

Since (2.11) is a continuous integral, while only \( N \) discrete \( k_x \) and \( M \) discrete \( k_y \) points are sampled, (2.11) is approximated at a time \( t = l\Delta t \) (the \( l \)-th time-step of the FDTD method) by the sum:

\[
\vec{E}_0(\tau_0, l\Delta t) \approx \frac{1}{NM} \sum_{n=-N/2}^{N/2} \sum_{m=-M/2}^{M/2} \vec{E}_{\text{array}}(\tau_0, \hat{x} \frac{2\pi n}{Nd_x} + \hat{y} \frac{2\pi m}{Md_y}, l\Delta t). \tag{2.12}
\]

Particularly, a modified form of (2.12) can be employed to determine the electric field at points outside the simulated unit cell, by invoking the PBCs (2.1a). In particular,

\[
\vec{E}_0(\tau_0 + \vec{p}_{I,J}, l\Delta t) \approx \frac{1}{NM} \sum_{n=-N/2}^{N/2} \sum_{m=-M/2}^{M/2} \vec{E}_{\text{array}}(\tau_0, \hat{x} \frac{2\pi n}{Nd_x} + \hat{y} \frac{2\pi m}{Md_y}, l\Delta t) \\
\cdot \exp \left( -j\vec{k}_p \cdot \vec{p}_{I,J} \right) \tag{2.13}
\]

with \( \vec{p}_{I,J} = \hat{x}Id_x + \hat{y}Jd_y \), for integer \( I, J \).

### 2.4 Summary

The sine-cosine method enables the FDTD modeling of periodic structures by simulating a single unit cell. The wideband validity of the method was rigorously proved, and the method was combined with the array-scanning technique to incorporate the existence of non-periodic sources in FDTD. Thus, a fast and accurate approach for the time-domain modeling of driven periodic structures was formulated, with the potential to offer a simplified modeling scheme for periodic structure related problems. The efficiency and accuracy of the proposed scheme will be analyzed in detail in the next chapter, along with extensions of the method to several classes of practical applications.
Chapter 3

Sine-Cosine Array-Scanning FDTD
Modeling of Driven Linear Periodic Structures

In this chapter, the sine-cosine method is combined with the time-domain array-scanning method to efficiently solve several practical classes of problems. The ability of the methodology to characterize an infinitely periodic structure under a non-periodic excitation based on a number of small, low-cost simulations is first demonstrated with the example of a transmission-line based “perfect lens”. Then, such a numerical scheme is generalized to include non-periodic metallic objects, thus extending its application to finite planar microstrip-line structures, by introducing a novel, composite periodic/absorbing boundary condition. Finally, the modeling of antennas over periodic structures via the proposed methodology is discussed in detail.
3.1 Modeling of Periodic Microstrip-Line Structure: Negative-Refractive Index Transmission-Line “Perfect Lens”

Figure 3.1: The top view of an NRI-TL microwave “perfect lens” with infinite number of unit cells in the $x$–direction.

In this section, the sine-cosine method and the array-scanning Finite-Difference Time-Domain (FDTD) is applied to analyze the microwave implementation of Pendry’s concept of a “perfect lens” [13] that has been recently proposed and experimentally demonstrated [47]. The structure utilizes the unit cells of two-dimensional (2D) positive and negative-refractive-index transmission lines (NRI-TLs)

A microwave “perfect lens” contains several infinite layers of NRI cells presented in Fig. 2.4 of Section 2.2.2, embedded in the positive-refractive-index transmission line (PRI-TL) network, shown in Fig. 3.1. Thus, the structure is periodic in the transverse direction, naturally lending itself to a periodic FDTD scheme.

First, the convergence properties of the sine-cosine based array-scanning FDTD are evaluated with a domain consisting of 18 PRI-TL cells in the $y$–direction. The geometry
Chapter 3.

Figure 3.2: Electric field $E_z$ in the middle of the substrate and along the $y$–axis in a PRI-TL which is periodic in the $x$–direction. The sine-cosine array-scanning FDTD with a variable number of $k_x$-points, $N$, is used. A sinusoidal $E_z = 1$ V/m is applied within the substrate of the first unit cell.

is treated as a one-dimensional (1D) periodic structure in the $x$–direction and simulated by the sine-cosine method, using one unit cell along the direction of periodicity, terminated at periodic boundary conditions (PBCs). The vertical electric field ($E_z$) nodes within the substrate of the first cell are excited by a sinusoidal hard source at 1 GHz. Then, the vertical electric field $E_z$ at the center of each subsequent cell is determined, in the middle of the substrate, from the array-scanning equation. The standard approach to this problem, namely the use of a finite number of cells along the $x$–direction until a convergent solution is attained, has also been implemented. In both simulations, the time step is set to 0.723 ps and the total number of time steps is 16,384.

The results of the two approaches are presented in Figs. 3.2, 3.3, respectively, which include diagrams of the computational domains used. It is noted that the sine-cosine based array-scanning FDTD converges with $N = 16$ $k_x$-points, or a sampling rate of $0.125\pi$ rad/m in the wave number domain. On the other hand, 17 cells are needed for
Figure 3.3: Electric field $E_z$ in the middle of the substrate and along the $y$–axis in a PRI-TL, for 5-31 unit cells in the $x$–direction. A sinusoidal $E_z = 1$ V/m is applied within the substrate of the first unit cell.

The field in the finite structure in the $x$–direction to converge within 1 % of the fields of the infinite periodic one.

The convergence properties of the two methods are summarized in Fig. 3.4, which depicts the relative error norm:

$$\mathcal{E} = \sum_j \left( \frac{E_z(j) - E_z^{ref}(j)}{E_z^{ref}(j)} \right)^2$$  \hspace{1cm} (3.1)

where $E_z(j)$ is the $z$-component of the electric field in the middle of the substrate and along the $y$–axis, calculated with the array-scanning FDTD and finite structure simulations (plotted in Figs. 3.2, 3.3, respectively) and $E_z^{ref}$ is the same field calculated with a 32-cell finite structure FDTD simulation. The error norm $\mathcal{E}$ is plotted with respect to the number of $k_x$ points used for the array-scanning based field calculation and with respect to the number of cells in the transverse direction used for the finite structure field calculation.
Figure 3.4: Error norm $E$ of eq. (3.1) with respect to the number of $k_x$ points used for the array-scanning based field calculation and with respect to the number of cells in the transverse direction used for the finite structure field calculation. ©(2008)IEEE.

The electric field amplitude decays away from the source, as expected. As discussed in [47], this amplitude decay, and the resulting loss of the evanescent spectral components of the source, can be compensated for by introducing a layer occupied by the NRI-TL cells of Fig. 2.4(a). To achieve the matching of this layer to the PRI-TL half-spaces (to the left and right of it) at 1 GHz, the choice of the loading elements is the same as in last section. Then, the characteristic impedance of both lines becomes 50 Ω. The domain is excited by a 1 GHz sinusoidal hard source, that is placed two and a half unit cells away from the first interface. Note that the NRI region occupies five cells, twice as many as the distance of the source and the image plane from the positive-to-negative index interfaces.

The expected electric field ($E_z$) amplitude growth within the NRI slab is verified by the sine-cosine based array-scanning FDTD, as shown in Fig. 3.5, which includes a diagram of the computational domain. For these results, 16 $k_x$-points have been calculated. For comparison, the results of a finite structure simulation, employing 17 cells in
Figure 3.5: Vertical electric field $E_z$ in the middle of the substrate and along the $y-$axis in a planar microwave lens geometry, calculated via the sine-cosine array-scanning FDTD (N=16) and a finite structure simulation, using 17 cells in the $x-$direction.

the transverse $x-$direction, are appended, being in good agreement with the sine-cosine based array-scanning results. It is noted that the field amplitude growth effect is due to resonant coupling between the two interfaces and therefore builds up rather slowly during the time-domain simulation. The steady-state is reached in 60,000 time steps.

The sine-cosine based array-scanning FDTD simulation is run on a grid server. Each wavenumber simulation takes 2454 second, as opposed to 20513 seconds with the finite structure simulation running on a single server.

The field pattern of Fig. 3.5 indicates that the matching of the PRI and the NRI regions is imperfect, mainly because the excitation has a finite spatial period due to the implementation of the array-scanning method. It should be noted that the cause of the mismatch is different from that in the experimental results of [47]. The latter is mainly
caused by the finiteness of the structure in the transverse direction. Such a mismatch leads to an imperfect restoration of the source at the image plane (two and a half unit cells from the second interface), which is still better than the conventional diffraction-limited case. Indeed, Fig. 3.6 shows the electric field \( E_z \) amplitude at the source and the image plane (along the transverse direction), determined via the aforementioned sine-cosine based array-scanning FDTD and finite structure simulations. The 2D diffraction-limited source image \( V_{diff}^2 \) (for an all positive-index space) considering the exponential decay of the evanescent components is also appended, which is given by \[48\]

\[
V_{diff}^2(\nu_d) = I_0 Z_p k_p d_x \frac{\exp[-j(k_{py} + k_{ny})D - jk_x \nu_d]}{k_{py}} \int_{-\pi/d_x}^{\pi/d_x} dk_x (3.2)
\]

where \( Z_p \) and \( k_p \) are the effective impedance and wave number in the positive-refractive-index region, \( D \) is the distance between the source plane and the focal plane, and \( k_{py} \) and \( k_{ny} \) are the \( y \)-directional wave number in the free-propagation and the lens region, chosen so that \( k_{ny} = k_{py} \) in the propagation spectrum and \( k_{ny} = -k_{py} \) in the evanescent spectrum. It is noted that the half-power beam-width of the source image extends over four cells, whereas the diffraction-limited image extends over six cells. These patterns are in excellent agreement with the experimental results of [47] for the same structure and offer the first full-wave validation of those.

The vertical field values in the transverse direction, beyond the simulated unit cell, shown in Fig. 3.6 have been calculated by means of (2.13). Note that there are significant field values in up to about 6 unit cells in the \( \pm x \)-direction. As a result, applying (3.7) with \( W_x \approx 6d_x \), yields \( N \geq 12 \), as a limit for the number of \( k_x \) points needed for the reconstruction of the field profile in the spatial domain.

### 3.2 Discussion about Accuracy and Efficiency

Beside the computational complexity arising from the unit cell of the structure itself, the accuracy of the proposed method is largely influenced by the sampling numbers of
Figure 3.6: Electric field $E_z$ in the middle of the substrate along the $x$–axis in a planar microwave lens geometry, calculated via the sine-cosine array-scanning FDTD (N=16) and a finite structure simulation, using 17 cells in the $x$–direction, at the source and the image (focal) plane. All fields have been normalized to their maximum amplitude.

points inside the Brillouin zone. So does the efficiency of the method, in the sense that the sampling number actually determines the number of the low-cost simulations to run.

For a 2D structure implementing the array-scanning FDTD with $N$ and $M$ uniform samples in the $k_x$ and $k_y$ axis, the sampling error can be expressed in terms of alias terms in the space-domain due to the finite sampling rate in the spectral domain as [49]:

$$
\epsilon(\tau_0, t) = \frac{|\sum_{h,l\neq0} F_{ref}(\tau_0 + hN d_x \hat{x} + lM d_y \hat{y}, t)|}{|F_{ref}(\tau_0, t)|}. \quad (3.3)
$$

In (3.3), the vector $F_{ref}(\tau, t)$ represents a reference solution to the problem at hand. If an analytical solution exists, it can be directly used in the estimate of (3.3). Alternatively, $F_{ref}(\tau, t)$ can be obtained from an FDTD simulation with a dense mesh and a large number of cells, to prevent waves reflected from the terminating boundaries from affecting the working volume. Both alternatives are useful primarily for benchmarking the method.
in canonical problems.

The PRI-TL cell mentioned in last section is simulated to validate (3.3). The same computational domain setup used in the convergence analysis, consisting an array of 18 unit cells in the $y$-direction and terminated in sine-cosine periodic boundaries in the $x$-direction, is simulated. Such a transmission-line grid is analogous to a homogeneous medium, whose properties are determined by the parameters of the microstrip line. Thus, by implementing the array-scanning method with $N$ points in the $k_x$ domain, the total field at the center of the $m$-th cell can be calculated by:

$$E_z(0, md_y) = E_0 \sum_{h=-\infty}^{\infty} G(hN d_x \hat{x} + md_y \hat{y} | 0).$$  \hfill (3.4)$$

Here $G(\vec{r} | \vec{r}')$ is the 2D Green’s function

$$G(\vec{r} | \vec{r}') = \frac{j}{4} H_0^{(2)}(k | \vec{r} - \vec{r}'|)$$  \hfill (3.5)$$

where $H_0^{(2)}$ is the Hankel function of the second-kind. The calculation takes into account all significant terms larger than 0.1 percent of $E_0$. The analytical calculation is plotted in Fig. 3.7 along with the result from array-scanning FDTD. The two sets of results match well.

Moreover, (3.3) implies that as long as the actual fields tend to zero $N$ periods away in the $x$-direction and $M$ periods away in the $y$-direction, respectively, the error related to the proposed lattice termination should also go to zero. This offers a guidance in the choice of the sampling rate in practical problems. If the fields in the driven periodic structure under study are spatially limited within the area ($-W_x \leq x \leq W_x, -W_y \leq y \leq W_y$), then the sampling rates $S_x = N/(2\pi/d_x)$ samples/(rad/m) and $S_y = M/(2\pi/d_y)$ samples/(rad/m) should obey the inequalities:

$$2\pi S_x \geq 2W_x, \quad 2\pi S_y \geq 2W_y$$  \hfill (3.6)$$

which leads to:

$$N \geq 2\frac{W_x}{d_x}, \quad M \geq 2\frac{W_y}{d_y}.$$  \hfill (3.7)$$
Chapter 3.

Practically, safe bounds for $W_x$ and $W_y$ can be derived from the physics of the problem at hand. For example, in the presence of a driven microstrip line printed over a periodic structure, the spatial extent of the fields can be estimated by the well-known Wheeler formula for the microstrip width correction due to field fringing. On the other hand, if the periodic structure itself is driven, its cells acting as coupled resonators, a larger number of $N, M$ may be needed. Then, a convergence study is necessary. It is noted though that all sine-cosine FDTD simulations for different $k_x$’s are independent from each other and therefore lend themselves to perfect parallelization with no inter-processor communication overhead.

It is also important to mention the trade-offs between the time and memory efficiency involved in practical applications with the proposed method. Notably, this method allows for a significant reduction of the computational domain. On the other hand, it requires multiple simulations of a reduced domain, in order to complete the sampling of the
wavevectors needed for the array-scanning integral (2.12) to converge. It is also important to observe that these simulations are totally independent and perfectly parallelizable as such. Hence, this technique can be interpreted as a “spectral decomposition” method, whereby a given source is decomposed into wavevectors that are individually modeled (in parallel if possible) in a small computational domain. Let us compare this approach to its conventional alternative, the finite version of the periodic problem with a number of unit cells, for single and multiple processor environments, respectively.

For a single processor, the array-scanning method is preferable when the size of the corresponding finite problem is large, either exceeding the available memory resources or becoming extremely time-consuming.

For multiple processors, the “spectral decomposition” approach compares favorably to a domain decomposition of the finite periodic problem, as it totally eliminates the communication overhead between sub-domains. While state of the art domain decomposition techniques may lead to almost linear speed-ups, the sine-cosine array-scanning FDTD leads to a perfectly linear speed-up due to the independence of each $k$—simulation.

### 3.3 Modeling of Non-Periodic Metallic Structures over Periodic Substrates

#### 3.3.1 The Composite Periodic/Absobing Boundary: Methodology

The presence of non-periodic metallic structures, i.e. microstrip lines or antennas, on periodic substrates, is yet another category of problems which is obviously not compatible with periodic boundaries. In Method of Moments (MoM), Since the surface electric current density on metallic planes is treated as a primary source, the problem naturally lends itself to the application of the array-scanning technique [37]. However, in FDTD, a
crucial difference from the MoM arises [50] as the field components tangential to metallic surfaces are set to zero. Hence, if the computational domain is terminated in PBCs, these metallic surfaces are periodically reproduced; their presence cannot be eliminated by array-scanning. Figure 3.8 demonstrates the aforementioned situation with a typical example of a microstrip line residing on a substrate periodic in the \( x \)-direction. Here, \( \phi_x \) represents the phase progression for a Floquet mode across one unit cell. Direct application of the array-scanning FDTD on one unit cell of the structure along with the metallic object merely leads to the reproduction of an infinite array of the object.

While previous research on periodic FDTD formulations has focused on the application of *either* periodic or absorbing boundary conditions at each boundary of a given computational domain (a feature inherited by commercial packages as well), the problem at hand is best served by terminating the substrate at PBCs and the space above it, including the nodes of the metallic guide, in absorbing boundary conditions (or Per-
Figure 3.9: Combination of periodic and absorbing boundary conditions with array scanning ensures that the original structure can be simulated through the reduced computational domain. ©(IEEE)2008.

fectly Matched Layers, PMLs). This approach corresponds to the configuration shown in Fig. 3.9. Thus, the periodic imaging of the metallic boundaries is prevented, while the array-scanning method can still be employed to isolate the effect of the original source excitation.

When a PML absorber is used for the implementation of the absorbing boundary over the periodic boundary, special care needs to be taken for the update of the electric field nodes that are tangential to the interface between the absorber and the periodic substrate. Normally, the exterior boundaries of PMLs are terminated with perfect electric walls. However, in this case, the “lower” boundary of the absorbing layer is the extension of the air-substrate interface within the computational domain occupied by the PML. Thus, the tangential electric field on the wall of the absorber cannot be set to zero. Instead, it has to be updated.

These updates are performed in a way that is depicted in Fig. 3.10. Auxiliary
magnetic field nodes are introduced within the periodic substrate along the interface with the absorber, which are easily updated by PBCs using magnetic field values within the unit cell. Consequently, in the PML update, these magnetic fields are used to ensure the regular Yee updates for the tangential electric fields. It is important to notice that these auxiliary field update does not add any significant computational cost, in the sense that at this region of the substrate, which is beyond the boundaries of the simulated single unit cell, no other nodes (except for these auxiliary ones) need to be updated. Note that this method is only valid when the metallic surface does not contact the boundary of termination, so that the continuity at the air-substrate interface is not interrupted. Otherwise, extra unit cells in the direction of periodicity is necessary.
3.3.2 Numerical Application: Microstrip Line Over an Electromagnetic Bandgap Substrate

The numerical example studied in [37] to verify the application of the array-scanning method in MoM is investigated to validate the proposed methodology. The example consists of a microstrip line printed on an electromagnetic bandgap (EBG) substrate. The three-layer periodic substrate is shown in Fig. 3.11. All three layers are $h_1 = h_2 = h_3 = 0.635$ mm high and their dielectric constants are 9.8, 3.2 and 9.8, respectively. The center layer includes periodic rectangular air blocks of $6.5 \times 6.5 \times 0.635$ mm. The spacing between the neighboring blocks is $\alpha = 14$ mm in both directions. The width of the microstrip line, which is aligned with the air blocks underneath it, is 3 mm.

First, the structure is modeled by a single unit cell terminated with sine-cosine based PBCs throughout the $x$–direction, as shown in Fig. 3.8 (b), and excited with a 2-10 GHz modulated Gaussian source. The $x$–component of the electric field is sampled at the plane of the air-substrate interface, which is the plane where the microstrip line lies
Figure 3.12: Euclidean norm of the $x$-component of the electric field on the air-substrate interface of: a microstrip line over a unit cell of the periodic substrate of Fig. 3.11 terminated in PBCs; a finite structure consisting of unit cells of the same periodic substrate, with microstrip lines printed on each one of these cells. The position of the microstrip lines in this finite structure is also shown. ©(2008)IEEE.

as well. This is compared to the $E_x$ component in a structure consisting of seven unit cells of the periodic substrate in the $x-$direction, including the microstrip (similar to Fig. 3.8). The Euclidian norms of the two:

$$||E_x||_2 = \sqrt{\sum_n |E_x(n\Delta t)|^2} \quad (3.8)$$

are shown to be identical in Fig. 3.12. The plot of this norm also clearly shows that the middle strip (and the associated boundary condition $E_x = 0$) is periodically reproduced by the PBCs, after the application of array scanning (which in [37] was sufficient to eliminate the presence of these strips). The result numerically confirms that this problem cannot be solved by the application of the sine-cosine array-scanning FDTD alone.

To correctly model the numerical problem using the proposed composite boundary
Figure 3.13: Euclidean norm of the $x$-component of the electric field one Yee cell below the air-substrate interface of: a microstrip line over a unit cell of the periodic substrate of Fig. 3.11 terminated in PBCs within the substrate and an absorber from the air-substrate interface on; a finite structure consisting of seven unit cells of the same periodic substrate, with microstrip lines printed on the center cell. The position of the microstrip line is also shown. ©(2008)IEEE.

scheme, the structure is again modeled with one unit cell in the $x$–direction. However, this time it is terminated in sine-cosine PBCs within the substrate and PMLs above. The scattering parameters of five unit cells in the $y$–direction are computed. One unit cell, without air blocks, is added before and after these five cells, to provide space for the excitation and probe points, giving rise to a domain of seven unit cells in total, terminated at a PML as well. The Yee cell size is $0.5\text{ mm} \times 0.5\text{ mm} \times 0.318\text{ mm}$ and hence, a single unit cell of the structure contains $28 \times 28 \times 30$ cells. A 2-10 GHz modulated Gaussian hard source excitation is applied 14 Yee cells from the first set of air-blocks in the propagation direction and the vertical ($E_z$) electric field is probed one cell beneath the microstrip at the two boundaries of the perforated substrate. The time-step
Figure 3.14: Scattering parameters of the electromagnetic band-gap substrate microstrip line of Fig. 3.11, calculated by the sine-cosine based array-scanning technique (with $N=16$ $k_x$ points) and a finite structure simulation, with 7 cells in the $x$-direction.
is $\Delta t = 0.602$ ps and 16384 time steps are run. For the sine-cosine based array-scanning FDTD, $N = 16$ points are used to sample $k_x$, and each wavenumber simulation takes 863 seconds. For comparison, a finite structure with seven cells in the $x -$direction is also modeled in 4107 sec.

To confirm that the spurious periodic reproduction of the microstrip line, observed in Fig. 3.12, is avoided, the Euclidian norm of the $x -$component of the electric field is sampled one cell below the air-substrate interface and plotted in Fig. 3.13. Note that in this case, the plane of the air-substrate interface is not terminated in PBCs; therefore, the array-scanning method does not determine the values of the field beyond the limits of one unit cell in the transverse direction and hence, $E_x$ is now sampled just one cell below this plane within the periodic substrate. Clearly, the field pattern is now free of the spikes that appeared in Fig. 3.12, correctly decaying to zero away from the microstrip.
Furthermore, the scattering parameters are computed from both the array-scanning method and the finite structure simulation. The results of the two methods are in good agreement, as shown in Fig. 3.14, and are corroborated by the theoretical and experimental results of [37]. This agreement can also be observed in the time-domain. To that end, Fig. 3.15 presents the time-domain waveform of the transmitted vertical ($E_z$) electric field at the output of the simulated five unit cell geometry (one cell beneath the microstrip), as determined by the sine-cosine based array-scanning method and the corresponding finite structure simulation.

3.4 Antennas over Periodic Substrates

The previous section extended the methodology of array-scanning FDTD to account for the presence of non-periodic metallic objects. The scheme offers great convenience in modeling antennas over periodic substrates. In such cases, the unconventional form of the proposed computational domain requires the modification of the well-known near-to-far-field transformation for the determination of antenna radiation patterns in FDTD. Such a modification, along with the guidelines on proper modeling of antenna feeds with periodic boundaries, is outlined within the following section. Furthermore, next section offers numerical validations of the proposed methodology via examples of integrated and wire antennas over periodic or homogeneous dispersive substrates (as a form of periodic substrates with arbitrary periodicity).

3.4.1 Radiation Pattern Calculation

In FDTD-based antenna simulations, a near-field to far-field transformation is necessarily employed for the extraction of radiation patterns. This transformation is based on the surface equivalence theorem, whereby equivalent surface electric and magnetic current densities $\mathbf{J}_s = \hat{n} \times \mathbf{H}$, $\mathbf{M}_s = -\mathbf{E} \times \hat{n}$ can be used to calculate the radiated fields of
the antenna-periodic-structure system as a whole. To that end, a planar surface right above the antenna is chosen, with \( \hat{n} \equiv \hat{z} \) (Fig. 3.16). Fields radiated in the half-space bounded by this infinite surface are found by evaluating the appropriate radiation integrals [51] and thus the radiation pattern of the antenna is also computed. Practically, the confinement of \( J_s, M_s \) over a finite portion of the surface enables the truncation of the infinite radiation integrals. For example, in a three-dimensional (3D) free space, the electric field pattern in the \( \theta \) plane is computed by

\[
F(\theta) = |L_\phi + \eta_0 N_\theta|, \tag{3.9}
\]

Here

\[
\begin{align*}
N &= \iiint_S \nabla \cdot J_s \exp(jkr'\cos\Phi)ds' \\
L &= \iiint_S \nabla \cdot M_s \exp(jkr'\cos\Phi)ds'
\end{align*} \tag{3.10}
\]

where \( r' \) denotes the distance between the origin and the far-field observation point, \( \Phi \) denotes the angle between the observation direction and the direction from origin to the point where surface currents are computed, and \( S \) is the equivalent surface.

By applying the methodology proposed in last section, i.e., terminating the metallic antenna on a periodic substrate with a combination of periodic boundaries and absorbing boundaries, the effective domain is limited. To perform a near-to-far-field transformation, the equivalent current surface may practically have to extend beyond the boundaries of the domain, to allow for a sufficient decay of the surface currents, which in turn enables the truncation of the radiation integrals. Hence, the values of \( J_s, M_s \) on the surface cannot be computed directly. Instead, an indirect, yet straightforward methodology has been devised.

Note that for metallic surfaces at the air-substrate interface that spread across the complete computational domain in the direction of periodicity, the tangential field is no longer continuous at the interface (i.e. the field within the substrate never couples to the free space). Thus, the extrapolation method mentioned is not applicable.

To express this idea in mathematical form, consider the computation of the equivalent
Figure 3.16: Definition and update of electric and magnetic equivalent surface current densities, involved in the near to far-field transformation. ©(2011)IEEE.

Surface electric current at a point \( \mathbf{r}_0 \) \((i\Delta x + M d_x, l\Delta y + N d_y, q_s \Delta z)\) outside the computational domain, with \( \Delta x, \Delta y, \Delta z \) being the Yee cell dimensions, \( d_x \) and \( d_y \) the periods of the 2D periodic structure, while \( q_s = z_s/\Delta z \) is the \( z \)--index of the Yee cells with tangential magnetic field components on the surface. If the computational domain in the substrate includes \( N_x \times N_y \) cells, \( i \leq N_x, l \leq N_y \). Finally, let cells \((i, l, q)\) with \( 0 \leq q < q_{s_{\text{max}}_{\text{sub}}} \) belong to the substrate, where \( q_{s_{\text{max}}_{\text{sub}}} < q_s \), yet the difference \( (q_s - q_{s_{\text{max}}_{\text{sub}}}) \Delta z = \delta \) is electrically small (typically 1-2 cells).

Under these assumptions, \( \overline{H}_t(\mathbf{r}_0) \) can be determined in two steps. First, it can be expressed as an extrapolation function of \( \overline{H}_t \) nodes inside the substrate, yet still outside the computational domain:

\[
\overline{H}_t(\mathbf{r}_0) = f (\overline{H}_t(\mathbf{r}_0 - \delta \hat{z}), \overline{H}_t(\mathbf{r}_0 - (\delta + \Delta z) \hat{z}), \ldots)
\]  

(3.11)
tric fields $\mathbf{E}_t$ required for the computation of the surface magnetic current density $\mathbf{M}_s$ on the surface $z = q_s \Delta z$.

Second, the values of the transverse fields included in these extrapolations can be computed from nodes that do belong to the computational domain through the Floquet boundary condition. For instance, for the magnetic field phasor:

$$\vec{H}_t(i \Delta x + m \Delta x, l \Delta y + n \Delta y, q \Delta z) = \vec{H}_t(i \Delta x, l \Delta y, q \Delta z) \exp(-j (k_x m \Delta x + k_y n \Delta y)).$$

(3.12)

Substituting (3.12) and the corresponding electric field expression into (3.10) and collecting all the terms, we have

$$\mathbf{N} = M \sum_{m=-M}^{M} \sum_{n=-N}^{N} \int \int_S \nabla \cdot \mathbf{J}_s \exp[j(k r' \cos \Phi - k_x m \Delta x - k_y n \Delta y)] ds'$$

$$\mathbf{L} = M \sum_{m=-M}^{M} \sum_{n=-N}^{N} \int \int_S \nabla \cdot \mathbf{M}_s \exp[j(k r' \cos \Phi - k_x m \Delta x - k_y n \Delta y)] ds'$$

(3.13)

where $\mathbf{J}_s$ and $\mathbf{M}_s$ are the surface currents computed from the extrapolated fields in the computational domain, provided by the sine-cosine method, and $M, N$ are the number of unit cells to which the surface current practically vanishes.

### 3.4.2 Antenna Feed Modeling

In addition to simple voltage sources, several other feed methods such as microstrip lines and coaxial feeds, are often employed in designs of antennas over periodic structures. Such feeds can be incorporated into the proposed methodology as follows.

One commonly adopted feed for most patch antennas is the microstrip line feed (Fig. 3.17 (a)). Microstrip-fed patch antennas are necessarily treated as 1D periodic structures in the transverse direction with the proposed methodology. Along the direction of the microstrip, the computational domain is terminated in absorbing boundary conditions, which allows for the calculation of the antenna input impedance. As long as the microstrip is either at the back (e.g. in cases of coupled microstrip line feed) or on top of
Figure 3.17: The numerical configuration of antennas with different feeds: (a) a patch antenna with a microstrip line feed, and (b) a wire antenna with a coaxial feed. ©(2011)IEEE.

the substrate, it would be terminated at absorbing boundary conditions in one certain direction. Hence, the use of PBCs for the termination of the substrate in the transverse direction is possible.

A more complicated case arises in the study of antennas fed with coaxial cables. Fig. 3.17(b) shows a typical case in which the coaxial cable is connected to the feed point of a wire antenna above the substrate. In practice, such a coaxial cable usually penetrates the periodic substrate. In this case, the presence of the coaxial cable inside the substrate cancels the periodicity of the substrate and hence, prohibits the application of PBCs. To overcome this problem, the following approximate solution has been devised. The coaxial cable is modeled by a 1D transmission line separately from the main computational domain. The coaxial cable is then connected to the feed point, i.e. one end of the wire antenna, using the thin-wire feed model [52]. Suppose the coaxial feed is aligned along the $x-$direction and connected to the computational domain at Yee cell index $(I, J, K)$,
the magnetic field around the probe (for instance, $H_z$) can be updated with

$$H_z|_{I+1/2,J+1/2,K}^{n+1/2} = H_z|_{I+1/2,J+1/2,K}^{n-1/2} - \frac{\Delta t}{\mu_0 \Delta x} \left[ E_y|_{I+1,J+1/2,K}^{n} - \frac{2V_0^n}{\Delta y \ln(\Delta y/a)} \right]$$

at the point around the connection point of the coaxial feed and

$$H_z|_{I+1/2,J+1/2,K}^{n+1/2} = H_z|_{I+1/2,J+1/2,K}^{n-1/2} - \frac{\Delta t}{\mu_0 \Delta x} \left[ E_y|_{I+1,J+1/2,K}^{n} - E_y|_{I,J+1/2,K}^{n} \right]$$

at points along the probe. Here $V_0^n$ is the Voltage at the end of the 1D transmission line, and $a$ is the radius of the excitation probe. Afterward, the current at the end of the transmission line model $I|_{K+1/2}^{n+1/2}$ is updated from the magnetic field inside the computational domain using the Ampere’s Law. Since the feed point is above the periodic substrate, the excitation is applied to the antenna, while the substrate periodicity remains intact. Such a scheme can also be applied in other circumstances, for example, antennas fed by microstrip co-planar waveguides.

The aforementioned approach does not account for the interaction between the antenna and the feed itself (for example, scattering of near fields from the metallic feed boundaries), as the feed has been removed from the mesh. This may affect the numerical result in various aspects. If the actual feed is connected to the antenna through the substrate, the interaction between the scattered field from the coaxial cable and the periodic structure inside the substrate cannot be captured; or, if there is radiation from the coaxial cable, its contribution to the antenna pattern is also ignored. However, the results from next section demonstrate that in most cases, as long as the actual antenna is the major design concern, the proposed method can still lead to the accurate computation of the input impedance and the radiation pattern of coaxial-fed structures. On the other hand, this methodology would not be suitable for the study of the feed itself.
Figure 3.18: The horizontal monopole mounted on an periodic mushroom structure acting as a high impedance surface [53]. ©(2011)IEEE.

3.5 Numerical Applications for Antennas over Periodic Substrates

3.5.1 Horizontal Monopole over a High-Impedance Surface

The first example, used as a benchmark application, is a horizontal monopole antenna, mounted on a high-impedance ground plane (a 2D periodic “mushroom surface”) that is shown in Fig. 3.18 [53]. The 2.4 cm × 2.4 cm unit cell of the high-impedance surface consists of a square metallic plate and a metallic via of a 0.36 mm diameter. The gap between neighboring plates is 0.15 mm. The unit cell of the mushroom structure resides in a 1.6 mm thick homogeneous substrate with \( \varepsilon_r = 2.2 \). The wire antenna is 1 cm long and is mounted 1 mm above the interface between the substrate and air. It is fed by a 50 Ω coaxial cable.

This example is slightly different from what was discussed in the previous section in the sense that the antenna is not located at the air-substrate interface, but above the interface. Moreover, it is a wire antenna instead of an integrated one. To model the antenna, the periodic boundaries in the \( x - \) and \( y - \)directions extend along the \( z - \)axis up to half a cell beneath the horizontal wire.

The unit cell of the computational domain is modeled by \( 16 \times 16 \times 26 \) Yee’s cells. Three
Figure 3.19: The $S_{11}$ of the horizontal monopole using the proposed method and the finite structure simulation, compared with the measured results from [53]. ©(2011)IEEE.

Yee’s cells in the $z-$direction are used to model the substrate. The 0.1 mm diameter monopole is modeled by the thin wire model [17], and the coaxial feed is modeled by a 1D transmission line with 100 cells. The transmission-line model is connected to the input of the antenna at point A (Fig. 3.18) above the periodic surface. The computational domain at and above the horizontal plane where the antenna is located is terminated by 10-cell PMLs, while PBCs are employed below the plane, in both the $x-$ and the $y-$directions. A modulated 8-18 GHz Gaussian pulse is applied at the 50-th cell of the transmission line. The time step is set to 0.88ps and 25000 time steps are executed.

A computational domain of $2 \times 6$ unit cells in the $x-$ and the $y-$directions respectively is used, in order to enclose the wire antenna. Uniform sampling of 16 $k_x$ points and 16 $k_y$ points within the irreducible Brillouin zone of the high-impedance surface is applied, resulting in a total of 256 samples of the Floquet wave vector. For comparison, a finite structure, $3 \text{ cm} \times 3 \text{ cm}$ in the $x-$ and the $y-$directions respectively, is also simulated. The same finite structure is simulated and measured in [53].

Figure 3.19 shows the reflection coefficient ($S_{11}$) at the input of the wire antenna,
computed by the proposed method and the finite-structure simulation, along with measured results of [53]. The agreement between the three sets of data is excellent. The proposed computation takes 855 seconds for each simulation, while the finite structure simulation needs 6587 seconds.

To compute the far-field pattern, surface currents are recorded on a 14.4 mm × 14.4 mm planar surface right above the wire antenna, with zeroth-order extrapolation. Figure 3.20 depicts the E-plane pattern at 13 GHz using FDTD (proposed method and finite structure simulation) along with the measured results of [53], corroborating the excellent agreement observed in the $S_{11}$ results of Fig. 3.19.
3.5.2 Patch Antenna over an Electromagnetic Bandgap Substrate

The next example is a patch antenna printed on an EBG substrate, which was presented in [54]. The geometry of the structure is shown in Fig. 3.21. The substrate includes two layers with thickness $h_1 = h_2 = 0.787$ mm and the dielectric constant $\varepsilon_r = 4.6$. The bottom layer of the substrate consists of an array of mushroom structures with a unit cell size of 7 mm. The size of the metallic patch is $4.5$ mm $\times$ $4.5$ mm, and the radius of the via is 0.2 mm. The patch antenna is printed on the surface of the upper substrate layer, with dimensions $L = 22.14$ mm and $W = 31.59$ mm. The antenna is excited by a coupled microstrip line of 1.2 mm width along the $y$–direction, printed on the interface of the two substrate layers and aligned with the center of the patch.

In FDTD, each unit cell is modeled by $36 \times 36 \times 32$ Yee’s cells, and the thickness of each layer of the substrate is represented by 6 Yee’s cells. A modulated 2-4 GHz Gaussian pulse is applied as the excitation. The time step is set to be 0.77 ps, and 32768 steps are performed. The computational domain is set to 6 unit cells in the $x$–direction and 4 unit cells in the $y$–direction. In the $x$–direction, the computational domain is terminated...
Figure 3.22: The $S_{11}$ of the patch antenna on an EBG substrate using the proposed method, compared with finite structure simulation results and the measured results of [54]. ©(2011)IEEE.

in PBCs within the lower layer of the substrate, and in 10-cell PMLs elsewhere. In the $y$–direction, PMLs are applied at both ends of the domain. In the $x$–direction, $32 k_x$ points are sampled in the Brillouin zone. A finite structure with $6 \times 8$ unit cells is also simulated for comparison.

Figure 3.22 shows the $S_{11}$ obtained using the proposed method and the finite structure simulation, along with the measured results of [54]. Again, good agreement is demonstrated. The execution time for the sine-cosine array-scanning FDTD was 2351 seconds for each simulation. The finite structure simulation took 22478 seconds.

Furthermore, the radiation pattern is computed, by applying a near-to-far-field transformation on a surface of $10 \times 8$ unit cells in the $x$– and the $y$–directions and symmetrically placed with respect to the proposed computational domain and half a Yee’s cell above the patch antenna. Figure 3.23 shows the E-plane radiation pattern of the patch antenna at 2.5 GHz using the proposed method (with zeroth-order extrapolation) and the finite structure simulation, being again in good agreement with the measured results.
of [54].

![Graph showing the E-plane far-field pattern of the patch antenna of [54] at 2.5 GHz using the proposed method, compared with finite simulation results and the measured results of [54]. ©(2011)IEEE.](image)

**Figure 3.23:** The E-plane far-field pattern of the patch antenna of [54] at 2.5 GHz using the proposed method, compared with finite simulation results and the measured results of [54]. ©(2011)IEEE.

### 3.6 Summary

The combination of the sine-cosine method with the array-scanning method offers an effective approach to model a series of periodic structure based problems. For periodic structures with non-periodic excitations, such a methodology enables the FDTD modeling of the structure by simulating a single unit cell. The method is shown to be an efficient and accurate alternative for the time-domain modeling of driven periodic structures.

The methodology is further extended to include the modeling of non-periodic metallic objects, such as microstrip lines and integrated or wire antennas, over periodic or dispersive structures. Such an extension is based on a novel computational domain by applying PBCs to model the latter, absorbing boundary conditions to terminate the space above the antenna and the array-scanning technique to enable source modeling. This combina-
tion has been enhanced by an efficient scheme for near-to-far-field transformation which leads to the fast calculation of antenna radiation patterns, based on the assumption that the distance of the antenna from the periodic structure is electrically small.

The proposed method can be practically viewed as a “spectrum decomposition” method, as it decomposes the total field into a number of independent low-cost solutions from plane wave expansions. Thus, it is perfectly scalable and its convergence depends on the number of the simulated wavevectors within the Brillouin zone. If multiple processors are available to a user, the “spectral decomposition” would be clearly preferable over classical domain decomposition applied on a finite version of the periodic structure.
Chapter 4

Periodic Boundary Conditions as a Lattice Truncation Method in FDTD

4.1 Array-Scanning Method from an FDTD Mesh Truncation Perspective of View

In this chapter, a feasibility study is presented on the use of periodic boundary conditions (PBCs) for the application of Finite-Difference Time-Domain (FDTD) lattice truncation. Such exploration is motivated by the fact that the state-of-the-art in FDTD lattice truncation, involving analytical absorbing boundary conditions [55–57] and Perfectly Matched Layer absorber (PML, [58]), inevitably trades accuracy for complexity. Particularly, although PML has established itself as the method of choice for FDTD lattice termination due to its low reflectivity, drawbacks still exist: a dispersive media version of PML employs multiple auxiliary variables in addition to field vectors, which produces non-trivial memory and execution time overhead; close proximity of the source to the PML interface still causes inevitable reflections. Moreover, the performance of the PML in problems involving spatially dispersive media and backward-wave metamaterials has recently come under scrutiny [59,60]. These questions are particularly important for the application of
FDTD to the modeling of optical structures. To this end, the sine-cosine array-scanning FDTD is proposed as an alternative technique that may strike a better balance between accuracy, complexity and versatility.

From the discussion in Chapters 2 and 3, it is obvious that, from an FDTD mesh truncation point of view, the sine-cosine based array-scanning FDTD can serve as a good candidate in terminating unbounded periodic structures (or homogeneous structures, acting as virtual periodic structures with arbitrary lattice vectors) excited by any spatially limited excitation. It is also important to notice that according to Section 3.3, the presence of non-periodic metallic objects, for example, microstrip lines or antennas printed on periodic substrates, can be accurately modeled under the array-scanning scheme by introducing a combination of PBCs and PMLs.

An obvious prerequisite for the applicability of such an approach is that the working volume be periodic in the direction of termination (or non-periodic metallic objects reside on the surface of the periodic structures, and thus can be accounted for by the periodic/PML boundary combination). This condition is met in many practical cases of temporally and spatially periodic media either used as substrates or as stand-alone devices. On the other hand, since the Fourier transform in the array-scanning method is in effect a linear superposition of Floquet modes, the aforementioned method is clearly not applicable to non-linear media.

Since the array-scanning method involves only the Fourier transform of Floquet modes, it is not limited by the presence of dispersion or conductivity of the media it truncates. A uniform treatment of the lattice termination can thus be applied on a wide range of structures and media provided that the periodicity of the structure is preserved.

The most intriguing feature of the proposed scheme is that it is not limited by the presence of dispersion or conductivity, nor does the actual complexity and computational work involved grow in these cases [61]. A uniform treatment of the lattice termination can thus be applied to a wide range of structures and media provided that the periodicity
of the structure is preserved. Such a treatment is valid even when the material has an unusual dispersion or constitutive relationship (i.e. \( n < 0 \), as in [60]), and conventional PMLs cannot be applied. This feature renders the sine-cosine array-scanning FDTD a promising alternative to PML for many practical cases.

Another important observation for such a lattice termination scheme is that, according to (3.3), the accuracy of the method is primarily limited by the sampling error of the Floquet wave, provided the FDTD discretization error is small. Thus, the accuracy of the proposed truncation scheme is relatively unaffected by the proximity of sources to the boundary. In the following examples, it will further been shown that the accuracy performance of the proposed scheme is typically similar to that of the PML, except when the source is very close to the absorbing boundary. Then, it actually becomes better, as PML reflectivity increases dramatically due to the strong presence of near-grazing incident waves.

4.2 Numerical Results: Validation

4.2.1 Two-Dimensional Conducting Half Space

A two-dimensional (2D) benchmark problem from [17] is used here to assess the performance of the sine-cosine array-scanning FDTD as a mesh truncation method. The geometry consists of a conducting half-space with \( \varepsilon_r = 10 \) and \( \sigma = 0.3 \text{ S/m} \), over a free space region (Fig. 4.1). The excitation is a modulated Gaussian current source, spectrally supported from 0.5 to 10 GHz. The 24 mm wide computational domain is discretized by 40 Yee cells in the \( x \)-direction. As the geometry is infinite in that direction, we can also consider it as infinitely periodic with a period of 24 mm. To that end, PBCs are applied and 16 to 32 \( k_x \)-wavenumbers are uniformly sampled within the Brillouin zone. For error comparison, an identical domain terminated in a 10-cell uniaxial PML in the \( x \)-direction is simulated. The PML conductivity profile follows a polynomial
grading $\sigma(l) = (l/d)^m \sigma_{\text{max}}$ and $\sigma_{\text{max}} = -(m + 1) \ln R(0)/(2\eta d)$ where $d$ is the thickness of the PML, $m = 4$, $R(0) = e^{-16}$, and $\eta$ is the characteristic wave impedance of the region terminated in the PML. Notably, the presence of conductivity necessitates the augmentation of the conventional PML formulation with additional auxiliary variables, as detailed in [17]. As for the $y$–direction, 2000 Yee cells are used to eliminate reflections from the terminal boundaries, in order to ensure that our error study will include the $x$–boundary alone. Finally, the time step is set to 0.925 ps and 4096 time steps are run. Each wavevector simulation takes 533 seconds, while the PML simulation takes 712 seconds.

The error of both termination methods is evaluated by comparing to a reference solution in a domain of $2000 \times 2000$ Yee cells, and computing the norm:

$$\epsilon(n\Delta t) = \max_{i,j} \left( \frac{|E_z|_{i,j}^n - |E_z(\text{ref})|_{i,j}^n}{|E_{z(\text{ref})\text{max}}|_{i,j}} \right)$$  \hspace{1cm} (4.1)

where $E_{z(\text{ref})}$ is the $z$–component of the electric field obtained by the reference simulation, in two cases. First, the current source is placed at point A at the center of the interface between the two half spaces, and second, at point B in the upper half space one Yee cell away from the boundary and 12 cm from the conducting medium interface. Figure 4.2
Figure 4.2: The frequency-domain relative error of the structure in Fig. 4.1(a) using the proposed method with 16 and 32 $k_x$ samples, compared with the relative error of a 10-cell uniaxial PML. ©(2010)IEEE.

shows the corresponding errors in the frequency domain. It is clear that the change of the accuracy level of the sine-cosine array-scanning FDTD caused by the proximity of the source to the boundaries is much smaller than that of the PML. In the case of 32 sample points with source A, the accuracy level of the method is comparable to that of the PML. With a source close to the boundary, the performance of the proposed method clearly surpasses that of the PML.

The effect of the size of the computational domain on efficiency and accuracy of the proposed method is further examined by applying the source at point A and gradually decreasing the domain size in the $x$–direction. Figure 4.3(a) shows the maximum time domain error within the computational domain using (4.1) with respect to the number of Yee cells in the $x$–direction. It is clear that the proposed method is relatively insensitive to the change of the size of the working volume. Furthermore, Fig. 4.3(b) shows the relationship between the CPU time with respect to the change of the working volume,
Figure 4.3: The (a) maximum error and (b) computational time of the structure in Fig. 4.1(a) using the proposed method with 32 $k_z$ samples and excitation at point A, compared with results using a 10-cell uniaxial PML. ©(2010)IEEE.
using the PML termination and the proposed method, with both a single $k$ and the complete simulation if the program were executed serially. This “toy” problem, considered for benchmarking purposes, can be efficiently solved by the PML. Hence, while single $k$-simulations remain faster than the PML-based ones, the total time spent on all $k$’s exceeds the PML simulation time for the same level of accuracy.

4.2.2 Dipole Antenna within a Dispersive Substrate

Figure 4.4: The geometry of a Hertzian dipole source embedded in a dispersive substrate. ©(2010)IEEE.

The second example is a Hertzian dipole embedded in a dispersive substrate [62], shown in Fig. 4.4. The substrate permittivity follows the Drude model: $\varepsilon_r(f) = 1 - f_p^2/f^2$ where $f_p = 19.49$ GHz. Such a homogenous dispersive media may represent artificial dielectric structures, for example, periodic metallic cylinder rows [63], in suitable frequency ranges for simplicity of numerical investigation. The height of the substrate is $h = 33.32$ mm, with a horizontally oriented dipole source placed at $h_s = h/2$ below the air-substrate interface.

The size of the FDTD computational domain in the $x-$ and the $y-$directions is $3.6 \text{ cm} \times 3.6 \text{ cm}$, and is discretized in $48 \times 48 \times 75$ Yee cells. The dipole is represented by
This geometry is periodic (as infinite) in the $x-$ and the $y-$directions, hence the proposed method is applicable. To that end, $16 \, k_x$ and $16 \, k_y$ samples are considered. A 10-cell uniaxial PML is used in the $z-$direction. The reference solution is extracted by a structure that is $12 \, \text{cm} \times 12 \, \text{cm}$ long in the $x-$ and the $y-$direction respectively, and terminated in 10-cell uniaxial PMLs in all directions, using the same polynomial grading profile as in the previous example. The simulations are executed in parallel, each one taking 7740 seconds, while the reference solution simulation is run on a single console and takes 32830 seconds.

Several representative sets of results are shown. The radiation patterns of the dipole on the $x-y$ plane and the $x-z$ plane, calculated using the methodology in Section 3.4, are shown in Fig. 4.5. The agreement between the sine-cosine array-scanning FDTD results and the corresponding reference simulation is very good. Moreover, to compare the error
between the proposed method and the PML termination, an alternative working volume is set up with uniaxial PML termination along the directions of periodicity, and with an identical computational domain size of 3.6 cm × 3.6 cm in the x− and the y−directions. The z−component of the electric field is sampled at point A, which is 1 cm above the air-substrate interface. The time-domain normalized error is computed using (4.1) and is plotted in Fig. 4.6. The result clearly demonstrates that close proximity of the source to the periodic boundaries does not compromise the accuracy of the proposed method. On the other hand, the error of the PML-based solution is substantially higher than the proposed method. In particular, it is noted that the accuracy of the PML-based simulation is not substantially improved even when the number of PML cells increases significantly.
Figure 4.7: The required CPU time of the proposed method versus the maximum normalized error of \( E_z \) sampled at point A in the geometry of Fig. 4.4, compared with the 10-cell PML termination. ©(2010)IEEE.

The trade-off between the simulation time and the corresponding maximum error achieved using both the proposed method and the PML termination is further illustrated in Fig. 4.7. This is done by gradually increasing the size of the working volume using both the proposed method and the PML termination, and recording the simulation time associated with the particular size as well as the maximum time-domain error at point A. Figure 4.7 shows the relationship between the CPU time and the maximum normalized error achieved, both with respect to a single \( k \) and to the complete simulation, if the program is executed serially. The result is compared to the performance of a domain terminated in 10-cell PMLs. Again, the insensitivity of the proposed method to the working volume change is observed. In terms of execution time, the proposed method is preferable if multiple processors are available, as its serial execution remains slower than the PML.
4.3 Numerical Results: Applications

4.3.1 One-Dimensional Bragg Filter

Figure 4.8: The computational domain of a structure with 1D periodic permittivities excited by an infinite line source, terminated in periodic boundaries or PMLs in the \( y \)-direction. ©(2010)IEEE.

The first application, which has been studied in [59], is shown in Fig. 4.8(b). The objective is to simulate a one-dimensional (1D) Bragg filter with a periodic dielectric permittivity of the form \( \varepsilon_r(y) = 6 + 5 \sin(2\pi y/a) \) in the \( y \)-direction, where \( a = 1 \) cm, within a computational domain of 10 cm \( \times \) 10 cm. The presence of an inhomogeneous dielectric permittivity raises a question as to which particular \( \varepsilon \) should the PML be matched to. Studies of various PML-based alternatives were carried out in [59], indicating a substantially increased level of reflection errors in all cases.

On the other hand, the application of PBCs along the \( y \)-direction seems a natural way to terminate the FDTD lattice in this case, as the presence of a finite source can be modeled. This is indeed possible via the proposed method, whereby the computational domain is terminated by PBCs in the \( y \)-direction and in perfect magnetic conductors in the \( x \)-direction. For comparison, an alternative set-up with 10-cell uniaxial PMLs
terminating the \( y \)-direction, with fourth-order polynomial grading of the conductivity profile, is also simulated. A uniform line source \( J_z \), of a 5-25 GHz modulated Gaussian waveform in time, is applied at \( y = 5 \) cm. The time step is set to 5.869 ps and 2048 steps are run. For the proposed method, 16-32 \( k_y \)'s are sampled uniformly within the Brillouin zone in both the \( x \)- and the \( y \)-directions. Each of these simulations takes 32 seconds. The alternative setup with PML termination takes 41 seconds to execute.

The reference fields, used for error estimation, are obtained using a large computational domain of 2000 \( \times \) 2000 Yee cells, so that no reflections from the boundary can reach the positions of interest during the complete simulation time.

Figure 4.9: The numerical error with respect to time of the array-scanning method with different sampling densities, compared with 10-cell PMLs, in the geometry of Fig. 4.8. ©(2010)IEEE.

The results of these simulations are shown in Fig. 4.9, which corroborates the significantly increased reflections from the PML reported in [59]. On the other hand, the sine-cosine based array-scanning FDTD delivers again a relative error of about 0.1\%, with 16 and 32 \( k_y \) samples. The effect of the sampling density of \( k_y \) on the accuracy of the proposed method is also shown in the figure. The results indicate that the numerical
error tends to decrease as the sampling density increases, as expected.

### 4.3.2 Negative Refractive Index Lens

![Figure 4.10: A 2D dispersive metamaterial lens with negative refractive index $n = -1$ at 16 GHz. ©(2010)IEEE.](image)

The proposed method is applied to simulate the geometry of a doubly dispersive negative-refractive index (NRI) lens [60], in the time domain. Figure 4.10 shows the 2D computational domain. A dispersive slab with 2 cm thickness is placed in free space, with both magnetic and electric plasma response following the Drude model: 

$$\mu_r = \varepsilon_r = 1 - \omega_p^2 / [\omega(\omega - j\Gamma_0)]$$

with $\omega_p = 2\pi \times 22.6 \times 10^9$ rad/s. The setting yields a negative refractive index $n_N = -1$ at 15.98 GHz, with a small loss introduced by the $\Gamma_0$ term. The fact that yet another modification of the conventional PML formulation is necessary for backward-wave media, to avoid numerical instability, has been discussed in [60]. On the contrary, the sine-cosine array-scanning FDTD is readily applicable in this case as well.

In FDTD, the computational domain is discretized with $118 \times 120$ Yee cells. The dispersive slab is modeled using the $z$-transform method of [64]. The time step is set to
Figure 4.11: The electric field $E_z$ at the first and second interfaces of the dispersive slab of Fig. 4.10 and at $x = 2.95$ cm, using the proposed method for FDTD lattice termination in the $±y$-directions. ©(2010)IEEE.

0.83 ps. For the proposed method, the computational domain is terminated in 10-cell uniaxial PMLs in the $x$-direction, and in PBCs in the $y$-direction, which also includes the NRI region occupied by the slab. The array-scanning integral is approximated with 16 $k_y$’s, which are simulated in parallel. For comparison, an identical domain is terminated in 10-cell dispersive uniaxial PMLs in the $±y$-directions. The form of the complex permittivity in the PML region is:

$$\tilde{\varepsilon} = \varepsilon_0 \varepsilon_r(\omega) \left( \kappa + \frac{\sigma(y)}{j\omega\varepsilon_0} \right)$$

where $\kappa$ is used as a parameter to control the numerical instability observed in [60]. Finally, a time-harmonic current source is placed 1 cm from the first interface between free space and the slab, while the parameter $\Gamma_0 = 2\pi \times 100$ rad/s.

Figure 4.11 shows the time evolution of the transverse electric field $E_z$ at the first and the second interface of the slab using the proposed method, which indeed remains absolutely stable. On the other hand, Fig. 4.12 shows $E_z$ at the second interface, as computed with the dispersive PML in the $y$-direction for different values of $\kappa$. Evidently,
increasing the value of $\kappa$ delays the onset of the numerical instability observed in [60] for $\kappa = 1$, yet it cannot eliminate it totally.

With a stable simulation technique at hand, some interesting aspects of this superlens geometry can be further explored. For example, Fig. 4.11 indicates the growth in amplitude of $E_z$ at the second interface, compared to the first. This resonant effect is due to multiple reflections between the two interfaces; its transient evolution can be clearly observed in the time domain. Figure 4.13 depicts the magnitude of $E_z$, recorded throughout the computational domain at various time steps. Evidently, in the beginning, $E_z$ starts as a space wave attenuating away from the source (steps 400-600). However, as multiple reflections build up, the wave attenuation is still featured in the free-space regions, but starts being inverted within the NRI slab, until the steady-state of Fig. 4.11 is eventually reached. More specifically, this growth is indicated in Fig. 4.14, which demonstrates the temporal evolution of the exponentially growing pattern of the field inside the NRI slab. In this case, $n_N = -1 - 0.01j$, while the theoretical result has been obtained from [65].
Figure 4.13: The electric field $E_z$ in the computational domain of Fig. 4.10, at different time steps. The lens interfaces are marked by solid lines in the diagrams.

As in every resonant effect, the timing of the exponential field growth depends on the losses. This dependence is illustrated in Fig. 4.15, which shows the temporal evolution of the electric field at the second interface of the lens for different imaginary parts of the refractive index of the slab. Three cases are considered, tuning $\Gamma_0$: $n_N = -1 - 0.001j$, $-1 - 0.01j$, and $-1 - 0.1j$. Obviously, the higher the losses, the faster the steady-state is reached. Moreover, the timing predictions from FDTD are in agreement with the Laplace transform based calculation of [66], which indicated that the time required for an NRI lens to reach steady state is in the order of $1/\text{Im}(\varepsilon_r\mu_r)\omega$. Therefore, if the NRI lens becomes lossless, the time required to achieve convergence approaches infinity. Such a tendency is clearly shown in Fig. 4.15.

4.4 Summary

The application of periodic boundaries, effected by the sine-cosine FDTD method, was further extended as a potential alternative to absorbing boundary conditions and PMLs
for FDTD lattice termination. It was found that as long as PBCs are applicable, they can deliver at least comparable and potentially better absorptivity than the PML, overcoming existing constraints of conventional absorbers. Moreover, the proposed formulation remains the same regardless of the dispersion or loss of the working volume. This feature is in contrast with PML, which needs additional variables to properly account for electric or magnetic dispersion.

Moreover, it was demonstrated that a periodic FDTD code, augmented with the array-scanning method, can be recycled as a lattice termination technique for cases where ordinary PMLs would either fail (NRI media) or need substantial modifications (conducting/dispersive media). The very same formulation applies to all linear media, regardless of dispersion, offering FDTD users a convenient, if not always faster, alternative to the PML absorber.
Figure 4.15: The electric field $E_z$ in the computational domain of Fig. 4.10, at the second interface and at $y = 2.95$ cm, with refractive index of the NRI slab being $n_N = (a) -1 - 0.1j$, (b) $-1 - 0.01j$, and (c) $-1 - 0.001j$. ©(2010)IEEE.
Chapter 5

Efficient Analysis of Nonlinear Periodic Structures with Extended Stability FDTD Schemes

Unlike linear periodic structures, nonlinear periodic structures do not lend themselves to the application of periodic boundaries, since all periodic boundary conditions (PBCs) are in effect based on the assumption that the total field is a linear superposition of Floquet modes. Typically, these structures are simulated with a finite number of unit cells. Possible acceleration techniques are focused on alleviating the high computational cost introduced by the extra-fine spatial and time meshing required for accurate resolution of higher order modes.

In this chapter, two methodologies are presented, including a nonlinear Alternating-Direction Implicit Finite-Difference Time-Domain (ADI-FDTD) scheme and a spatial filtering method, both attempting to reduce the computational cost by extending the FDTD time step size beyond the Courant-Friedrichs-Lewy (CFL) limit. The efficiency and accuracy of the methods are compared to conventional nonlinear FDTD. Both methodologies are applied to simulate a spatial soliton inside a weakly nonlinear dielectric stack.
5.1 Auxiliary Differential Equation FDTD (ADE-FDTD) for Nonlinear Dispersive Materials

The time-domain Faraday’s Law and Ampere’s Law of a one-dimensional (1D) non-magnetic nonlinear medium with field components $E_x$ and $H_y$ can be expressed as (the spatial dependence of the field is suppressed for simplicity):

$$\nabla \times E_x(t) = -\mu_0 \frac{\partial}{\partial t} H_y(t). \tag{5.1a}$$

$$\nabla \times H_y(t) = \frac{\partial}{\partial t} \left[ \varepsilon_0 \varepsilon_{\infty} E_x(t) + P_{NL}^x(t) + P_L^x(t) \right] + \sigma E_x(t)$$

$$= \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} E_x(t) + \sigma E_x(t) + J_{NL}^x(t) + J_L^x(t) \tag{5.1b}$$

where $J_L^x(t)$ is the linear dispersion polarization current and $J_{NL}^x(t)$ is the nonlinear polarization current. For linear dispersion, the polarization current is expressed as

$$J_L^x(t) = \varepsilon_0 \frac{\partial}{\partial t} \int_0^t E_x(t - \tau) \chi^{(1)}(\tau) d\tau \tag{5.2}$$

where $\chi^{(1)}$ is the linear susceptibility function. For nonlinearity, only the third-order effect is considered. Thus, $J_{NL}^x(t)$ can be written as

$$J_{NL}^x(t) = \varepsilon_0 \frac{\partial}{\partial t} \int_0^t \int_0^t \int_0^t E_x(t - \tau) E_x(t - \tau_1) E_x(t - \tau_2) \chi^{(3)}(t, \tau, \tau_1, \tau_2) d\tau d\tau_1 d\tau_2. \tag{5.3}$$

In (5.3), the third-order susceptibility function $\chi^{(3)}(t, \tau, \tau_1, \tau_2)$ can be reduced to a simplified form using the Born-Oppenheimer approximation [67]

$$\chi^{(3)}(t, \tau, \tau_1, \tau_2) = \delta(t - \tau_1) \delta(\tau - \tau_2) \chi_0^{(3)} [(1 - \alpha) g_R(\tau_1 - \tau_2) + \alpha \delta(t - \tau_2)] \tag{5.4}$$

where the first and second term of $\chi^{(3)}$ represent Raman and Kerr effect, respectively, and $\chi_0^{(3)}$ is the magnitude of the third-order susceptibility function. Here, the Raman nonlinearity kernel function is given by

$$g_R(t) = \frac{t_1^2 + t_2^2}{t_1 t_2} \exp \left( -\frac{t}{t_2} \right) \sin \left( \frac{t}{t_1} \right) u(t) \tag{5.5}$$
where $t_1, t_2$ are time delay factors for the Raman effect, and $u(t)$ is the step function. Substitute (5.4) into (5.3), and the polarization current reduces to two terms

$$J_{x}^{NL}(t) = \varepsilon_0 \frac{\partial}{\partial t} \left\{ E_x(t) \chi_0^{(3)} \int_0^t (1 - \alpha) g_R(t - \tau) |E_x(\tau)|^2 \, d\tau \right\} + \varepsilon_0 \frac{\partial}{\partial t} \left[ \alpha \chi_0^{(3)} E_x(t)^3 \right]$$

$$= J_x^R(t) + J_x^K(t) \tag{5.6}$$

where $J_x^R(t)$ and $J_x^K(t)$ stand for the currents induced by Raman and Kerr effect, respectively. These two terms are treated separately in the auxiliary update equations for the polarization currents, which will be derived in the following.

### 5.1.1 Auxiliary Update Equation for Linear Dispersive Media

Consider a linear medium with Lorentz dispersion. By performing a Fourier transform on (5.2), the frequency domain polarization current is given by (\tilde{\text{denoting frequency-domain components}})

$$\tilde{J}_x^L(\omega) = j \omega \varepsilon_0 \chi^{(1)}(\omega) \tilde{E}_x(\omega) = \left( \frac{\varepsilon_0 \Delta \varepsilon_L \omega^2 + j \omega}{\omega^2 + 2 j \omega \delta_L - \omega^2} \right) \tilde{E}_x(\omega) \tag{5.7}$$

where $\Delta \varepsilon_L$ is the change in relative permittivity due to the dispersion, $\omega_L$ is the undamped resonant frequency, and $\delta_L$ is the damping coefficient. Performing an inverse Fourier transform on (5.7) leads to

$$\omega_L^2 J_x^L(t) + 2 \delta_L \frac{\partial}{\partial t} J_x^L(t) + \frac{\partial^2}{\partial t^2} J_x^L(t) = \varepsilon_0 \Delta \varepsilon_L \omega_L^2 \frac{\partial}{\partial t} E_x(t). \tag{5.8}$$

In preparation for the ADI scheme derivation, (5.8) is discretized at numerical time step $n$ and spatial index $k$ with half time step. Collect all terms and we have:

$$J_{x}^{L,n+1/2} = \alpha_L J_{x}^{L,n} + \xi_L J_{x}^{L,n-1/2} + \frac{\gamma_L}{\Delta t} \left[ E_{x,k}^{n+1/2} - E_{x,k}^{n-1/2} \right] \tag{5.9}$$

where

$$\alpha_L = \frac{8 - \omega_L^2 \Delta t^2}{4 + 2 \delta_L \Delta t}, \ \xi_L = \frac{\delta_L \Delta t - 2}{\delta_L \Delta t + 2}, \ \gamma_L = \frac{\varepsilon_0 \Delta \varepsilon_L \omega_L^2 \Delta t^2}{4 + 2 \delta_L \Delta t}. \tag{5.10}$$


5.1.2 Auxiliary Update Equation for Kerr Nonlinearity

According to (5.6), the polarization current associated with Kerr nonlinearity can be expressed as

\[ J^K_x(t) = 3\varepsilon_0\alpha\chi_0^{(3)}E_x(t)^2 \frac{\partial E_x(t)}{\partial t}. \]  

(5.11)

Again, to synchronize with the ADI scheme in the following section, (5.11) is discretized at numerical time step \( n \) and spatial index \( k \) with half time step. Thus, the update equation can be written as

\[ J^K_{n+1/2} = 6\varepsilon_0\alpha\chi_0^{(3)} \frac{E_{n,k}^2}{\Delta t} \left[ E_{n+1/2,k} - E_{n-1/2,k} \right] - J^K_{n-1/2}. \]

(5.12)

Note that (5.12) can be also used to update \( J^K_n \) at integer time steps.

5.1.3 Auxiliary Update Equation for Raman Nonlinearity

To simplify the update scheme for the Raman nonlinearity polarization current \( J^R_x(t) \), an additional auxiliary variable \( S^R(t) \) is introduced [68]:

\[ J^R_x(t) = \frac{\partial}{\partial t} \left[ E_x(t)S^R(t) \right] \]

(5.13)

and

\[ S^R(t) = \varepsilon_0\chi_0^{(3)} \int_0^t (1 - \alpha)g_R(t - \tau) [E_x(\tau)]^2 d\tau. \]

(5.14)

Transfer (5.14) into the frequency domain following [68], and we have

\[ \tilde{S}^R(\omega) = \varepsilon_0 A\tilde{g}_R(\omega)\mathcal{F}[E_x(t)^2] = \left( \frac{\varepsilon_0 A\omega_R^2}{\omega_R^2 + 2j\omega\delta_R - \omega^2} \right) \mathcal{F}[E_x(t)^2] \]

(5.15)

where \( A = (1 - \alpha)\chi_0^{(3)} \) is the nonlinear coefficient, \( \omega_R \) is the undamped resonant frequency, and \( \delta_R \) is the damping coefficient. Here, \( \omega_R \) and \( \delta_R \) are associated with (5.5) by

\[ \omega_R = \sqrt{\frac{\tau_1^2 + \tau_2^2}{\tau_1^2\tau_2}}, \delta_R = \frac{1}{\tau_2}. \]  

(5.16)

Multiplying both sides of (5.15) by \( \omega_R^2 + 2j\omega\delta_R - \omega^2 \), performing an inverse Fourier transform and collecting all the terms, we have:

\[ \omega_R^2 S^R(t) + 2\delta_R \frac{\partial}{\partial t} S^R(t) + \frac{\partial^2}{\partial t^2} S^R(t) = \varepsilon_0 A\omega_R^2 E_x(t)^2. \]

(5.17)
Discretizing (5.17) at time step $n$ and spatial index $k$ with half time step leads to:

$$
\omega_R^2 S^R_n + 2 \delta_R \left[ \frac{S^R_{n+1/2} - S^R_{n-1/2}}{\Delta t} \right] \left( \frac{S^R_{n+1/2} - S^R_{n-1/2}}{(\Delta t/2)^2} \right) + \varepsilon_0 A^2 \omega_R^2 \left[ E_{x,k}^n \right]^2.
$$  

(5.18)

Solving (5.18), we have

$$
S^R_{n+1/2} = \alpha_R S^R_n + \xi_R S^R_{n-1/2} + A \gamma_R \left[ E_{x,k}^n \right]^2.
$$  

(5.19)

where

$$
\alpha_R = \frac{8 - \omega_R^2 \Delta t^2}{4 + 2 \delta_R \Delta t}, \quad \xi_R = \frac{\delta_R \Delta t - 2}{\delta_R \Delta t + 2}, \quad \gamma_R = \frac{\varepsilon_0 \omega_R^2 \Delta t^2}{4 + 2 \delta_R \Delta t}.
$$  

(5.20)

Note that (5.20) has exactly the same form as (5.10).

Finally, discretizing (5.13) at time step $n$ leads to an explicit update equation for the $J^R_{n+1/2}$:

$$
J^R_{n+1/2} = 2 \frac{\Delta t}{\Delta t} \left( E_{x,k}^{n+1/2} S^R_{n+1/2} - E_{x,k}^{n-1/2} S^R_{n-1/2} \right) - J^R_{n-1/2}.
$$  

(5.21)

### 5.2 ADI-FDTD Based on the Auxiliary Differential Equation Method

#### 5.2.1 Methodology

Originally developed for simulating linear computational domain, the ADI-FDTD [69] constructs an FDTD update procedure with two stages, namely, the backward finite-difference (FD) stage and the forward FD stage, each based on half FDTD time step. By arranging the forward FD stage and backward FD alternatingly, the ADI-FDTD is able to force the numerical growth factor within one discrete time step equal to one disregarding the time step size. Thus, it totally eliminates the CFL limit condition. Conventionally, the merit makes the ADI-FDTD especially suitable for applications with
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fine FDTD meshes, for which the efficiency of the simulation is largely limited by the maximum time step size according to the CFL limit.

In this section, the ADI-FDTD is rigorously formulated with nonlinear dispersive media, thus reducing the simulation cost of such media introduced by the extra-fine spatial meshing.

Discretizing (5.1a) and (5.1b) in time and space, for the backward FD stage we have

\[ -\frac{E_{x,k+1}^{n+1/2} - E_{x,k}^{n+1/2}}{\Delta z} = \frac{H_{y,k+1/2}^{n+1/2} - H_{y,k+1/2}^n}{\Delta t/2} \]  
\[ -\frac{H_{y,k+1/2}^{n+1/2} - H_{y,k-1/2}^{n+1/2}}{\Delta z} = \varepsilon_0 \varepsilon_\infty \frac{E_{x,k}^{n+1/2} - E_{x,k}^n}{\Delta t/2} + \sigma E_{x,k}^{n+1/2} + J_{k}^{R,n+1/2} + J_{k}^{K,n+1/2} + J_{k}^{L,n+1/2} \]  

where \( k \) is the spatial index. Here, \( J_{k}^{L,n+1/2}, J_{k}^{K,n+1/2} \) and \( J_{k}^{R,n+1/2} \) are associated with \( E_{x} \) through (5.9), (5.12), and (5.21).

Substituting (5.9), (5.12) and (5.21) into (5.22b) and rearranging the terms, the update equations for the backward FD stage can be written as

\[ E_{x,k}^{n+1/2} = C_{1,k} E_{x,k}^n + C_{2,k} E_{x,k}^{n-1/2} + C_{3,k} \left\{ \frac{H_{y,k+1/2}^{n+1/2} - H_{y,k-1/2}^{n+1/2}}{\Delta z} \right\} \]  
\[ H_{y,k+1/2}^{n+1/2} = H_{y,k+1/2}^n - \frac{\Delta t}{2\mu_0} \frac{E_{x,k+1}^{n+1/2} - E_{x,k}^{n+1/2}}{\Delta z} \]  

where

\[ C_{1,k} = \frac{2\varepsilon_0 \varepsilon_\infty}{2\varepsilon_0 \varepsilon_\infty + \gamma_L + 2S_k^{R,n+1/2} + 6\varepsilon_0 \alpha \chi_0^{(3)} \left[ E_{x,k}^n \right]^2 + \sigma \Delta t} \]  
\[ C_{2,k} = \frac{\gamma_L + 2S_k^{R,n+1/2} + 6\varepsilon_0 \alpha \chi_0^{(3)} \left[ E_{x,k}^n \right]^2}{2\varepsilon_0 \varepsilon_\infty + \gamma_L + 2S_k^{R,n+1/2} + 6\varepsilon_0 \alpha \chi_0^{(3)} \left[ E_{x,k}^n \right]^2 + \sigma \Delta t} \]  
\[ C_{3,k} = \frac{\Delta t}{2\varepsilon_0 \varepsilon_\infty + \gamma_L + 2S_k^{R,n+1/2} + 6\varepsilon_0 \alpha \chi_0^{(3)} \left[ E_{x,k}^n \right]^2 + \sigma \Delta t} \]
Equation (5.23a) and (5.23b) cannot be used for direct numerical update, as they
contain different unknown field components at time step \((n + 1/2)\) in both sides. For
example, in (5.23a), the update of \(E_x^{n+1/2}\) requires \(H_y^{n+1/2}\), which is not at then available.
By substituting (5.23b) into (5.23a), the \(H_y^{n+1/2}\) components are eliminated, resulting an
update equation for only the \(E_x^{n+1/2}\) component:

\[
A_{1,k}E_{x,k-1}^{n+1/2} + A_{2,k}E_{x,k}^{n+1/2} + A_{3,k}E_{x,k+1}^{n+1/2} = f_k(E_x^n, E_x^{n-1/2}, H_y^n) \tag{5.25}
\]

where

\[
A_{1,k} = A_{3,k} = -\frac{C_{3,k} \Delta t}{2 \mu_0 \Delta z^2}, A_{2,k} = 1 + \frac{C_{5,k} \Delta t}{\mu_0 \Delta z^2} \tag{5.26}
\]

and

\[
f_k(E_x^n, E_x^{n-1/2}, H_y^n) = C_{1,k}E_x^n(k) + C_{2,k}E_x^{n-1/2}\]
\[-C_{3,k}\left\{ \frac{H_y^{n+1/2} - H_y^{n-1/2}}{\Delta z} \right. \]
\[-J_{K,n-1/2} - J_{K,n-1/2}^L + \alpha_L J_{K,n}^L + \xi_L J_{K,n-1/2}^L \} \tag{5.27}
\]

The above equations yield a system of equations with a tridiagonal system matrix of the
form

\[
\begin{bmatrix}
A_{2,1} & A_{3,1} & \cdots & 0 & 0 \\
A_{1,2} & A_{2,2} & \cdots & 0 & 0 \\
& & \ddots & & \\
0 & 0 & \cdots & A_{2,K-1} & A_{3,K-1} \\
0 & 0 & \cdots & A_{1,K} & A_{2,K}
\end{bmatrix}
\begin{bmatrix}
E_{x,1}^{n+1/2} \\
E_{x,2}^{n+1/2} \\
\vdots \\
E_{x,K-1}^{n+1/2} \\
E_{x,K}^{n+1/2}
\end{bmatrix}
= \begin{bmatrix}
f_1 \\
f_2 \\
\vdots \\
f_{K-1} \\
f_K
\end{bmatrix} \tag{5.28}
\]

Such a system of equations can be efficiently solved by an LU factorization solver taking
advantage of the bandedness and sparsity [70, 71]. Thereafter, (5.23b) can be calculated
directly using \(E_x^{n+1/2}\).
For the forward FD stage, the equations are

\[
- \frac{E^{n+1/2}_{x,k+1} - E^{n+1/2}_{x,k}}{\Delta z} = \mu_0 \frac{H^{n+1/2}_{y,k+1/2} - H^{n+1/2}_{y,k+1/2}}{\Delta t/2} \tag{5.29a}
\]

\[
- \frac{H^{n+1/2}_{y,k+1/2} - H^{n+1/2}_{y,k-1/2}}{\Delta z} = \varepsilon_0\varepsilon_\infty \frac{E^{n+1/2}_{x,k} - E^{n+1/2}_{x,k}}{\Delta t/2} + \sigma E^{n+1/2}_{x,k} + J^{R,n+1/2}_k + J^{K,n+1/2}_k + J^{L,n+1/2}_k. \tag{5.29b}
\]

Combining (5.21) with (5.29a) and (5.29b) leads to

\[
E^{n+1}_{x,k} = C_{4,k} E^{n+1/2}_{x,k} + C_{5,k} E^{n-1/2}_{x,k} + C_{6,k} \left\{ - \frac{H^{n+1/2}_{y,k+1/2} - H^{n+1/2}_{y,k-1/2}}{\Delta z} + J^{R,n-1/2}_k + J^{K,n-1/2}_k - \left[ \alpha_L J^{L,n}_k + \xi_L J^{L,n-1/2}_k \right] \right\} \tag{5.30a}
\]

\[
H^{n+1}_{y,k+1/2} = H^{n+1/2}_{y,k+1/2} - \frac{\Delta t}{2\mu_0} \frac{E^{n+1/2}_{x,k+1} - E^{n+1/2}_{x,k}}{\Delta z} \tag{5.30b}
\]

where

\[
C_{4,k} = \frac{2\varepsilon_0\varepsilon_\infty - \gamma_L - \left( 2S^{R,n+1/2}_k + 6\varepsilon_0\alpha\chi^{(3)}_0 \left[ E^n_{x,k} \right]^2 \right)}{2\varepsilon_0\varepsilon_\infty} - \sigma \Delta t \tag{5.31a}
\]

\[
C_{5,k} = \frac{\gamma_L + 2S^{R,n-1/2}_k + 6\varepsilon_0\alpha\chi^{(3)}_0 \left[ E^n_{x,k} \right]^2}{2\varepsilon_0\varepsilon_\infty} \tag{5.31b}
\]

\[
C_{6,k} = \frac{\Delta t}{2\varepsilon_0\varepsilon_\infty}. \tag{5.31c}
\]

To summarize, the implementation of the nonlinear auxiliary equation method based ADI-FDTD over one discrete time step consists of the following procedures:

1. Calculate field components at half time step \( E^{n+1/2}_{x,k} \) and \( H^{n+1/2}_{y,k} \) based on (5.28) and (5.23b) (i.e. the backward FD stage).

2. Obtain \( J^{L,n+1/2}_k, S^{R,n+1/2}_k, J^{R,n+1/2}_k, \) and \( J^{K,n+1/2}_k \) based on (5.9), (5.19), (5.21), and (5.12).

3. Calculate field components at integer time step \( E^{n+1}_{x,k} \) and \( H^{n+1}_{y,k} \) based on (5.30a) and (5.30b) (i.e. the forward FD stage).
5.2.2 Numerical Validation: Nonlinear Homogenous Medium

The proposed method is tested for validity with a benchmark example of a nonlinear homogeneous medium possessing both Kerr and Raman nonlinearity [72,73]. The medium is assumed to have linear and nonlinear dispersive susceptibilities with $\varepsilon_\infty = 2.25$. For linear dispersion, a Lorentz model is used with $\Delta\varepsilon_L = 3$, $\omega_L = 4 \times 10^{14}$ rad/s, and $\delta_L = 2 \times 10^9$ rad/s in (5.7). For the third-order nonlinearity, the quantities used in the Born-Oppenheimer model are $\chi_0^{(3)} = 0.07$ (V/m)$^{-2}$, $\alpha = 70\%$, $t_1 = 12.2$ fs, and $t_2 = 32$ fs in (5.4) and (5.5).

![Graphs showing field distribution](image)

Figure 5.1: The spatial field distribution at $t = 0.6$ ps inside the homogeneous medium with both Kerr and Raman nonlinearity, using (a) conventional FDTD with auxiliary variable method and nonlinear ADI-FDTD with (b) $R_{\Delta t} = 2$, (c) $R_{\Delta t} = 5$, and (d) $R_{\Delta t} = 10$. 
The 1D computational domain is discretized into 60000 Yee cells with size of 5 nm. The size of the computational domain is chosen so that the wave never propagates to the boundaries during the simulation time span. Thus, simple perfect electric conductors are used to terminate the domain. A modulated hyperbolic secant pulse with a carrier frequency \( f_c = 137 \) THz and a characteristic time constant of 14.6 fs is injected at the center of the domain. The structure is simulated up to a 1000 fs time span. Since the maximum time step size of nonlinear FDTD cannot be determined by the CFL limit, it is selected from a stability test, i.e. reducing the time step size from the CFL limit until the result is stabilized. The time step used is \( \Delta t_0 = 0.0165 \) fs, corresponding to 0.66 times of the CFL limit, and 60000 steps were run. Both conventional ADE-FDTD and the proposed ADI-FDTD are used to simulate the structure. For the ADI-FDTD, the time step ratio \( R_{\Delta t} = \Delta t / \Delta t_0 \) is set to be 2, 5, and 10.

Figure 5.1 shows the corresponding time-domain field at 6.0 ps within the right half of the computational domain, with results from both conventional ADE-FDTD and nonlinear ADI-FDTD with different time step sizes. The temporal soliton, which retains its amplitude and width along propagation, as well as the precursor containing third-order components, are clearly observed. Also, the electric field spectrum 55 \( \mu \)m and 126 \( \mu \)m away from the excitation point is plotted in Fig. 5.2, clearly showing the redshift and sharpening of the spectrum distribution along the direction of propagation.

Figure 5.3 gives a comparison of the maximum relative time domain error

\[
\epsilon = \left| \frac{E_x(n\Delta t) - E_{0x}(n\Delta t)}{E_{0x}(n\Delta t)} \right|_{\text{max}}
\]  

(5.32)

where \( E_{0x}(n\Delta t) \) is the reference field value obtained from conventional ADE-FDTD, as well as the total CPU time required to simulate a fixed time span, between ADI-FDTD with different time step sizes. The error calculation uses the ADE-FDTD result as a reference. Similar to the linear case of [74], the error quickly increases along with the time step size. It is noted that around \( \Delta t = 5\Delta t_0 \), the ADI-FDTD is about two times faster than the ADE-FDTD, with a maximum deviation of less than 1 percent. This
Figure 5.2: The spectrum of the field at (a) 55 µm and (b) 126 µm away from the excitation inside the homogeneous medium with both Kerr and Raman nonlinearity, using conventional ADE-FDTD and ADI-FDTD with different time step sizes.
Figure 5.3: The maximum relative error at the center of the stack area and the relative total CPU execution time of the nonlinear ADI-FDTD, using the ADE-FDTD result as a reference.

point emerges to be an optimum choice of $\Delta t$.

5.3 A Spatial Filtering Method Extending the Stability Limit of FDTD

5.3.1 Methodology in Linear Media

In this section, an FDTD method based on a spatial filtering process is introduced to extend the stability limit of FDTD. Such a method has been indicated in finite-different schemes in fluid dynamic [75,76], and was introduced into electromagnetics regime in [77].

For simplicity, consider a 1D linear computational domain along the $z$–axis with field components $E_x$, $H_y$, discretized in uniform Yee cells. The numerical dispersion relationship of FDTD can thus be expressed as

$$
\sin^2 \left( \frac{\omega \Delta t}{2} \right) = \left( \frac{v_p \Delta t}{\Delta z} \right)^2 \sin^2 \left( \frac{\tilde{k} \Delta z}{2} \right)
$$

(5.33)
for a numerical plane wave with numerical frequency $\tilde{\omega}$ and numerical wavenumber $\tilde{k}$, where

$$v_p = \frac{1}{\sqrt{\varepsilon \mu}}.$$  \hfill (5.34)

In conventional stability analysis [78], to guarantee an accurate and stable solution, the numerical frequency must be real. This is true under the condition

$$\left(\frac{v_p \Delta t}{\Delta z}\right) \left| \sin \frac{\tilde{k} \Delta z}{2} \right| \leq 1. \hfill (5.35)$$

With the sinusoidal term in (5.35) bounded by 1, we have

$$\left(\frac{v_p \Delta t}{\Delta z}\right) \leq 1 \hfill (5.36)$$

which is the conventional CFL limit.

There is one key assumption when deriving (5.36), that the sinusoidal term in (5.35) can take any value between 0 and 1, which implies that stability is enforced for any wavenumber component between 0 and the Nyquist limit $\pi/\Delta z$. In FDTD, despite the fact that bandlimited signals are typically simulated, this is virtually necessary considering that: first, the simulation is carried out in a computational domain which is spatially limited, and thus, spectrally infinite; and second, the field value is a series of discrete samples at the grid of Yee cells, interpreted to an infinitely periodic spectrum. On the other hand, in FDTD, the useful wavenumber component is typically limited by the mesh fineness. Let $\Lambda = \lambda_{\text{min}}/\Delta z$ be the spatial discretization rate of the FDTD meshing, which is typically at least 10 and can potentially be even higher with the presence of temporal dispersion and nonlinearity. The part of the spatial frequency spectrum which can be accurately resolved is given by

$$0 \leq \tilde{k} \Delta z \leq \frac{2\pi}{\Lambda}. \hfill (5.37)$$

The rest wavenumber components in the higher end of the spectrum are very weakly excited and are corrupted by dispersion errors.
However, if we assume that the spectrum of the signal can be truncated up to the maximum “useful” component $\tilde{k}_{\text{max}} = 2\pi/\lambda_{\text{min}}$, which can be easily realized by spectrum filtering, thus, by filtering out the rest of harmonics, (5.35) becomes
\[
\left(\frac{v_p \Delta t}{\Delta z}\right) \left| \sin \frac{\tilde{k}_{\text{max}} \Delta z}{2} \right| \leq 1.
\] (5.38)
To this end, the CFL limit is effectively extended by a “CFL enhancement factor”
\[
CE = \frac{1}{\sin \frac{\tilde{k}_{\text{max}} \Delta z}{2}}.
\] (5.39)
Combining (5.39) and (5.37), we have
\[
CE = \frac{1}{\sin (\pi/\Lambda)}.
\] (5.40)
Figure 5.4 plots the relationship of the $CE$ factor and the spatial discretization rate. When $\Lambda$ is large enough, the $CE$ factor is approximately proportional to the FDTD meshing fineness.

The aforementioned relaxation is based on the truncation of the spatial frequency spectrum of the field. Here, a simple solution is adopted by introducing a rectangular filter
\[
F(\tilde{k}) = \begin{cases} 
1 & \tilde{k} \leq \tilde{k}' \\
0 & \tilde{k} > \tilde{k}' 
\end{cases}.
\] (5.41)
During each time step, the $E$ field and $H$ fields are first updated following the conventional FDTD equations. Then, a Discrete Fourier Transform (DFT) is performed on the spatial distribution of the field and the rectangular filter is applied to the resulting spectrum. Finally, an Inverse Discrete Fourier Transform (IDFT) is performed on the filtered spectrum to obtain the updated field distribution in the computational domain. It is also noted that enforcing $\tilde{k}' = \tilde{k}_{\text{max}}$ may not be necessary, and may introduce additional truncation errors according to the derivation in the next section. For a specific time step ratio $R_{\Delta t} = \Delta t/\Delta t_{\text{CFL}}$, where $\Delta t_{\text{CFL}}$ is the maximum time step size under conventional
CFL limit, (5.38) can be rewritten as

$$R_{\Delta t} \left| \sin \frac{k'\Delta z}{2} \right| \leq 1.$$  \hspace{1cm} (5.42)

Therefore, the maximum cutoff wavenumber allowed is

$$\tilde{k}' = \frac{2 \sin^{-1} (1/R_{\Delta t})}{\Delta z}.$$ \hspace{1cm} (5.43)

### 5.3.2 Error Estimation

The numerical error introduced by the spatial filtering method is mainly due to the truncation of the field spectrum during the filtering process. Let $E_x^n(k)$ be the electric field at time step $n$ and spatial index $k$ in a 1D computational domain. The spectrum of the field can be found by applying a DFT on the spatial field distribution

$$\hat{E}_x^n = \sum_{k=0}^{K-1} E_x^n(k) \exp \left( j \frac{2\pi pk}{L} \right).$$ \hspace{1cm} (5.44)
where $p$ is the spectrum index, $K$ is the total number of spatial indices in the computational domain, and $L$ is the number of DFT samples. Here, for simplicity, we choose $L = K$.

by applying a spectrum filter, the DFT samples between $M$ and $K - M$ are eliminated, where $M = \frac{k' \Delta z K}{2\pi}$. An IDFT is then performed to obtain the updated field distribution with the unnecessary wavenumber components filtered out. Thus, the reconstructed field distribution can be expressed as

$$
\hat{E}_{x,k}^n = \frac{1}{K} \left[ \sum_{p=0}^{M-1} \hat{E}_{x,p}^n \exp \left( -j \frac{2\pi pk}{K} \right) + \sum_{p=K-M+1}^{K-1} \hat{E}_{x,p}^n \exp \left( -j \frac{2\pi pk}{K} \right) \right]. \quad (5.45)
$$

Note that since the time-domain field is real, $E_x^n(K-p) = [E_x^n(p)]^*$. To this end, the truncation error for the field at spatial index $k$ accumulated at each time step can be expressed as

$$
\mathcal{E}_k = \frac{1}{K} \sum_{p=M}^{K-M} \hat{E}_{x,k}^n \exp \left( -j \frac{2\pi pk}{K} \right). \quad (5.46)
$$

Substitute (5.44) into (5.46), and we have

$$
\mathcal{E}(k) = \frac{1}{K} \sum_{p=M}^{K-M} \sum_{l=0}^{K-1} E_{x,l}^n \exp \left( j \frac{2\pi pl}{K} \right) \exp \left( -j \frac{2\pi pk}{K} \right)
= \frac{1}{K} \sum_{l=0}^{K-1} E_{x,l}^n \sum_{p=M}^{K-M} \exp \left( j \frac{2\pi p(l - k)}{K} \right)
= \frac{1}{K} \sum_{l=0}^{K-1} (-1)^{(l-k)} E_{x,l}^n \frac{\sin \left( 2\pi \left( \frac{K+1}{2} - M \right) (l-k) \right)}{\sin \frac{\pi (l-k)}{K}}. \quad (5.47)
$$

Also, since

$$
\frac{1}{K} \sum_{l=0}^{K-1} (-1)^{(l-k)} E_{x,l}^n \frac{\sin \left( \frac{2\pi}{K} \left( \frac{K+1}{2} - M \right) (l-k) \right)}{\sin \frac{\pi (l-k)}{K}}
\leq \| E_{x,l}^n \|_\infty \frac{1}{K} \sum_{l=0}^{K-1} (-1)^{(l-k)} \frac{\sin \left( \frac{2\pi}{K} \left( \frac{K+1}{2} - M \right) (l-k) \right)}{\sin \frac{\pi (l-k)}{K}}. \quad (5.48)
$$
Figure 5.5: The upper bound of the relative error introduced by the spatial filtering method during a single FDTD time step, within a computational domain of 16384 cells with (a) $R_{\Delta t} = 2$, (b) $R_{\Delta t} = 5$, (c) $R_{\Delta t} = 10$, and (d) $R_{\Delta t} = 20$.

The upper bound of the relative error accumulated at each time step can be written in the form of

$$
\epsilon(k) = \frac{E_k}{\|E_{x,l}\|_\infty} \leq \frac{1}{K} K^{K-1} \sum_{l=0}^{K-1} (-1)^{(l-k)} \sin \left( \frac{2\pi}{K} \left( \frac{K}{2} - M \right) (l-k) \right) \sin \left( \frac{\pi(l-k)}{K} \right).
$$

At this point it can be concluded that the upper bound of the relative error of the spatial filtering method is solely determined by the size of the computational domain $K$ and the filter parameter $M$, which depends on the ratio $R_{\Delta t} = \Delta t/\Delta t_{CFL}$. Figure 5.5 shows the upper bound of the relative error with a 1D computational domain of 16384 cells, with different values of $R_{\Delta t}$. It can be observed that the upper bound of the error increases significantly along with $R_{\Delta t}$, and the most significant error occurs near the boundary of...
the computational domain.

5.3.3 Extension to Nonlinear Media: Numerical Validation

With the established spatial filtering method in Section 5.3.1, it is an important question whether this method can be extended to simulate nonlinear structures. Such an extension is extremely promising since in nonlinear structures, to accurately resolve the higher order modes, very dense spatial discretization is typically required, leading to potentially large $CE$ factors according to (5.40), and thus time savings comparable to the nonlinear ADI-FDTD with a much simpler algorithm.

To numerically investigate this possibility, a numerical example of 1D medium with Kerr nonlinearity is set up to demonstrate the performance of the spatial filtering method in solving nonlinear problem. The 1D computational domain has a length of 20.5 $\mu$m, and a relative permittivity of $\varepsilon_r = 2.25$. A nonlinear dielectric slab occupies the domain from 6 $\mu$m to 14 $\mu$m, with a Kerr nonlinearity $\varepsilon_r(z) = \varepsilon_{r0}(1 + \lambda |E_x(z)|^2)$ where $\varepsilon_{r0} = 2.25$ and $\lambda = 0.02$. A modulated Gaussian pulse from 200-400 THz is applied 4 $\mu$m away in front of the first interface of the nonlinear slab.

The standard ADE-FDTD with or without spatial filtering is used to simulate the nonlinear structure. The whole computational domain is discretized into 16384 Yee cells, including one uniaxial Perfectly Matched Layer (PML) with a fourth-order polynomial grading and optimized parameters at each end of the domain. Since the Yee cell size is relatively small compared to the wavelength, the uniaxial PML is chosen to be 100-cell thick, which is equivalent to about a quarter of the minimum wavelength. For ADE-FDTD without spatial filtering, again, a stability test is performed to determine the maximum time step size, which is $\Delta t_0 = 0.46\Delta t_{CFL} = 0.003$ fs. For the spatial filtering method, $\Delta t = 2\Delta t_0$, $5\Delta t_0$, and $10\Delta t_0$ are used. The cutoff wavenumbers used in these cases are $\tilde{k}'\Delta z = 0.333\pi$, $0.128\pi$, and $0.064\pi$, respectively.

Figure 5.6 shows the frequency domain spectrum of the field at the center of the
nonlinear slab, obtained using ADE-FDTD without the spatial filtering method, as well as ADE-FDTD with the spatial filtering method with different time step sizes. It can be observed that the result from the proposed method is in good agreement with the conventional FDTD. Figure 5.7 depicts the error of the electric field inside the computational domain using the spatial filtering method, at $t = 31$ fs and 62 fs, using the ADE-FDTD result (without spatial filtering) as a reference. The theoretical error obtained from (5.47) is also plotted in the figure. It is obvious that the error estimation equation predicts the error of the proposed method perfectly. Moreover, Fig. 5.8 compares the maximum time domain error computed from (5.32), again using ADE-FDTD without spatial filtering as a reference, and the total CPU time required to simulate a fixed time span, between different time step sizes of the spatial filtering method.
Figure 5.7: The error of the electric field inside the nonlinear slab using the spatial filtering method, using the result of the conventional ADE-FDTD without spatial filtering as a reference, along with the theoretical calculation from (5.47) (indicated with triangles) at $t = 31$ ps (left column) and 62 ps (right column) with different values of $R_{\Delta t}$. 
Figure 5.8: The maximum relative error within the computational domain and the relative total CPU execution time of the spatial filtering method, using the result of the ADE-FDTD without spatial filtering as a reference.

5.4 Application: Gap Soliton in Finite Periodic Nonlinear Stack

The proposed nonlinear ADI-FDTD method, as well as the spatial filtering method, is applied to simulate a finite nonlinear periodic structure. The structure under study is a Bragg reflector consisting of a finite length of a weakly nonlinear optical stack with Kerr nonlinearity, shown in Fig. 5.9.

If a linear version of such a stack is illuminated by normal incident radiation within a stop gap, the envelope of the field magnitude decays exponentially while propagating in the stack. With enough Bragg reflector layers, the transmissivity of the structure is considerably small. However, it has been shown numerically in [79, 80] that with one layer in each unit cell with a weak Kerr nonlinearity of suitable parameters, the incident power can partially close the bandgap. In such a situation, if the incident wave frequency is originally at the edge of the bandgap, the gap edge may move past the frequency of
Figure 5.9: The geometry of a finite periodic nonlinear stack with plane wave incidence.

incidence, allowing the system to switch to a transmitting state. With proper incident power intensity, the transmissivity becomes equal to one, while the incident field couples to a soliton-like resonance inside the stack region.

Such a numerical observation has been further investigated theoretically in [81]. By separating the solution of the nonlinear stack problem into a fast Bloch-like component and a slowly varying envelope function, it is rigorously proved that as long as only the envelope is concerned, the stack can be viewed as a homogenous nonlinear medium. Thus, its solution follows the nonlinear Schrodinger’s equation.

The nonlinear stack presented in [79] is 1D with a periodicity of 0.25 µm. Each unit cell consists of a linear layer with $\varepsilon_{r1} = 2.25$ attached to a nonlinear layer with a linear permittivity $\varepsilon_{r2} = 4.5$ and a pure Kerr nonlinearity, so that $\varepsilon_r(z) = \varepsilon_{r2}(1 + \lambda |E_x(z)|^2)$.

The two layers have the same thickness. The finite periodic stack consists of 40 unit cells of such layers.

To characterize the dispersion of this structure in the linear regime, one unit cell of the stack with both layers chosen to be linear, i.e. $\lambda = 0$, is analyzed with sine-cosine periodic boundaries. Figure 5.10 displays the dispersion diagram, showing a bandgap
Figure 5.10: The dispersion diagram of the unit cell of the linear stack, where $d_z$ is the periodicity of the stack.

with a lower edge at 293 THz. An incident field at a frequency slightly higher than the lower bandgap edge, i.e. 300 THz, will cause significant reflections. Figure 5.11 shows the magnitude of the scattering parameters of the linear stack with 20 layers. The transmission coefficient at 300 THz is below -25 dB.

Next, we simulate 20 layers of the structure with a Kerr nonlinearity factor $\lambda = -0.004 \text{ m}^2/\text{V}^2$ in the second layer of the unit cell. A monochromatic source of 300 THz is placed 1.25 µm away in front of the stack. The computational domain is discretized with 16384 unit cells with size of 0.625 nm ($\approx \lambda_{\text{min}}/1000$) to limit the numerical phase velocity error induced by higher-order terms, and is terminated in 100-cell PMLs with a fourth-order polynomial grading and optimized parameters. In both methods, $R_{\Delta t} = \Delta t/\Delta t_0 = 5$ is used. For the spatial filtering method, this corresponds to a cutoff wavenumber of $\tilde{k}'\Delta z = 0.128\pi$. Here $\Delta t_0$ is the maximum time step size yielding a stable solution of the nonlinear structure using conventional ADE-FDTD. As mentioned in previous sections, it is decided by a stability test and equals to 0.001875 fs, which is 0.6 times of the CFL limit.
Figure 5.11: The S-parameters of the unit cell of the finite linear stack with 20 unit cells.

Figure 5.12 shows the theoretical transmissivity of the nonlinear stack at 300 THz as a function of the normalized incident power $\tilde{P} = \lambda E_0^2$ from [79], where $E_0$ is the magnitude of the incident field at the front interface of the nonlinear stack. The thick dashed line in the figure shows the transmissivity when the system is in the highly reflecting state. The bi-stable nature of the problem is clearly observed. At point $P_1$ and $P_2$, the transmissivity is effectively unity, and the gap soliton is formed inside the stack area.

To reach the state $P_1$, an incident wave with a carrier frequency 300 THz and a slowly varying envelope is injected. The envelope of the incident field is a superposition of a constant and a Gaussian pulse, so that the normalized power $\tilde{P}$ of the envelope varies between -0.004 and -0.08. A total number of $1.8 \times 10^5$ time steps are run, which are equivalent to the time span of $9 \times 10^5 \Delta t_0$ with conventional ADE-FDTD. Figure 5.13 shows the envelope of the incident plane wave with respect to the time step. Thus, when the magnitude of the incident power increases, the transmissivity of the stack first follows the thick dash line in Fig. 5.12. When $|\tilde{P}| > 0.075$, the transmissivity will switch to the next state, and, when the magnitude decreases, follow the solid line to $P_1$, where the gap
Figure 5.12: The transmissivity of the finite nonlinear stack with 20 unit cells at 300 THz as a function of the normalized incident power.

The total CPU time for the nonlinear ADI-FDTD and the spatial filtering method with $R_{\Delta t} = 5$ is 422 seconds and 355 seconds, respectively, while the conventional FDTD takes 676 seconds to simulate an equivalent time span. Figure 5.14, 5.15, and 5.16 show the electric field in the computational domain, inside and outside the nonlinear stack, at 28000-th, 92000-th, and 175000-th time step, obtained using the nonlinear ADI-FDTD and the spatial filtering method. The transmissivity in these figures corresponds to points A, B, and P$_1$ in Fig. 5.12, respectively. In Fig. 5.16, the shape of a gap soliton inside the nonlinear stack region is clearly observed using both methods. The intensity $P = |E^2_x|$ inside the stack area at the 175000-th time step, normalized to the incident intensity at the first interface of the stack $E^2_{x0}$, is also plotted in Fig. 5.17, which is identical to the result shown in [79].
5.5 Summary

The ADI-FDTD, originally designed to solve linear problems, is combined with the non-linear auxiliary variable equation method to offer an efficient solution for structures with third-order nonlinearity, induced by either Kerr or Raman effect. Such a scheme is free from Courant stability limit. Moreover, another methodology to extend the stability limit of the FDTD beyond conventional with linear and nonlinear structures is also proposed, which is based on filtering out unnecessary spatial frequency spectrum components during each time step of FDTD.

Both approaches are able to allow a time step size larger than conventional FDTD. To this end, they are especially useful for nonlinear applications, since the minimum FDTD cell size required to accurately resolve the response inside a nonlinear structure is much smaller than the minimum wavelength. The accuracy and efficiency of both algorithms are investigated through two numerical benchmark examples. It has been shown that the two proposed methods can substantially decrease the computation time while maintain a reasonable level of accuracy. The two approaches are applied to simulate a gap soliton.
Figure 5.14: The instantaneous electric field inside the computational domain at the 28000-th time step, obtained using nonlinear ADI-FDTD and the spatial filtering method.

inside a nonlinear periodic stack, both obtaining satisfactory results while reducing the required computational time significantly.
Figure 5.15: The instantaneous electric field inside the computational domain at the 92000-th time step, obtained using nonlinear ADI-FDTD the spatial filtering method.

Figure 5.16: The instantaneous electric field inside the computational domain at the 175000-th time step, obtained using nonlinear ADI-FDTD the spatial filtering method.
Figure 5.17: The normalized power intensity of the electric field inside the nonlinear stack region at the 175000-th time step, obtained using nonlinear ADI-FDTD and the spatial filtering method, along with the theoretical calculation result from [79].
Chapter 6

Conclusions

6.1 Summary

The efficient modeling of periodic-structure-based geometries in the time domain has always been an important research area. For periodic structures with non-periodic elements, conventional periodic boundary conditions (PBCs) are not applicable due to the incompatibility of the PBCs with complex non-periodic sources and boundaries. This work offered several fast and accurate tools to solve different classes of problems based on periodic structures, including driven periodic structures, microstrip lines and antennas over periodic substrates, as well as finite nonlinear dielectric stacks.

For linear media, the thesis proposed a combination of the sine-cosine Finite-Difference Time-Domain (FDTD) and time-domain form of the array-scanning method. For infinitely periodic structures with non-periodic sources, this methodology was able to decompose the problem into a number of low-cost simulations with one unit cell of the structure. Such a method has the potential to achieve significant savings in both computation time and memory, especially under a multiple-processor environment. The accuracy and efficiency of the proposed methodology was testified by a numerical application of the negative-refractive index (NRI) “perfect lens”.

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The aforementioned scheme was then further extended to include the modeling of non-periodic metallic objects above periodic substrates, such as microstrip lines and antennas. This was done by means of the application of PBCs to model the latter, absorbing boundary conditions to terminate the space above the metallic object and the array-scanning technique to enable source modeling. For antenna applications, the methodology has been enhanced by an efficient scheme for near-to-far-field transformation which leads to the fast calculation of antenna radiation patterns, based on the assumption that the distance of the antenna from the periodic structure is electrically small.

Moreover, the potential of the proposed sine-cosine based array-scanning FDTD as a lattice termination method was also demonstrated. It has been shown that the method delivers at least the same, and potentially better, absorptivity than conventional Perfectly Matched Layers (PMLs), while remaining a simple and uniform formulation regardless of the conductivity and dispersion of the enclosed medium. These features, along with the fact that it overcomes various limitations of conventional boundary conditions, make the method a useful alternative for FDTD lattice termination.

For nonlinear media, on the other hand, due to the dependence of material properties on local field intensities, the conventional PBCs are no longer available. Thus, instead of seeking a periodic boundary compatible solution, this work has focused on alleviating the heavy computational load introduced by the fine spatial and time mesh in FDTD with general nonlinear media. Such an objective was accomplished by a nonlinear version of the Alternating-Direction Implicit FDTD (ADI-FDTD) based on auxiliary differential equations, as well as a spatial filtering method to filter out unstable spatial harmonics in the computational domain. Both methods are able to use time step sizes well beyond the Courant-Friedrichs-Lewy (CFL) limit, thus potentially improving the efficiency of FDTD simulations. The application of both methods in periodic structure characterizations was validated with the example of a gap soliton inside a weakly nonlinear periodic dielectric stack.
6.2 Contributions

This section lists refereed journal and conference papers, and other academic contributions made during the course of this thesis work.

6.2.1 Journal Papers


6.2.2 Conference Papers

[C1] **D. Li** and C. D. Sarris, “FDTD lattice termination with periodic boundary conditions,” in *IEEE Microwave Theory and Techniques Society 2009 International Microwave Symposium Digest*, (Boston, MA, USA), June 2009.


### 6.3 Future Work

The methodologies proposed in this work have successfully addressed the interaction between various non-periodic objects and infinitely periodic structures. In practice, such classes of problems serve as idealized approximations, as actual periodic structures are always finite along the direction of periodicity. Thus, how to efficiently extract time-domain responses in finite periodic structures utilizing the information obtained by periodic analyses remains an intriguing question. One possible solution is to find the surface impedance at the boundary of one unit cell as the combination of the Bloch impedance and free-space impedance. Then, the surface impedance can be used to characterize the impedance boundary condition in FDTD.

For the efficient characterization of nonlinear media, the two methodologies proposed
in this work were both derived from their linear counterparts. The stability and numerical
dispersion of the ADI-FDTD, as well as the spatial filtering method, has been rigorously
demonstrated with linear media. For nonlinear media, the rigorous analysis of stability
conditions of the ADI-FDTD and the spatial filtering method remains to be explored.
Such an analysis may be based on the numerical energy analysis.
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