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Analysis of periodic structures using finite-difference time-domain method

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ANALYSIS OF PERIODIC STRUCTURES USING FINITE-DIFFERENCE TIME-DOMAIN METHOD

By

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ABSTRACT

Periodic structures are of great importance in electromagnetics these days due to their wide range of applications such as frequency selective surfaces (FSS), electromagnetic band gap, periodic absorbers, metamaterials and many others.

The aim of this work is to develop several algorithms to analyze different types of electromagnetic periodic structures using the constant horizontal wavenumber finite-difference time-domain periodic boundary condition (FDTD/PBC). A new FDTD/PBC approach is introduced to analyze the scattering properties of general skewed grid periodic structures. The approach is simple to implement and efficient in terms of both computational time and memory usage.

In addition, an efficient hybrid FDTD generalized scattering matrix (GSM) technique is developed to analyze multilayer periodic structure. The technique is based on the FDTD constant horizontal wavenumber approach to compute the scattering parameters of each layer. The new technique saves computational time and storage memory.

Moreover, a new algorithm is developed to analyze dispersive periodic structures, the algorithm is easy to implement and efficient in both computational time and memory usage. All the developed algorithms are validated through several numerical test cases.
LIST OF ABBREVIATIONS

ABC  Absorbing Boundary Condition
ADE  Auxiliary Differential Equation
CPML Convolutional Perfect Matched Layer
CPU  Central Processing Unit
DFT  Discrete Fourier Transform
DPBC Dispersive Periodic Boundary Condition
EBG  Electromagnetic Band Gap
FDTD Finite-Difference Time-Domain
FEM  Finite Element Method
FSS  Frequency Selective Surface
GB   Giga Byte
GSM  Generalized Scattering Matrix
HFSS High Frequency Structure Simulator
JC   Jerusalem Cross
MB   Mega Byte
MoM  Method of Moments
PBC  Periodic Boundary Condition
PBCs Periodic Boundary Conditions
PEC  Perfect Electric Conductor
PML  Perfect Matched Layer
RAM  Random Access Memory
RC   Recursive Convolution
RCS  Radar Cross Section
RFID Radio Frequency Identification
TE   Transverse Electric
TM   Transverse Magnetic
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University, Mississippi
December, 2010

Khaled ElMahgoub
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CHAPTER I

1 INTRODUCTION

1.1 Background

The finite-difference time-domain (FDTD) method has gained great popularity as a tool for solving Maxwell’s equations. The FDTD method is based on a simple formulation that does not require complex asymptotic or Green’s functions. Although it is based on a time-domain solution, it provides a wideband frequency-domain response using time-domain to frequency-domain transformation. It can easily handle composite geometries consisting of different types of materials. In addition, it can be easily implemented using parallel computational algorithms. These features of FDTD have made it one of the most attractive techniques in computational electromagnetics for many applications. FDTD has been used to solve numerous types of problems such as scattering, radar cross section, microwave circuits, waveguides, antennas, propagation, non-linear and other special materials, and many other applications [1].

Periodic electromagnetic structures are of great importance due to their applications in the design of frequency selective surfaces (FSS), electromagnetic band gap (EBG) structures, corrugated surfaces, phased antenna arrays, periodic absorbers, negative index materials, and many other applications. Many versions of the FDTD algorithms have been developed to analyze such structures and to make use of the periodicity of these structures. Periodic boundary conditions (PBC) were implemented in many forms such that only one unit cell can be analyzed instead of the entire structure. These techniques are divided into two main categories in [2]: field-transformation methods and direct field methods. Field transformation methods introduce auxiliary fields to eliminate the need for time-advanced data; the transformed field equations are
then discretized and solved using FDTD techniques. The split-field method [3] and multi-spatial grid method [4] are useful approaches in the field-transformation category. There are two main limitations with these methods: First, the transformed equations have additional terms that require special handling such as splitting the field and the use of a multi-grid algorithm to implement the FDTD, which increases the complexity of the problem. Second, as the angle of incidence increases from normal incidence ($\theta = 0^\circ$) to grazing incidence ($\theta = 90^\circ$), the stability factor needs to be reduced, so the FDTD time step decreases significantly [2]. As a result, smaller time steps are needed for oblique incidence to generate stable results, which increases the computational time for such cases.

As for the direct field category, these methods work directly with Maxwell’s equations, and there is no need for any field transformation. An example of these methods is the sine-cosine method [5], in which the structure is excited simultaneously with sine and cosine waveforms. The PBC for oblique incidence can be implemented using this method. The stability criterion for this technique is the same as the conventional FDTD (angle-independent), which provides stable analysis for incidence near grazing. However, it is a single frequency method and loses an important property of FDTD, the wide-band capability.

In [6]-[8] a simple and efficient FDTD/PBC algorithm was introduced that belongs to the direct field category and yet has a wideband capability. In this new approach, the FDTD simulation is performed by setting a constant horizontal wavenumber instead of a specific angle of incidence. The idea of using a constant wavenumber in FDTD originated from guided wave structure analysis and eigenvalue problems in [9], and it was extended to the plane wave scattering problems in [10]-[12]. The approach offers many advantages, such as implementation simplicity, stability condition and numerical errors similar to the conventional FDTD,
computational efficiency near the grazing incident angles, and the wide-band capability. Due to
the advantages offered by the constant horizontal wavenumber PBC, the algorithm is used in this
dissertation to solve some challenges in the simulation of periodic structures, such as a skewed
grid periodic structure, multilayered periodic structure, and dispersive periodic structures. This
dissertation starts with a description of the FDTD constant horizontal wavenumber approach.
The main advantages and disadvantages of the approach are discussed. The FDTD updating
equations are derived and numerical results are provided to verify the validity of the approach.

1.2 Contributions

It’s worthwhile to point out that most previous FDTD PBCs were developed to analyze axial
grid periodic structure. However, there are numerous applications where the grid of the periodic
structures is a general skewed grid. In Chapter 3, the constant horizontal wavenumber approach
is extended to analyze periodic structures with an arbitrary skewed grid. The new approach is
described and the FDTD updating equations are derived for both the cases in which the skewed
shift is coincident and non-coincident with the FDTD grid. Numerical results proving the validity
of the new approach are provided.

In today’s applications, many periodic structures are often built up of layers, each layer being
either a diffraction grating, periodic in one or two directions, or a homogenous dielectric slab
which acts as a separator or support. In Chapter 4, a complete analysis of a multilayer periodic
structure using the constant horizontal wavenumber is illustrated. The generalized scattering
matrix (GSM) cascading technique is used to analyze different kinds of multilayered periodic
structures. In addition, complete harmonic analysis using FDTD is presented and an algorithm
for determining whether the separation between different layers is large or small is provided.
Different cases of multilayer periodic structures are analyzed and numerical results are provided to prove the validity and efficiency of the new proposed algorithms.

Most previous PBCs for the FDTD technique were developed to analyze periodic structures where dispersive materials are not located on the boundaries of the unit cell. However, there are numerous applications where periodic structures with dispersive media on the boundaries of the unit cell must be used. In Chapter 5, a new dispersive periodic boundary condition (DPBC) for the FDTD technique is developed to solve the above challenge. The algorithm utilizes the auxiliary differential equation (ADE) technique with two-term Debye relaxation equation to simulate the general dispersive property in the medium. In addition, the constant horizontal wavenumber approach is modified accordingly to implement the periodic boundary conditions. The new algorithm offers many advantages such as implementation simplicity, stability condition and numerical errors similar to the conventional FDTD in addition to the computational efficiency. The validity of this algorithm is verified through several numerical examples.
CHAPTER II

2 FDTD METHOD AND PERIODIC BOUNDARY CONDITIONS

2.1 Basic Equations of the FDTD Method

The FDTD method belongs to the general class of grid-based differential time-domain numerical modeling methods. The time-dependent Maxwell's equations (in partial differential form) are discretized using central-difference approximations to the space and time partial derivatives.

The Time-domain Maxwell’s equations can be stated as follows:

\[ \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}, \]  \hspace{1cm} (2.1a)

\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \vec{M}, \]  \hspace{1cm} (2.1b)

\[ \nabla \cdot \vec{D} = \rho_e, \]  \hspace{1cm} (2.1c)

\[ \nabla \cdot \vec{B} = \rho_m, \]  \hspace{1cm} (2.1d)

where \( \vec{E} \) is the electric field intensity vector in \( \text{V/m} \), \( \vec{D} \) is the electric displacement vector in \( \text{C/m}^2 \), \( \vec{H} \) is the magnetic field intensity vector in \( \text{A/m} \), \( \vec{B} \) is the magnetic flux density vector in \( \text{Weber/m}^2 \), \( \vec{J} \) electric current density vector in \( \text{A/m}^2 \), \( \vec{M} \) is the magnetic current density vector in \( \text{V/m}^2 \), \( \rho_e \) is the electric charge density in \( \text{C/m}^3 \), and \( \rho_m \) is the magnetic charge density in \( \text{Weber/m}^3 \). For linear, isotropic, and non-dispersive materials the electric displacement vector and the magnetic flux density vector can be written as
\[ \vec{D} = \varepsilon \vec{E}, \quad \text{(2.2a)} \]

\[ \vec{B} = \mu \vec{H}, \quad \text{(2.2b)} \]

where \( \varepsilon \) is permittivity and \( \mu \) is permeability of the material. The electric current density \( \vec{J} \) is the sum of the conduction current density \( \vec{J}_c = \sigma^e \vec{E} \) and the impressed current density \( \vec{J}_i \) as \( \vec{J} = \vec{J}_c + \vec{J}_i \). Similarly, for the magnetic current density \( \vec{M} = \vec{M}_c + \vec{M}_i \), where \( \vec{M}_c = \sigma^m \vec{H} \).

Here \( \sigma^e \) is the electric conductivity of the material in S/m and \( \sigma^m \) is the magnetic conductivity of the material in \( \Omega/m \). Using the two curl equations (2.1) and the equation (2.2), one can rewrite Maxwell’s curl equations as

\[ \nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t} + \sigma^e \vec{E} + \vec{J}_i, \quad \text{(2.3a)} \]

\[ \nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t} - \sigma^m \vec{H} - \vec{M}_i. \quad \text{(2.3b)} \]

Equation (2.3) consists of two vector equations and each vector equation can be decomposed to three scalar equations for three dimensional space. Therefore, Maxwell’s curl equations can be represented with six scalar equations in a Cartesian coordinate system \((x, y, z)\) as follows:

\[ \frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon_x} \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma^e_x E_x - J_x \right), \quad \text{(2.4a)} \]

\[ \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_y} \left( \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} - \sigma^e_y E_y - J_y \right), \quad \text{(2.4b)} \]

\[ \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_z} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma^e_z E_z - J_z \right), \quad \text{(2.4c)} \]
\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu_x} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma_s^x H_x - M_{ix} \right), \quad (2.4d)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu_y} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \sigma_s^y H_y - M_{iy} \right), \quad (2.4e)
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu_z} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma_s^z H_z - M_{iz} \right). \quad (2.4f)
\]

The material parameters \( \varepsilon_x, \varepsilon_y, \) and \( \varepsilon_z \) are associated with electric field components \( E_x, E_y, \) and \( E_z \) through the equation (2.2a). Similarly the material parameters \( \mu_x, \mu_y, \) and \( \mu_z \) are associated with magnetic field components \( H_x, H_y, \) and \( H_z \) through the equation (2.2b) [1].

The first step in the FDTD algorithm is approximating the time and space derivatives appearing in Maxwell’s equations by finite-differences; the central finite-difference is used as an approximation of the space and time derivatives of both the electric and magnetic fields. The derivative of a function \( f(x) \) at a point \( x_0 \) using central finite-difference can be written as

\[
f'(x_0) \approx \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}, \quad (2.5)
\]

where \( \Delta x \) is the sampling period.

Secondly, electric and the magnetic field components are assigned to certain positions in each cell. In 1966, Yee was the first to set up an algorithm to solve both the electric and magnetic Maxwell’s curl equations [13].
In the Yee cell shown in Fig. 2.1, the three components of electric and magnetic fields are placed in certain positions in the cell such that they simulate Maxwell’s equations. From Fig. 2.1, it should be noticed that the electric field vectors form loops around the magnetic field vectors, which simulates Faraday’s law. On the other hand, the magnetic field vectors form loops around the electric field vectors, which simulates Ampere’s law. The electric field vectors are assigned to the center of the edges of the cells, while the magnetic field vectors are assigned to the center of the faces of the cells. The calculations of the electric and magnetic fields are not only offset in position but also in time. The electric field components are calculated at a certain time instant \((n+1) \Delta t\), while the magnetic field components are calculated at the time instant \((n+0.5) \Delta t\).
Equations (2.4) and (2.5) are used to construct six FDTD updating equations for the six components of electromagnetic fields by the introduction of respective coefficient terms as follows [1]:

For the $E_x$ component:

$$E^{n+1}_x(i,j,k) = C_{exc}(i,j,k) \times E^n_x(i,j,k)$$
$$+ C_{edc}(i,j,k) \times \left( H^{n+\frac{1}{2}}(i,j,k) - H^{n+\frac{1}{2}}(i,j-1,k) \right)$$
$$+ C_{edy}(i,j,k) \times \left( H^{n+\frac{1}{2}}(i,j,k) - H^{n+\frac{1}{2}}(i,j,k-1) \right)$$
$$+ C_{cxy}(i,j,k) \times J^{n+\frac{1}{2}}_{ix}(i,j,k),$$

where

$$C_{exc}(i,j,k) = \frac{2\varepsilon_x(i,j,k) - \Delta t \sigma^e_x(i,j,k)}{2\varepsilon_x(i,j,k) + \Delta t \sigma^e_x(i,j,k)},$$
$$C_{edc}(i,j,k) = \frac{2\Delta t}{(2\varepsilon_x(i,j,k) + \Delta t \sigma^e_x(i,j,k))\Delta y},$$
$$C_{edy}(i,j,k) = \frac{-2\Delta t}{(2\varepsilon_x(i,j,k) + \Delta t \sigma^e_x(i,j,k))\Delta z},$$
$$C_{cxy}(i,j,k) = \frac{-2\Delta t}{2\varepsilon_x(i,j,k) + \Delta t \sigma^e_x(i,j,k)}.$$

For the $E_y$ component:

$$E^{n+1}_y(i,j,k) = C_{cxy}(i,j,k) \times E^n_y(i,j,k)$$
$$+ C_{cyh}(i,j,k) \times \left( H^{n+\frac{1}{2}}(i,j,k) - H^{n+\frac{1}{2}}(i,j,k-1) \right)$$
$$+ C_{ceh}(i,j,k) \times \left( H^{n+\frac{1}{2}}(i,j,k) - H^{n+\frac{1}{2}}(i-1,j,k) \right)$$
$$+ C_{cxy}(i,j,k) \times J^{n+\frac{1}{2}}_{iy}(i,j,k),$$

where
\[
C_{eiy}(i,j,k) = \frac{2\varepsilon_y(i,j,k) - \Delta t\sigma^e_y(i,j,k)}{2\varepsilon_y(i,j,k) + \Delta t\sigma^e_y(i,j,k)}, \quad C_{eix}(i,j,k) = \frac{2\Delta t}{(2\varepsilon_y(i,j,k) + \Delta t\sigma^e_y(i,j,k))\Delta z},
\]
\[
C_{eyh}(i,j,k) = \frac{-2\Delta t}{(2\varepsilon_y(i,j,k) + \Delta t\sigma^e_y(i,j,k))\Delta x}, \quad C_{eiy}(i,j,k) = \frac{-2\Delta t}{2\varepsilon_y(i,j,k) + \Delta t\sigma^e_y(i,j,k)}.
\]

For the \(E_z\) component:

\[
E_{z}^{n+1}(i,j,k) = C_{eex}(i,j,k) \times E_{z}^{n}(i,j,k)
+ C_{ecx}(i,j,k) \times \left( H_{y}^{n+\frac{1}{2}}(i,j,k) - H_{y}^{n+\frac{1}{2}}(i-1,j,k) \right)
+ C_{ecz}(i,j,k) \times \left( H_{x}^{n+\frac{1}{2}}(i,j,k) - H_{x}^{n+\frac{1}{2}}(i,j-1,k) \right)
+ C_{eey}(i,j,k) \times J_{iz}^{n+\frac{1}{2}}(i,j,k),
\]

where

\[
C_{eex}(i,j,k) = \frac{2\varepsilon_x(i,j,k) - \Delta t\sigma^e_x(i,j,k)}{2\varepsilon_x(i,j,k) + \Delta t\sigma^e_x(i,j,k)}, \quad C_{ecx}(i,j,k) = \frac{2\Delta t}{(2\varepsilon_x(i,j,k) + \Delta t\sigma^e_x(i,j,k))\Delta y}, \quad C_{ecz}(i,j,k) = \frac{-2\Delta t}{2\varepsilon_x(i,j,k) + \Delta t\sigma^e_x(i,j,k)}.
\]

For the \(H_x\) component:

\[
H_{x}^{n+\frac{1}{2}}(i,j,k) = C_{heh}(i,j,k) \times H_{x}^{n-\frac{1}{2}}(i,j,k)
+ C_{hexy}(i,j,k) \times \left( E_{y}^{n}(i,j,k+1) - E_{y}^{n}(i,j,k) \right)
+ C_{hexz}(i,j,k) \times \left( E_{z}^{n}(i,j+1,k) - E_{z}^{n}(i,j,k) \right)
+ C_{hexm}(i,j,k) \times M_{iz}^{n}(i,j,k),
\]

where

\[
C_{heh}(i,j,k) = \frac{2\mu_x(i,j,k) - \Delta t\sigma^m_x(i,j,k)}{2\mu_x(i,j,k) + \Delta t\sigma^m_x(i,j,k)}, \quad C_{hexy}(i,j,k) = \frac{2\Delta t}{(2\mu_x(i,j,k) + \Delta t\sigma^m_x(i,j,k))\Delta z},
\]
\[
C_{hexz}(i,j,k) = \frac{-2\Delta t}{(2\mu_x(i,j,k) + \Delta t\sigma^m_x(i,j,k))\Delta y}, \quad C_{hexm}(i,j,k) = \frac{-2\Delta t}{2\mu_x(i,j,k) + \Delta t\sigma^m_x(i,j,k)}.
\]
For the $H_y$ component:

$$H_{y}^{n+\frac{1}{2}}(i, j, k) = C_{hyh}(i, j, k) \times H_{y}^{n-\frac{1}{2}}(i, j, k) + C_{hye}(i, j, k) \times \left( E_{n}^{x}(i+1, j, k) - E_{n}^{x}(i, j, k) \right) + C_{hye}(i, j, k) \times \left( E_{n}^{y}(i, j, k+1) - E_{n}^{y}(i, j, k) \right) + C_{hye}(i, j, k) \times M_{O}^{n}(i, j, k),$$

(2.10)

where

$$C_{hyh}(i, j, k) = \frac{2\mu_{y}(i, j, k) - \Delta t\sigma_{m}^{n}(i, j, k)}{2\mu_{y}(i, j, k) + \Delta t\sigma_{m}^{y}(i, j, k)}, C_{hye}(i, j, k) = \frac{2\Delta t}{2\mu_{y}(i, j, k) + \Delta t\sigma_{m}^{y}(i, j, k)} \Delta x,$$

$$C_{hye}(i, j, k) = \frac{-2\Delta t}{2\mu_{y}(i, j, k) + \Delta t\sigma_{m}^{y}(i, j, k)} \Delta y, C_{hye}(i, j, k) = \frac{-2\Delta t}{2\mu_{y}(i, j, k) + \Delta t\sigma_{m}^{y}(i, j, k)} \Delta z.$$

For the $H_z$ component:

$$H_{z}^{n+\frac{1}{2}}(i, j, k) = C_{hzh}(i, j, k) \times H_{z}^{n-\frac{1}{2}}(i, j, k) + C_{hzx}(i, j, k) \times \left( E_{n}^{x}(i, j + 1, k) - E_{n}^{x}(i, j, k) \right) + C_{hzy}(i, j, k) \times \left( E_{n}^{y}(i, j, k+1) - E_{n}^{y}(i, j, k) \right) + C_{hzm}(i, j, k) \times M_{O}^{n}(i, j, k),$$

(2.11)

where

$$C_{hzh}(i, j, k) = \frac{2\mu_{z}(i, j, k) - \Delta t\sigma_{m}^{n}(i, j, k)}{2\mu_{z}(i, j, k) + \Delta t\sigma_{m}^{z}(i, j, k)}, C_{hzx}(i, j, k) = \frac{2\Delta t}{2\mu_{z}(i, j, k) + \Delta t\sigma_{m}^{z}(i, j, k)} \Delta x,$$

$$C_{hzy}(i, j, k) = \frac{-2\Delta t}{2\mu_{z}(i, j, k) + \Delta t\sigma_{m}^{z}(i, j, k)} \Delta y, C_{hzm}(i, j, k) = \frac{-2\Delta t}{2\mu_{z}(i, j, k) + \Delta t\sigma_{m}^{z}(i, j, k)} \Delta z.$$

After deriving the six FDTD updating equations (2.6) – (2.11), a time-marching algorithm can be constructed, as shown in Fig. 2.2.
The first step in this algorithm is setting up the problem space, including objects, material type, sources, etc., and defining any other parameters that will be used during the FDTD computation. The problem space usually has a finite size and specific boundary conditions can be enforced on the boundaries of the problem space. Therefore, the field components on the boundaries of the problem are treated according to the type of the boundary conditions during the

Fig. 2.2 The flowchart of the conventional FDTD code [1].
iteration. After the fields are updated and boundary conditions are enforced, the current values of the desired field components are captured and stored as output data, and this data can be used for real time processing and/or post-processing in order to calculate other desired parameters. The FDTD iterations can be continued until some stopping criteria are achieved.

### 2.2 Periodic Boundary Conditions

The speed of the simulation and the storage space depends mainly on the size of the computational domain. For the free space scattering problem, the computational domain must be extended to infinity, which means an infinite number of cells in the computational domain are needed. The solution of this problem is to truncate the domain by a set of artificial boundaries at a certain distance from the objects. Various boundary conditions were developed to solve this problem, such as perfect electric conductor (PEC) boundaries, which can be used to simulate cavity structures, and absorbing boundary conditions (ABC), which can be used to simulate open boundary problems. Different methods have been used to simulate an absorbing boundary condition in FDTD calculations. The most common ones are Mur [14], Liao [15], perfect matched layer (PML) [16], and convolutional perfect matched layer (CPML) [17].

Periodic boundary conditions (PBCs) were developed to implement periodic structure using FDTD. The main idea is to make use of the periodic nature of the structure such that only one unit cell needs to be analyzed instead of the entire structure. The difference between a periodic boundary condition and a normal absorbing boundary condition is that electric field components outside the boundary are known for PBC due to the periodicity. Consider the 1-D periodic problem shown in Fig. 2.3, the fields in the unit cell \((i+N+1)\) have the same values as the fields in unit cell \((i+N)\) and \((i+N+2)\), etc.
From the above figure, it is obvious that $E_{z_{n+1}}$ component can be updated using the knowledge of $E_{z_0}$. According to the Floquet theory, the boundary electric field of a periodic structure with periodicity $P_x$ along the $x$-direction can be written in the frequency-domain as

$$E(x, y, z) = E(x = P_x, y, z) \times e^{j k_x P_x}. \tag{2.12}$$

### 2.3 Constant Horizontal Wavenumber Approach

To understand the constant horizontal wavenumber method, the case of an infinite dielectric slab shown in Fig. 2.4(a) should be considered. The slab is illuminated with a TM$^z$ plane wave.
Fig. 2.4 (a) $k_0$ direction and slab geometry, (b) Analytical reflection coefficient of infinite dielectric slab.

The thickness of the slab is $h = 0.2$ m, and its relative permittivity is $\varepsilon_r = 4$; the reflection coefficient of the infinite slab is shown in Fig. 2.4(b). Assuming the incident angle is $\theta$, the horizontal wavenumber $k_x$ is given by

$$k_x = k_0 \sin \theta$$  \hspace{1cm} (2.13)

where $k_0 = \omega/c$ is the free space wavenumber, and $c$ is wave speed in free space.

From Fig. 2.4, it should be noticed that the reflection coefficient plotted in the $k_x$-frequency plane provides a complete description of the scattering properties of the dielectric slab for all angles of incidence. In addition, Fig. 2.4 illustrates different FDTD methods, the solid line represents the split-field method, which simulates oblique incidence with fixed angle and a band of frequencies; the small star represents the sine-cosine method, which simulates the oblique
incidence at fixed angle and fixed frequency; the dotted horizontal line represents normal incidence, and the dashed line represents the constant horizontal wavenumber method, which simulates the oblique incidence for different angles of incidence and different frequencies, but with constant $k_x$. From Fig. 2.4 it could also be noticed that for certain $k_x$ value the simulation is only valid from a certain minimum frequency where the dashed line meets the $45^\circ$ line.

The constant horizontal wavenumber approach is to fix the value of the horizontal wavenumber $k_x$ in the FDTD simulation instead of the angle $\theta$, where $k_x$ is determined by both frequency and angle of incidence. Thus, the term $e^{jk_xP_x}$ is considered constant in (2.12). Using direct frequency-domain to time-domain transformation, the field in the time-domain can be represented as follows:

$$ E(x = 0, y, z, t) = E(x = P_x, y, z, t) \times e^{jk_xP_x} . \tag{2.14} $$

It also should be pointed out that both the $E$ and $H$ fields have complex values in the FDTD computation because of the PBC in (2.14) [6].

Therefore, by fixing $k_x$ (varying angle with frequency), the need for the knowledge time-advanced electric field component is eliminated. An important issue related to the constant wavenumber method is plane wave excitation. If the traditional total-field/scattered-field (TF/SF) formulation described in [18] is applied, a problem arises regarding the incident angle. For example, the tangential electric field component of a TM$^z$ incident wave depends on the incident angle. To overcome this problem, the TF/SF technique is modified. In the case of TM$^z$ excitation, only the tangential magnetic incident field component is imposed on the excitation plane $z = z_0$. The one-field excitation allows the plane wave to propagate in both directions $z > z_0$ and $z < z_0$ ($z_0$ is the excitation plane position). Thus, the entire computational domain becomes
the total field region, and there is no scattered field region. The scattered field can be calculated using the difference of the total and the incident field. Similarly for the TE\(_z\) case, only the tangential electric incident field component is imposed.

In addition, there exists a problem of horizontal resonance, where fields do not decay to zero over time. To avoid this problem, the proper frequency range for the excitation waveform must be chosen as follows [6]:

\[
f_C = \frac{k \cdot c}{2 \pi} + \frac{BW}{2}.
\]

(2.15)

where \(f_C\) is the center frequency of the Gaussian pulse and \(BW\) is the bandwidth of the Gaussian pulse. In this approach, the conventional Yee scheme shown in Fig. 2.1 is used to update the \(E\) and \(H\) fields, which offers several advantages, such as implementation simplicity and the same stability condition and numerical errors similar to the conventional FDTD. In addition, the computational efficiency for incident angles near grazing and wideband capability are achieved as well [6]. This makes the constant horizontal wavenumber approach a good choice for the analysis of periodic structures.

Fig. 2.5 Periodic structure geometry (square patch FSS).
The reflection and transmission properties of the periodic structure shown in Fig. 2.5 can be calculated using FDTD by simulating unit A only. The magnetic field components are updated using the conventional FDTD updating equations (2.9) – (2.11), while the electric field, non-boundary components will be updated using the conventional FDTD updating equations (2.6) – (2.8). The components on the boundaries will be updated using PBC equations based on the constant horizontal wavenumber approach. The updating equations for the boundary electric field components are organized as follows:

- Updating $E_x$ at $y = 0$ and $y = P_y$.
- Updating $E_y$ at $x = 0$ and $x = P_x$.
- Updating $E_z$ at $y = 0, y = P_y, x = 0$, and $x = P_x$, without the corners.
- Updating $E_z$ at the corners.
To update the $E_x$ on the boundary $y = 0$, the magnetic field components $H_z$ outside unit A are needed. However, due to the periodicity in the $y$-direction, one can use magnetic field components $H_z$ of interest inside unit A to update these electric fields as

$$E_{x}^{n+1}(i,1,k) = C_{exe}(i,1,k) \times E_{x}^{n}(i,1,k) + C_{exh}(i,1,k) \times [H_{z}^{n+1/2}(i,1,k) - H_{z}^{n+1/2}(i,0,k)]$$

$$+ C_{exh}(i,1,k) \times [H_{y}^{n+1/2}(i,1,k) - H_{y}^{n+1/2}(i,1,k-1)],$$

(2.16)

where the coefficients are stated as in (2.6), and $H_{z}^{n+1/2}(i,0,k) = H_{z}^{n+1/2}(i,n_y,k) \times e^{j \Delta y}$ due to the periodicity in the $y$-direction as shown in Fig. 2.6. The term $e^{j \Delta y}$ is used to compensate the phase shift due to general oblique incidence.

Then the updating equation for $E_x$ on the boundary $y = 0$ can be written as

$$E_{x}^{n+1}(i,1,k) = C_{exe}(i,1,k) \times E_{x}^{n}(i,1,k)$$

$$+ C_{exh}(i,1,k) \times [H_{z}^{n+1/2}(i,1,k) - H_{z}^{n+1/2}(i,n_y,k) \times e^{j \Delta y}]$$

$$+ C_{exh}(i,1,k) \times [H_{y}^{n+1/2}(i,1,k) - H_{y}^{n+1/2}(i,1,k-1)],$$

(2.17)

where $n_y$ is the total number of FDTD cells in the $y$-direction, and $\Delta y$ is the FDTD cell size in the $y$-direction. As for $E_x$ on the boundary $y = P_y$, the updating equation can be written as

$$E_{x}^{n+1}(i,n_y + 1,k) = E_{x}^{n+1}(i,1,k) \times e^{-j \Delta y}.$$  

(2.18)
Due to periodicity in $x$-direction as shown in Fig 2.7, the updating equation for the $E_y$ component on the boundary $x = 0$ can be written as

$$E_y^{n+1}(1, j, k) = C_{eyxe}(1, j, k) \times E_y^n(1, j, k) + C_{eyhx}(1, j, k) \times [H_x^{n+1/2}(1, j, k) - H_x^{n+1/2}(1, j, k - 1)] + C_{eyhz}(1, j, k) \times [H_z^{n+1/2}(1, j, k) - H_z^{n+1/2}(n_x, j, k) \times e^{jk_n,\Delta x}],$$

where $n_x$ is the total number of FDTD cells in the $x$-direction within the period $P_x$, and $\Delta x$ is the FDTD cell size in the $x$-direction.

As for $E_y$ on the boundary $x = P_x$, the updating equation can be written as

$$E_y^{n+1}(n_x + 1, j, k) = E_y^{n+1}(1, j, k) \times e^{-jk_n,\Delta x}. \quad (2.20)$$

A similar procedure is used for updating the $E_z$ components, but corner components are updated separately due to the presence of periodicity in both $x$- and $y$-directions. For $E_z$ on the boundaries $x = 0$ and $x = P_x$, the updating equation can be written for $j \neq 1$ and $j \neq n_y+1$ (avoiding the corners) as
\[ E_{z}^{n+1}(1, j, k) = C_{exc}(1, j, k) \times E_{z}^{n}(1, j, k) \]
\[ \quad + C_{ehy}(1, j, k) \times [H_{y}^{n+\frac{1}{2}}(1, j, k) - H_{y}^{n+\frac{1}{2}}(n_{y}, j, k) \times e^{jk_{x}n_{x}}] \]  
\[ \quad + C_{ehx}(1, j, k) \times [H_{x}^{n+\frac{1}{2}}(1, j, k) - H_{x}^{n+\frac{1}{2}}(1, j - 1, k)]. \]  

\[ E_{z}^{n+1}(n_{x} + 1, j, k) = E_{z}^{n+1}(1, j, k) \times e^{-jk_{x}n_{x}}. \]  

The updating equation for the \( E_{z} \) components on the boundaries \( y = 0 \), and \( y = P_{y} \) can be written for \( i \neq 1 \) and \( i \neq n_{x} + 1 \) (avoiding the corners) as

\[ E_{z}^{n+1}(i, 1, k) = C_{exc}(i, 1, k) \times E_{z}^{n}(i, 1, k) \]
\[ \quad + C_{ehy}(i, 1, k) \times [H_{y}^{n+\frac{1}{2}}(i, 1, k) - H_{y}^{n+\frac{1}{2}}(i - 1, 1, k)] \]
\[ \quad + C_{ehx}(i, 1, k) \times [H_{x}^{n+\frac{1}{2}}(i, 1, k) - H_{x}^{n+\frac{1}{2}}(i, n_{y}, k) \times e^{jk_{x}n_{x}}]. \]  

\[ E_{z}^{n+1}(i, n_{y} + 1, k) = E_{z}^{n+1}(i, 1, k) \times e^{-jk_{x}n_{x}}. \]  

The \( E_{z} \) components at the corners are updated as follows:

At \( x = 0 \) and \( y = 0 \),

\[ E_{z}^{n+1}(1, 1, k) = C_{exc}(1, 1, k) \times E_{z}^{n}(1, 1, k) \]
\[ \quad + C_{ehy}(1, 1, k) \times [H_{y}^{n+\frac{1}{2}}(1, 1, k) - H_{y}^{n+\frac{1}{2}}(n_{y}, 1, k) \times e^{jk_{x}n_{x}}] \]
\[ \quad + C_{ehx}(1, 1, k) \times [H_{x}^{n+\frac{1}{2}}(1, 1, k) - H_{x}^{n+\frac{1}{2}}(1, n_{y}, k) \times e^{jk_{x}n_{x}}]. \]  

At \( x = P_{x} \) and \( y = 0 \),

\[ E_{z}^{n+1}(n_{x} + 1, 1, k) = E_{z}^{n+1}(1, 1, k) \times e^{-jk_{x}n_{x}}. \]  

At \( x = 0 \) and \( y = P_{y} \),

\[ E_{z}^{n+1}(1, n_{y} + 1, k) = E_{z}^{n+1}(1, 1, k) \times e^{-jk_{x}n_{x}}. \]
At $x = P_x$ and $y = P_y$,

$$E_z^{n+1}(n_x + 1, n_y + 1, k) = E_z^n(1, 1, k) \times e^{-jk, n_y \Delta y} \times e^{-jk, n_x \Delta x}. \quad (2.28)$$

![Flowchart of the FDTD/PBC code](image)

Fig. 2.8 The flowchart of the FDTD/PBC code.
Equations (2.16) – (2.28) describe the constant horizontal wavenumber method. All these equations are derived for an obliquely incident plane wave. For a normally incident plane wave all the phase compensation terms should be set to one. After deriving the updating equations, a time marching algorithm can be constructed as shown in Fig. 2.8. The main difference between this algorithm and the conventional FDTD algorithm shown in Fig. 2.2, is the updating of the boundary electric field components.

### 2.4 Numerical Results

In this section, numerical results generated using the constant horizontal wavenumber method are presented. The FDTD code was developed using the MATLAB [19] programming language. All the test cases were executed using the same computer (Intel Core 2 CPU 6700 2.66GHz with 2 GB RAM). These results demonstrate the validity of the approach for determining reflection and transmission properties of periodic structures. The first example is an infinite dielectric slab excited by TM$^z$ and TE$^z$ plane waves. The second example is a dipole FSS, and the last example is a Jerusalem cross (JC) FSS. The results are compared with results obtained from analytical solutions for the dielectric slab and Ansoft Designer [20] (which is based on MoM) for the dipole and JC FSS. The numerical results are shown in two different representations. The first representation plots results of reflection coefficient magnitude versus frequency with certain horizontal wavenumber values. The second representation plots the results of the reflection coefficient magnitude versus frequency for a certain angle of incidence, which requires multiple runs of the code to generate such results. In addition, the MATLAB code is capable of generating the phase of the reflection coefficient. Moreover, the code is capable of extracting the magnitude and phase of the transmission coefficient and the reflection and transmission cross-polarization coefficients.
2.4.1 An Infinite Dielectric Slab

Due to its homogeneity, the infinite dielectric slab can be considered as a periodic structure with any periodicity. In addition, the analytical solution can be easily generated, which makes the infinite dielectric slab an appropriate verification case. The approach is first used to analyze an infinite dielectric slab with thickness $h = 9.375$ mm and relative permittivity $\varepsilon_r = 2.56$ (the reflection and transmission properties of an infinite dielectric slab can be calculated analytically). The slab is illuminated by TM$^z$ and TE$^z$ plane waves, respectively. The slab is excited using a cosine-modulated Gaussian pulse centered at 10 GHz with a 20 GHz bandwidth (in this dissertation the bandwidth of modulated Gaussian pulse is defined as the frequency band where the magnitude of the frequency domain reaches 10% of its maximum at the center of the pulse). Two cases are examined where the plane wave is incident normally ($k_x = k_y = 0$ m$^{-1}$) in the first case and obliquely ($k_x = 104.8$ m$^{-1}$, $k_y = 0$ m$^{-1}$ for minimum frequency of 5 GHz) in the second case. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.3125$ mm and the slab is represented by $5 \times 5$ cells. In the FDTD code, 2,500 time steps and a Courant factor [21] of 0.9 are used [1].

![Fig. 2.9 (a) The FDTD/PBC domain with different boundary conditions, (b) An infinite dielectric slab in the FDTD/PBC computational domain.](image)
Fig. 2.10 Reflection coefficient for infinite dielectric slab, (a) TM\textsuperscript{z} case, (b) TE\textsuperscript{z} case.

The CPML is used for the absorbing boundaries at the top and the bottom of the computational domain as shown in Fig. 2.9. In Fig. 2.10 the results are compared with analytical
results, where good agreement between the analytical solutions and results generated by the constant horizontal wavenumber method for both TMz and TEz cases (normal and oblique incidence) are observed. The stability of the algorithm can be noticed even at the angles of incidence near grazing ($\theta = 90^\circ$).

2.4.2 A Dipole FSS

The algorithm is then used to analyze an FSS structure consisting of dipole elements. The dipole length is 12 mm and width is 3 mm. The periodicity is 15 mm in both the $x$- and $y$-directions. The substrate has a thickness of 6 mm and relative permittivity $\varepsilon_r = 2.2$, as shown in Fig. 2.11 [22]. The structure is first illuminated by a normally incident plane wave (with polarization along the $y$-axis). Figure 2.12 provides the results for normal incidence. The structure is excited using a cosine-modulated Gaussian pulse centered at 8 GHz with a 16 GHz bandwidth.

Fig. 2.11 Dipole FSS geometry (all dimensions are in mm).
In the FDTD code, 2,500 time steps and a Courant factor of 0.9 are used. The CPML is used for absorbing boundaries at the top and the bottom of the computational domain. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.5$ mm. The results are compared with results obtained from Ansoft Designer. The computational time per simulation for the FDTD code is 4.53 minutes, and the memory usage is 0.2MB, while for Ansoft Designer the computational time per simulation is 45 minutes for 30 frequency points, and the memory usage is 21 MB.

To show the capabilities of the constant horizontal wavenumber code, results for several $k_x$’s versus frequency are generated, as shown in Figure 2.13. From the figure the reflection and transmission regions can be clearly identified. It should be noticed that near the light line ($\theta = 90^\circ$, $k_x = k_0$), there exists some oscillation. This is because the excitation signal is weak at that frequency region.
Fig. 2.13 The reflection coefficient for dipole FSS with TE$^z$ plane wave ($k_x = 0$ to 419.17 m$^{-1}$).

Figure 2.14 provides results for an oblique incidence case ($k_x = 20$ m$^{-1}$ and $k_y = 7.28$ m$^{-1}$ for minimum frequency of 2 GHz) where the structure is excited using a cosine-modulated Gaussian pulse centered at 9 GHz with a 14 GHz bandwidth. In the FDTD code, 2,500 time steps and a Courant factor of 0.9 are used. The computational time per simulation for the FDTD code is 5.023 minutes, and the memory usage is 0.9MB, while for Ansoft Designer the computational time per simulation is 50 minutes for 30 frequency points, and the memory usage is 21 MB. From Fig. 2.14 good agreement between the results generated using Ansoft Designer and results generated using the new algorithm for oblique incidence can be noticed.
2.4.3 A Jerusalem Cross FSS

Next, the algorithm is used to analyze an FSS structure consisting of Jerusalem cross (JC) elements. The periodicity is 15.2 mm in both the x- and y-directions. The dimensions of the elements are shown in Fig. 2.15 [23]. The structure is illuminated by a TE\(^z\) plane wave (polarized along the y-axis). Figure 2.16 provides results for normal incidence. The structure is excited using a cosine-modulated Gaussian pulse centered at 7 GHz with 8 GHz bandwidth. The grid cell size is \(\Delta x = \Delta y = 0.2285\) mm and \(\Delta z = 0.457\) mm. In the FDTD code, 3,000 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries at the top and the bottom. The results were compared with results obtained from Ansoft Designer. The computational time per simulation for the FDTD code is 4.53 minutes, and the memory usage is 0.2 MB, while for Ansoft Designer computational time per simulation is 45 minutes for 30 frequency points, and the memory usage is 21 MB using the same computer.

Fig. 2.14 The reflection coefficient for dipole FSS with oblique incident TE\(^z\) plane wave \((k_x = 20\ \text{m}^{-1}, k_y = 7.28\ \text{m}^{-1})\).
Fig. 2.15 JC FSS geometry (all dimensions are in mm).

Fig. 2.16 Co- and cross-polarization reflection coefficients for JC FSS with normal incident TE$_z$ plane.

Figure 2.17 provides results for oblique incidence ($\theta = 60^\circ$ and $\varphi = 45^\circ$) exciting a JC FSS structure. To generate results for a specific angle of incidence, multiple runs of the code are needed, which increases the computational time.
Fig. 2.17 Co- and cross-polarization reflection coefficient for JC FSS with oblique incident TE\(^z\) plane wave (\(\theta = 60^\circ, \varphi = 45^\circ\)).

Using 30 different \(k_x\) values (from 25.501 m\(^{-1}\) to 93.5036 m\(^{-1}\)), both co- and cross-polarization reflection coefficients were generated. The results were compared with results obtained from Ansoft Designer. Good agreement between the results generated using Ansoft Designer and results generated using the new algorithm for both normal and oblique incidence can be noticed from Figs. 2.16 and 2.17.

2.5 Summary

In this chapter, a description of the FDTD constant horizontal wavenumber approach was provided. The main advantages and disadvantages of the approach were discussed, and the FDTD updating equations were derived. The approach is simple to implement and efficient in terms of both computational time and memory usage. In addition, the stability criterion is essentially angle-independent. Therefore, it is efficient in implementing incidence with angle close to grazing as well as normal incidence. It is capable of calculating the co- and cross-
polarization reflection and transmission coefficients of normal and oblique incidence for both the TE^z and TM^z cases, and for different periodic structures with single or multiple k_x values. The numerical results show good agreement with results from the analytical solution for the dielectric slab and the MoM solutions for both dipole and JC FSS structures.
CHAPTER III

3 SKEWED GRID PERIODIC STRUCTURES

3.1 Introduction

It’s worthwhile to point out that most PBCs mentioned in the previous chapter are developed to analyze axial grid periodic structures. However, there are numerous applications where the grid of the periodic structures is a general skewed grid (used to decrease the grating lobes in phased arrays antenna, etc.). Figure 3.1 shows the geometries of both axial and skewed grid structures. The axial periodic structures are special cases of the general skewed grid structures, where the skew angle $\alpha = 90^\circ$. Although the analysis of a skewed grid periodic structure has been well developed using the MoM technique [22], it has not been fully solved with FDTD. A pioneering effort presented in [24] utilizes the sine-cosine method in the analysis of periodic phased arrays with skewed grids and thus loses the wideband capability of the FDTD. Furthermore, the work presented in [24] belongs to a special case where the amount of shift in the skew direction is an integer multiple of the FDTD cell size in the same direction. This special case is referred to as “coincident” in this dissertation.

Fig. 3.1 Geometries of (a) Axial, and (b) Skewed periodic structures.
In this chapter, the constant horizontal wavenumber approach is extended to analyze periodic structures with skewed grids. Two cases of skewed grid periodic structures are implemented. In the first case, the skew amount is coincident with the FDTD grid; and in the second case, the skew amount is non-coincident with the FDTD grid (the general skewed grid periodic structure). In addition, the new algorithm is very efficient and simple, and it retains the broadband capabilities of the FDTD.

This chapter is organized as follows: in Section 3.2, the FDTD updating equations are derived for both the coincident and the non-coincident skew amount cases. In Section 3.3, several numerical examples proving the validity of the new approach are presented, including an infinite dielectric slab, a dipole FSS, and a Jerusalem cross FSS. Various incident angles, skew angles, and polarizations have been tested in these examples, and the numerical results show good agreement with the analytical results or other numerical results obtained from the frequency-domain methods.

3.2 Constant Horizontal Wavenumber Approach for Skewed Grid Case

In this section the derivation of the different electric and magnetic field updating equations are presented for two cases: in the first case the shift is an integer number of FDTD grid cells (coincident), while in the second case the shift is not an integer number of FDTD grid cells (non-coincident).

3.2.1 The Coincident Skewed Shift

Figure 3.2 shows the FDTD grid for the coincident skewed shift periodic structure. In this specific example, the unit cell is discretized using 5x5 FDTD grid cells ($\Delta x \times \Delta y$); the unit A is the one to be simulated, while unit B and unit C are the adjacent periodic units. The structure has
periodicity of $P_x$ in the $x$-direction and $P_y$ in the $y$-direction. $S_x$ is the skewed shift which can be calculated as $S_x = P_y / \tan(\alpha)$, where $\alpha$ is the skew angle. Since the skewed shift $S_x$ is between 0 and $P_x$, the skew angle is between $90^\circ$ and $\tan^{-1}(P_y / P_x)$. For the periodic structures with a square unit cells ($P_y = P_x$), the skew angle is between $90^\circ$ and $45^\circ$. For a periodic structure with a rectangular unit cells, it is possible to get a small skew angle.

It should be noticed from Fig. 3.2, that in this case $S_x$ is an integer multiple of the discretization step in the $x$-direction ($\Delta x$). This configuration makes the shift coincident with the FDTD grid and this simplifies the calculation of the boundary electric fields. The magnetic field components are updated using the conventional FDTD updating equations (2.9) – (2.11). As for the electric field, non-boundary components are updated using the conventional FDTD updating equations (2.6) – (2.8).

![Fig. 3.2 FDTD grid for skewed periodic structure coincident case ($E_x$ components).](image)

Fig. 3.2 FDTD grid for skewed periodic structure coincident case ($E_x$ components).
The components at the boundaries are updated using PBC equations based on the new approach. In this specific case, the skewed shift is in the $x$-direction. A similar procedure can be used if the skewed shift is in the $y$-direction.

The updating equations for boundary electric field components are organized as follows:

- Updating $E_x$ at $y = 0$ and $y = P_y$.
- Updating $E_y$ at $x = 0$ and $x = P_x$.
- Updating $E_z$ at $y = 0, y = P_y, x = 0$, and $x = P_x$ without the corners.
- Updating $E_z$ at the corners.

To update $E_z$ on the boundary $y = 0$, the magnetic field components $H_z$ outside unit A are needed, as shown in Fig. 3.2. However, due to periodicity and taking into account the skewed shift, one can use magnetic field components $H_z$ inside unit A to update these electric fields.

For $i + (S_x / \Delta x) \leq n_x$

$$H_z^{n+1/2}(i, 0, k) = H_z^{n+1/2}(i + \frac{S_x}{\Delta x}, n_y, k) \times e^{i k_x S_x} \times e^{j k_y P_x}, \quad (3.1)$$

while for $i + (S_x / \Delta x) > n_x$

$$H_z^{n+1/2}(i, 0, k) = H_z^{n+1/2}(i + \frac{S_x}{\Delta x} - n_x, n_y, k) \times e^{i k_x (S_x - P_x)} \times e^{j k_y P_y}, \quad (3.2)$$

where $n_x$ and $n_y$ are the total number of cells in $x$- and $y$-directions, respectively. The two exponential terms are used to compensate the phase variations due to the oblique incidence. Using (3.1) and (3.2), the updating equation for the $E_x$ components on the boundary $y = 0$ can be written as
\[ E_{x}^{n+1}(i,1,k) = C_{ex}(i,1,k) \times E_{x}^{n}(i,1,k) + C_{ex}^{e}(i,1,k) \times [H_{x}^{n+1/2}(i,1,k) - H_{x}^{n+1/2}(i,0,k)] \\
+ C_{exy}(i,1,k) \times [H_{y}^{n+1/2}(i,1,k) - H_{y}^{n+1/2}(i,1,k-1)], \]  

(3.3)

where the coefficients are the same as in (2.6).

The updating equation for the \( E_{x} \) components on the boundary \( y = P_{y} \) can be written

for \( i - (S_{x} / \Delta x) \leq 0 \) as

\[ E_{x}^{n+1}(i,n_{y} + 1,k) = E_{x}^{n+1}(i + n_{y} - \frac{S_{x}}{\Delta x},1,k) \times e^{-jk_{y}(S_{y} - P_{y})} \times e^{-jk_{y}P_{y}}, \]  

(3.4)

while for \( i - (S_{x} / \Delta x) > 0 \)

\[ E_{x}^{n+1}(i,n_{y} + 1,k) = E_{x}^{n+1}(i - \frac{S_{x}}{\Delta x},1,k) \times e^{-jk_{y}S_{y}} \times e^{-jk_{y}P_{y}}, \]  

(3.5)

As for updating the \( E_{y} \) components on the boundaries \( x = 0 \) and \( x = P_{x} \), (2.19) and (2.20) are used with no further modification. For the \( E_{z} \) components on the boundaries \( x = 0 \) and \( x = P_{x} \), the updating equations (2.23) and (2.24) can be used for \( j \neq 1 \) and \( j \neq n_{y} + 1 \) (avoiding the corners). Updating the \( E_{z} \) components on the boundaries \( y = 0 \) and \( y = P_{y} \) is handled in a similar manner as the \( E_{x} \) components, as shown in Fig. 3.3, which requires taking into consideration the skewed shift.
Fig. 3.3 FDTD grid for coincident case $E_z$ components (avoiding the corners).

The updating equation for the $E_z$ components on the boundaries $y = 0$ can be written for $i \neq 1$ and $i \neq n_x + 1$ (avoiding the corners) as

$$E_z^{n+1}(i,1,k) = C_{ee}(i,1,k) \times E_z^n(i,1,k) + C_{ehy}(i,1,k) \times [H_y^{n+1/2}(i,1,k) - H_y^{n+1/2}(i-1,1,k)]$$
$$+ C_{ehy}(i,1,k) \times [H_x^{n+1/2}(i,1,k) - H_x^{n+1/2}(i,0,k)]. \quad (3.6)$$

For $i + (S_x/\Delta x) \leq n_x$

$$H_x^{n+1/2}(i,0,k) = H_x^{n+1/2}(i + \frac{S_x}{\Delta x}, n_y, k) \times e^{jk_i} \times e^{jk_y} \times e^{jk_z}, \quad (3.7)$$

while for $i + (S_x/\Delta x) > n_x$

$$H_x^{n+1/2}(i,0,k) = H_x^{n+1/2}(i + \frac{S_x}{\Delta x} - n_x, n_y, k) \times e^{jk_i} \times (S_x - P_x) \times e^{jk_y} \times e^{jk_z}. \quad (3.8)$$
Fig. 3.4 FDTD grid for coincident case $E_z$ corner components.

The $E_z$ components at the corners are updated according to Fig 3.4 as follows:

At $x = 0$ and $y = 0$

$$E_z^{n+1}(1,1,k) = C_{exc}(1,1,k) \times E_z^n(1,1,k)$$
$$+ C_{elec}(1,1,k) \times [H_y^{n+1/2}(1,1,k) - H_y^{n+1/2}(n_x,1,k) \times e^{jkx}]$$
$$+ C_{eh}(1,1,k) \times [H_x^{n+1/2}(1,1,k) - H_x^{n+1/2}(1 + \frac{S_y}{\Delta x},n_y,k) \times e^{jky}] .$$ (3.9)

At $x = P_x$ and $y = 0$

$$E_z^{n+1}(n_x+1,1,k) = E_z^{n+1}(1,1,k) \times e^{-jkx}.$$ (3.10)

At $x = 0$ and $y = P_y$

$$E_z^{n+1}(1,n_y+1,k) = E_z^{n+1}(1+n_x \frac{S_y}{\Delta x},1,k) \times e^{-jky} \times e^{-jkx} .$$ (3.11)
At \( x = P_x \) and \( y = P_y \)

\[
E_{z}^{n+1}(n_x+1, n_y+1, k) = E_{z}^{n+1}(1, n_y+1, k) \times e^{-jk \cdot P_x}.
\] (3.12)

The above procedure provides the six FDTD updating equations for the case of a coincident skewed shift. These updating equations can be used to update electric and magnetic fields in any region in the computational domain (boundary and non-boundary).

### 3.2.2 The Non-Coincident Skewed Shift

In this section the shift is considered to be a general shift, not an integer multiple of the discretization step in the \( x \)-direction (\( \Delta x \)) as shown in Fig. 3.5. In this case, two possible solutions can be used. The first solution is to decrease (\( \Delta x \)) so that the shift becomes coincident with the new discretization and use the above formulation, but this will increase the computational time. In addition, an appropriate \( \Delta x \) has to be chosen with every new skew angle.

Fig. 3.5 FDTD grid for skewed periodic structure non-coincident (\( E_x \) components).
The second method that will be described in this section uses an interpolation between adjacent field components to calculate the required field component. As shown in Fig. 3.5, the shift is not an integer multiple of the discretization step in the $x$-direction ($\Delta x$). So the skewed shift is considered non-coincident with the FDTD grid. As a result, to update the $E_x$ component in cell 1 (shown in the left top corner in Fig. 3.5), an interpolation between $H_z$ in cell 2 and $H_z$ in cell 3 is needed to get the corresponding $H_z$ for this $E_x$ component. The interpolation is linear interpolation based on the two distances $x_1$ and $x_2$ ($x_1$ is the distance between the magnetic field in cell 2 and the position of the corresponding magnetic field, and $x_2$ is the distance between the magnetic field in cell 3 and the position of the corresponding magnetic field). It should be noticed that the two $H_z$ components in cells 2 and 3 are outside the unit A. However, as described in the previous section, due to periodicity and taking into account the skewed shift, one can use magnetic field components $H_z$ inside the unit of interest to drive these two components. Then the $H_z$ component corresponding to $E_x$ in cell 1 can be written as

$$H_z^{\pi+1/2}(1,0,k) = w_1 H_z^{\pi+1/2}(1,\left\lceil \frac{S_x}{\Delta x} \right\rceil, n_y, k) + w_2 H_z^{\pi+1/2}\left(\left\lfloor \frac{S_x}{\Delta x} \right\rfloor, n_y, k\right) e^{j(kx_1 - S_x P_y)} e^{j(ky_1 P_y)},$$

(3.13)

where $\left\lceil x \right\rceil$ is the ceiling function, and $w_1$ and $w_2$ are the two weighting factors calculated based on distances $x_1$ and $x_2$: $w_1 = x_1 / \Delta x$, $w_2 = x_2 / \Delta x$. Using (3.13) and (3.3), the $E_x(1,1,k)$ can be updated. Similarly, all other $E_x$ components on the boundary $y = 0$ can be updated.

As for the $E_x$ components on the boundary $y = P_y$, consider the updating equation for the first component $E_x(1,n_y+1,k)$:

$$E_x^{\pi+1}(1,n_y+1,k) = w_1 E_x^{\pi+1}(1+n_x - \left\lfloor \frac{S_x}{\Delta x} \right\rfloor, 1, k) + w_2 E_x^{\pi+1}(2+n_x - \left\lfloor \frac{S_x}{\Delta x} \right\rfloor, 1, k) e^{-j(kx_1 - S_x P_y)} e^{-j(ky_1 P_y)}.$$

(3.14)
Similarly, all other $E_x$ components on the boundary $y = P_y$ can be updated. For updating the $E_y$ components on the boundaries $x = 0$ and $x = P_x$, equations (2.19) and (2.20) are used with no further modification. The $E_z$ components on the boundaries $x = 0$ and $x = P_x$, the updating equations (2.23) and (2.24) can be used for $j \neq 1$ and $j \neq n_y + 1$ (avoiding the corners).

Updating the $E_z$ components on the boundaries $y = 0$ and $y = P_y$ (avoiding the corners) will be handled in a similar manner as the $E_x$ components, as shown in Fig. 3.6, which requires taking into consideration the skewed shift. Note that the $H_x(i,0,k)$ is calculated from interpolation similar to the $H_z(1,0,k)$ in (3.13).

$$H_{x}^{n+1 \over 2}(2,0,k) = [w_1H_{x}^{n+1 \over 2}(2 + \left[ {S_y \over \Delta x} \right] ,n_y,k) + w_2H_{x}^{n+1 \over 2}(2 + \left[ {S_y \over \Delta x} \right] +1,n_y,k)] \times e^{jkS_y} \times e^{jkP_y} \quad (3.15)$$

Fig. 3.6 FDTD grid for non-coincident case ($E_z$ components).
Using (3.15) and (3.6) the electric field $E_z(2,1,k)$ can be updated. Similarly all other $E_z$ components on the boundary $y = 0$ can be updated. The $E_z$ component on the boundary $y = P_y$ can be updated as follows:

$$E_z^{n+1}(2,n_y+1,k) = w_1 E_z^{n+1}(2+n_x, 1, k) + w_2 E_z^{n+1}(3+n_x, 1, k) \times e^{-j\beta_y(S_x - P_y)} \times e^{-j\beta_y P_y}. \quad (3.16)$$

If $n_x = 5$ in equation (3.16), then for this specific case $\text{cei}(S_x/\Delta x)$ will be equal 2. The component $E_z^{n+1}(3+n_x, 1, k) = E_z^{n+1}(6,1,k)$ is a corner component so for the proper updating sequence, the corner $E_z$ components ($y = 0$) should be updated before updating the $E_z$ on the boundary $y = P_y$. Similar to the component $E_z^{n+1}(2,n_y+1,k)$, all other $E_z$ components on the boundary $y = P_y$ can be updated.

Fig. 3.7 FDTD grid for non-coincident case $E_z$ corner components.
The $E_z$ components at the corners are updated according to Fig. 3.7 as follows:

At $x = 0$ and $y = 0$

$$
E_{z}^{n+1}(1,1,k) = C_{eze}(1,1,k) \times E_{z}^{n}(1,1,k) + C_{ezy}(1,1,k) \times [H_{y}^{n+1/2}(1,1,k) - H_{y}^{n+1/2}(n_x,1,k) \times e^{jk_{y}P_{y}}]
$$

$$
+ C_{ezy}(1,1,k) \times [H_{x}^{n+1/2}(1,1,k) - H_{x}^{n+1/2}(1,0,k)],
$$

where

$$
H_{x}^{n+1/2}(1,0,k) = [w_{1}H_{x}^{n+1/2}(1+\left[\frac{S_{x}}{\Delta x}\right],n_{y},k) + w_{2}H_{x}^{n+1/2}(\left[\frac{S_{x}}{\Delta x}\right],n_{y},k)] \times e^{jk_{x}S_{x} \times e^{jk_{y}P_{y}}}. \tag{3.17}
$$

At $x = P_{x}$ and $y = 0$

$$
E_{z}^{n+1}(n_{x}+1,1,k) = E_{z}^{n+1}(1,1,k) \times e^{-jk_{y}P_{y}}. \tag{3.19}
$$

At $x = 0$ and $y = P_{y}$

$$
E_{z}^{n+1}(1,n_{y}+1,k) = \left[w_{1}E_{z}^{n+1}(1+n_{x} - \left[\frac{S_{x}}{\Delta x}\right],1,k) + w_{2}E_{z}^{n+1}(2+n_{x} - \left[\frac{S_{x}}{\Delta x}\right],1,k) \right] \times e^{-jk_{x}(S_{x}N_{x}) \times e^{-jk_{y}P_{y}}}. \tag{3.20}
$$

At $x = P_{x}$ and $y = P_{y}$

$$
E_{z}^{n+1}(n_{x}+1,n_{y}+1,k) = E_{z}^{n+1}(1,n_{y}+1,k) \times e^{-jk_{y}P_{y}}. \tag{3.21}
$$

The above procedure provides the six FDTD updating equations for the case of the non-coincident skewed shift. These updating equations can be used to update the electric and magnetic fields in any region in the computational domain (boundary and non-boundary).
3.3 Numerical Results

In this section, numerical results generated using the new algorithms are presented. The FDTD code was developed using the MATLAB programming language. All the test cases were executed using the same computer (Intel Core 2 CPU 6700 2.66GHz with 2 GB RAM). These results demonstrate the validity of the new algorithm for determining reflection and transmission properties of periodic structures with arbitrary skewed grids. The first example is an infinite dielectric slab excited by TM\textsuperscript{z} and TE\textsuperscript{z} plane waves. The second example is a dipole FSS, where the structure is analyzed with special skewed angles that can be simulated using the normal FDTD/PBC, and the third example is a JC FSS. The results obtained from the skewed FDTD code are compared with results obtained from an analytic solution, the axial FDTD method, and Ansoft Designer.

3.3.1 An Infinite Dielectric Slab

Due to its homogeneity, the infinite dielectric slab can be considered as a periodic structure with any skew angle. The algorithm is first used to analyze an infinite dielectric slab with thickness \( h = 9.375 \) mm and relative permittivity \( \varepsilon_r = 2.56 \). The slab is illuminated by TM\textsuperscript{z} and TE\textsuperscript{z} plane waves, respectively. The skew angle of the slab is set to 60°. The slab is excited using a cosine-modulated Gaussian pulse centered at 10 GHz with 20 GHz bandwidth. The plane wave is incident normally (\( k_x = k_y = 0 \) m\textsuperscript{-1}) and obliquely (\( k_x = 104.8 \) m\textsuperscript{-1}, \( k_y = 0 \) m\textsuperscript{-1} for minimum frequency of 5 GHz). The FDTD grid cell size is \( \Delta x = \Delta y = \Delta z = 0.3125 \) mm, and the slab is represented by 5x5 cells. In the FDTD code, 2,500 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries at the top and the bottom of the computational domain. The results are compared with analytical results in Fig. 3.8.
Fig. 3.8 Reflection coefficient for infinite dielectric slab, (a) TM\(^z\) case, (b) TE\(^z\) case.
From Fig. 3.8, good agreement between analytical solutions and results generated by the new algorithm for both TM$^z$ and TE$^z$ cases (normal and oblique incidence) can be noticed. The stability of the algorithm can be noticed even at the angles of incidence near grazing.

### 3.3.2 A Dipole FSS

The algorithm is then used to analyze an FSS structure consisting of dipole elements. The dipole length is 12 mm and width is 3 mm. The periodicity is 15 mm in both $x$- and $y$-directions. The substrate has a thickness of 6 mm and relative permittivity $\varepsilon_r = 2.2$, as shown in Fig. 3.9. The structure is first illuminated by a normally incident plane wave (with polarization along the $y$-axis), and the skew angle of the structure is set to 90° (axial case) and 63.43° (special case where the shift is a half unit cell in $x$-direction). These two cases are special cases that can also be simulated using the axial periodic boundary conditions.

![Dipole FSS geometry with skew angle $\alpha = 63.43^\circ$](image)

Fig. 3.9 Dipole FSS geometry with skew angle $\alpha = 63.43^\circ$ (all dimensions are in mm).
Fig. 3.10 Reflection coefficient for dipole FSS with normal incident TE\textsuperscript{z} plane wave with skew angle of 90° and 63.43°.

Figure 3.10 provides results for normal incidence. The structure is excited using a cosine-modulated Gaussian pulse centered at 8 GHz with 16 GHz bandwidth. In the FDTD code, 2,500 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries at the top and the bottom of the computational domain. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.5$ mm. The results are compared with results obtained from the axial FDTD code. The computational time per simulation for the skewed code is 4.28 minutes, and the memory usage is 0.2 MB. For the axial code with $\alpha = 63.43^\circ$; the time is doubled due to the increase in the computational domain size (the unit cell size is doubled in the $y$-direction as shown in Fig. 3.9).

Figure 3.11 provides results for an oblique incidence ($\theta = 30^\circ$ and $\varphi = 60^\circ$) exciting the dipole FSS structure with skew angle $\alpha = 50^\circ$ (a general skewed grid which can’t be implemented using the axial FDTD). To generate results for a specific angle of incidence, multiple runs of the code are needed.
Fig. 3.11 Reflection coefficient for dipole FSS with oblique incident TE\(^z\) plane wave (\(\theta = 30^\circ\), \(\varphi = 60^\circ\)) with skew angle of 50°.

The results are compared with results obtained from Ansoft Designer. From Fig. 3.11, the good agreement between the results generated using Ansoft Designer and those generated using the new algorithm for oblique incidence can be noticed. The new algorithm results in Fig. 3.11 are generated using 33 different \(k_x\) values (from 0.131 m\(^{-1}\) to 83.834 m\(^{-1}\)).

### 3.3.3 A Jerusalem Cross FSS

Next, the algorithm is used to analyze an FSS structure consisting of JC elements. The periodicity is 15.2 mm in both the \(x\)- and \(y\)-directions. The dimensions of the elements are shown in Fig. 3.12. The structure is illuminated by a TE\(^z\) plane wave (polarization along \(y\)-axis). Figure 3.13 provides results for normal incidence. The structure is excited using a cosine-modulated Gaussian pulse centered at 7 GHz with 8 GHz bandwidth. The grid cell size is \(\Delta x = \Delta y = 0.2285\) mm and \(\Delta z = 0.457\) mm.
Fig. 3.12 JC FSS geometry with skew angle $\alpha = 80^\circ$ (all dimensions are in mm).

In the FDTD code, 3,000 time steps and a Courant factor of 0.9 are used. CPML is used for the absorbing boundaries at the top and the bottom. The structure has a skew angle $\alpha = 80^\circ$ (general skewed grid). The results were compared with results obtained from Ansoft Designer. The computational time per simulation for the skewed code is 4.53 minutes, and the memory usage is 0.2 MB, while for Ansoft Designer computational time, per simulation is 45 minutes for 30 frequency points, and the memory usage is 21 MB using the same computer.

Figure 3.14 provides results for an oblique incidence plane wave ($\theta = 60^\circ$ and $\varphi = 45^\circ$) exciting a JC FSS structure with skew angle $\alpha = 80^\circ$. To generate results for a specific angle of incidence, multiple runs of the code are needed, which increases the computational time. Using 30 different $k_r$ values (from $38.5031 \text{ m}^{-1}$ to $141.1781 \text{ m}^{-1}$), both co- and cross-polarization reflection coefficients were generated. The results were compared with results obtained from Ansoft Designer. Good agreement between the results generated using Ansoft Designer and results generated using the new algorithm for both normal and oblique incidence can be noticed in Figs. 3.13 and 3.14.
Fig. 3.13 Co- and cross-polarization reflection coefficient for JC FSS with normal incident TE$_z$ plane wave with skew angle of 80°.

Fig. 3.14 Co- and cross-polarization reflection coefficient for JC FSS with oblique incident TE$_z$ plane wave ($\theta = 60^\circ$, $\phi = 45^\circ$) with skew angle $\alpha = 80^\circ$. 
3.4 Summary

This chapter introduces a new FDTD approach to analyze the scattering properties of general skewed grid periodic structures. The approach is developed based on the constant horizontal wavenumber technique. It is simple to implement and efficient in terms of both computational time and memory usage. In addition, the stability criterion is angle-independent. Therefore, the algorithm is efficient in implementing incidence with angle close to grazing as well as normal incidence. It is capable of calculating the co- and cross-polarization reflection and transmission coefficients of normal and oblique incidence, for both TE\textsuperscript{z} and TM\textsuperscript{z} cases, and for different skewed grid periodic structures. The numerical results show good agreement with results from the analytical solution for a dielectric slab, and the MoM solutions for dipole and JC FSS structures.
CHAPTER IV

4 MULTILAYERED PERIODIC STRUCTURES

4.1 Introduction

Many periodic structures are built up of several layers, each layer being either a diffraction grating, periodic in one or two directions, or a homogenous dielectric slab which acts as a separator or support [25]. Two approaches can be employed to analyze multilayered structures. One approach is to formulate and analyze a specific composite structure in its entirety [26]. This approach has serious practical limitations because the required amount of computation increases rapidly as the number of layers increases, and also because a complete new analysis is required every time a change is made in any layer. The other alternative is to compute the generalized scattering matrix (GSM) [27]-[29] for each layer and then obtain the total GSM of the entire structure by simple matrix calculations. This approach is more flexible and applicable to practical problems where several layers may be cascaded in an arbitrary sequence. The cascading technique allows one to take advantage of different methods in computing the GSM for each layer of a multilayered structure. In most of the previous work, the method of moments (MoM) and the finite element method (FEM) are used to compute the scattering parameters of each layer. In this chapter, the finite-difference time-domain (FDTD) with the constant horizontal wavenumber periodic boundary condition (PBC) approach described in Chapter 2 is used to compute the scattering parameters of each layer.

Usually, the GSM consists of scattering parameters of incident waves and their space harmonics, known as Floquet harmonics [30]-[31]. In previous chapters all the simulations were full wave simulations for single layer periodic structures and that is why the Floquet harmonics
were not mentioned. However, in multilayered periodic structures, the Floquet harmonics are particularly important due to the interactions between layers. Many parameters affect the behavior of the harmonics including the frequency range of interest, incident angle and polarization, periodicity and geometry of each layer, sequence of different layers, and separation between these layers. A complete Floquet harmonic analysis is presented in this chapter, where propagation and evanescent behaviors of harmonics are studied using the FDTD method. In addition, guidelines are provided to select proper higher order harmonics for certain separation sizes. It is worthwhile to point out that the FDTD algorithm used in this chapter is efficient for the harmonic analysis since the periodic boundary condition is handled by the constant horizontal wavenumber approach.

This chapter is organized as follows: In Section 4.2, different categories of multilayered periodic structures are defined. In Section 4.3, the hybrid FDTD/GSM approach is described and the definition, computation, and conversion of scattering and transmission matrices are provided. In Section 4.4, a complete Floquet harmonic analysis of periodic structure is presented and the propagation and evanescent behaviors of the Floquet harmonics are studied. In addition, guidelines for harmonics selection are provided. Section 4.5 provides numerical examples to prove the validity of the hybrid FDTD/GSM approach. The algorithm is used to simulate different test cases such as dipole and square patch FSS structures with different periodicities, and with normal and oblique incidences. The scattering properties of the entire multilayered structures are calculated for both co- and cross-polarization components. In Section 4.6, a summary of the proposed algorithm is provided.
4.2 Categories of Multilayered Periodic Structures

Multilayered periodic structures could be categorized according to the periodicities of the layers and the separation between layers. As shown in Fig. 4.1, three categories exist according to the periodicity of different layers: in the first category, all the layers have the same periodicities (which will be referred to as the 1:1 case); in the second category, the periodicities of the layers are integer multiples of each other (which will be referred to as the n:1 case); in the third category, the periodicities of the layers are not integer multiples of each other (which will be referred to as the n:m case). As shown in Fig. 4.1, in the first category (1:1), the two layers have the same periodicity: in this specific case, it is 15 mm × 15 mm. In the second category (n:1), the first layer has periodicity of 7.5 mm × 7.5 mm, and the second layer has periodicity of 15 mm × 15 mm (4 unit cells : 1 unit cell). In the third category (n:m), the first layer has periodicity of 10 mm × 10 mm, and the second layer has periodicity of 15 mm × 15 mm (9 unit cells : 4 unit cells).

Fig. 4.1 Three categories of multilayered periodic structures according to the periodicity.
4.2 Two categories of multilayered periodic structures according to the separation.

As shown in Fig. 4.2, two categories exist according to the separation between layers. In the first category, the separation between layers is large enough to neglect the effects of the higher order harmonics (which will be referred to as the large gap case). In the second category, the separation between layers is small so that the effects of the higher order harmonics cannot be neglected (which will be referred to as the small gap case).

4.3 Hybrid FDTD/GSM Method

In this section, the hybrid FDTD/GSM approach is described. The definition, computation, and conversion of scattering and transmission matrices are provided.

4.3.1 Procedure of Hybrid FDTD/GSM Method

As described here for multilayered periodic structures, the GSM technique can take into account propagating and non-propagating modes and interactions between them (including cross-polarization effects). It describes the reflection and transmission properties of each layer by a
scattering matrix for that layer and uses a cascading process to obtain a scattering matrix for the overall structure. The modes are the Floquet spatial harmonics of a plane-wave incident on a structure with specified periodicity. Each element in the scattering matrix is either a reflection or a transmission coefficient, which provides the linear relationship between a scattered harmonic and one of the incident harmonics that excites it. The scattering matrix for a single layer can be transformed into a transmission matrix, and the cascading procedure is applied to the single-layer transmission matrices to produce a transmission matrix for the overall structure. This matrix can then be transformed to produce a scattering matrix for the overall structure. In principle, any desired level of solution accuracy can be obtained by using a sufficiently large matrix for each layer. In practice, the objective is to choose the matrix size large enough for good accuracy but small enough to keep the expenditure of computing resources within acceptable limits.

Fig. 4.3 Flow chart of the proposed algorithm.
As shown in Fig. 4.3, the proposed algorithm can be summarized as follows:

(1) Using the constant horizontal wavenumber FDTD/PBC, the scattering parameters of the first layer are calculated and the scattering matrix is constructed.

(2) The scattering matrix of the first layer is transformed to a transmission matrix.

(3) Step 1 and 2 are repeated for all the layers.

(4) The total transmission matrix is calculated using matrix multiplication for all the transmission matrices.

(5) The total transmission matrix is transformed to a scattering matrix and all the scattering parameters are extracted from it.

For the layered medium shown in Fig. 4.4, the total composite transmission matrix is given by

$$T_{total} = T^{(N)} \ldots T^{(2)} T^{(1)},$$

(4.1)
where the transmission and scattering matrices are defined as

\[
\begin{bmatrix}
  b_1 \\
  a_1
\end{bmatrix} =
\begin{bmatrix}
  T_{11} & T_{12} \\
  T_{21} & T_{22}
\end{bmatrix}
\begin{bmatrix}
  a_2 \\
  b_2
\end{bmatrix},
\begin{bmatrix}
  b_1 \\
  a_2
\end{bmatrix} =
\begin{bmatrix}
  S_{11} & S_{12} \\
  S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
  a_1 \\
  b_2
\end{bmatrix}.
\]

(4.2)

The transformations between the \([S]\) and \([T]\) matrices are given by

\[
[T] = \begin{bmatrix}
  S_{12} - S_{11}S_{21}^{-1}S_{22} & S_{11}S_{21}^{-1} \\
  -S_{21}S_{22} & S_{21}^{-1}
\end{bmatrix},
\]

(4.3a)

\[
[S] = \begin{bmatrix}
  T_{12}T_{22}^{-1} & T_{11} - T_{12}T_{22}^{-1}T_{21} \\
  T_{22}^{-1} & -T_{22}^{-1}T_{21}
\end{bmatrix}.
\]

(4.3b)

When cross-polarization components or higher harmonics are included, \(T_{ij}\) and \(S_{ij}\) of (4.3) become sub-matrices, and the variables \(a_j\) and \(b_j\) become vectors. Equation (4.3) can be easily proved for the general case using matrix partitioning as shown in Appendix A.1.

### 4.3.2 Calculating Scattering Parameters Using FDTD/PBC

In this section, the scattering parameters of a single layer periodic structure are calculated using the constant horizontal wavenumber FDTD/PBC technique described in Chapter 2. We consider a case of a single layer periodic structure, where the layer has periodicity in both the \(x\)- and \(y\)-directions and is illuminated by a plane wave with general oblique incidence as shown in Fig. 4.5. Using the constant horizontal wavenumber FDTD/PBC technique, only one unit cell is simulated to get the scattering parameters of the entire layer. Let's start with a simple case where only the co- and cross-polarization components of the dominant mode (without any higher order Floquet harmonics) are calculated.
Fig. 4.5 Geometry of single layer periodic structure.

Fig. 4.6 Reflected and transmitted electric fields for co- and cross-polarized components of the dominant mode.

As shown in Fig. 4.6, $a_1$, $b_1$, $a_3$, and $b_3$ are related to the co-polarized electric field components of the dominant mode, while $a_2$, $b_2$, $a_4$, and $b_4$ are related to the cross-polarized electric field components of the dominant mode. Four different field components exist, so the scattering matrix will be of the size $4\times4$. The S-parameters are calculated as

$$S_{11} = \frac{E_{r}^{\text{Co-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{21} = \frac{E_{r}^{\text{X-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{31} = \frac{E_{t}^{\text{Co-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{41} = \frac{E_{t}^{\text{X-pol}}}{E_{i}^{\text{(top)}}}, \quad \text{(4.4a)}$$

$$S_{12} = \frac{E_{r}^{\text{Co-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{22} = \frac{E_{r}^{\text{X-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{32} = \frac{E_{t}^{\text{Co-pol}}}{E_{i}^{\text{(top)}}}, \quad S_{42} = \frac{E_{t}^{\text{X-pol}}}{E_{i}^{\text{(top)}}}. \quad \text{(4.4b)}$$
For the rest of the S-parameters, the plane wave excitation is placed below the layer, and then

\[ S_{13} = \frac{E_{t}^{\text{Co-pol}}}{E_{t}^{\text{Co-pol}(\text{bottom})}}, \quad S_{23} = \frac{E_{t}^{X-\text{pol}}}{E_{t}^{\text{Co-pol}(\text{bottom})}}, \quad S_{33} = \frac{E_{t}^{\text{Co-pol}}}{E_{t}^{\text{Co-pol}(\text{bottom})}}, \quad S_{43} = \frac{E_{t}^{X-\text{pol}}}{E_{t}^{\text{Co-pol}(\text{bottom})}}, \]  

\( S_{14} = \frac{E_{t}^{\text{Co-pol}}}{E_{t}^{X-\text{pol}(\text{bottom})}}, \quad S_{24} = \frac{E_{t}^{X-\text{pol}}}{E_{t}^{X-\text{pol}(\text{bottom})}}, \quad S_{34} = \frac{E_{t}^{\text{Co-pol}}}{E_{t}^{X-\text{pol}(\text{bottom})}}, \quad S_{44} = \frac{E_{t}^{X-\text{pol}}}{E_{t}^{X-\text{pol}(\text{bottom})}}, \]  

(4.4c, d)

where \( E_{t/r/i}^{\text{Co/x-pol}} \) are the complex amplitudes of the frequency-domain electric fields [32]-[33], which can be obtained from the time-domain electric field by using the discrete Fourier Transform (DFT). For the TE\(_z^x\) plane wave, the co- and cross-polarized components can be stated as follows:

\[ E_{t}^{\text{Co-pol}} = E_{y} \frac{k_{x}}{\sqrt{k_{x}^{2} + k_{y}^{2}}} - E_{x} \frac{k_{y}}{\sqrt{k_{x}^{2} + k_{y}^{2}}}, \]

\[ E_{t}^{X-\text{pol}} = E_{y} \frac{k_{x}}{\sqrt{k_{x}^{2} + k_{y}^{2}}} + E_{y} \frac{k_{y}}{\sqrt{k_{x}^{2} + k_{y}^{2}}}. \]

(4.4e)

The S-parameters for other layers can be calculated similarly and transformed to T-parameters as shown in (4.3). Symmetry can be used to reduce the calculation of S-parameters. As for dielectric layers or air gaps, the homogeneity of these layers decreases the S-parameter calculation simulation time (it can be also calculated analytically). Similar to the cross-polarization analysis, any number of higher order Floquet harmonics can be added, and the S-parameters due to these higher harmonics can be calculated. The decomposition of electric field periodic in two dimensions is of the form:

\[ \hat{E}(x, y, z) = \sum_{n} \sum_{m} \hat{A}_{m,n} e^{j(k_{m,n}x + k_{m,n}y + k_{m,n}z)}, \]

(4.5)
where the $\vec{A}_{m,n}$ are the vector coefficients of the decomposition, and $k_{x,m,n}^m$ and $k_{y,m,n}^m$ are the wavenumbers of the Floquet modes determined by the cell dimensions of the periodic structure and the wavenumber of the incident field as follows:

\[
k_{x,m,n}^m = k \sin \theta \cos \phi + \frac{2\pi m}{P_x}, \tag{4.6a}\n\]
\[
k_{y,m,n}^m = k \sin \theta \cos \phi + \frac{2\pi n}{P_y \sin \alpha} - \frac{2\pi m}{P_y \tan \alpha}, \tag{4.6b}\n\]

where $P_x$, $P_y$, and $\alpha$ describe the geometry of the unit cell as shown in Fig 4.7, and $\alpha$ is the skew angle of the grid. In this chapter, this angle will be taken as $90^\circ$ (axial case), so the equation (4.6b) will be rewritten as

\[
k_{y,m,n}^m = k \sin \theta \cos \phi + \frac{2\pi n}{b}, \tag{4.6c}\n\]

![Fig. 4.7](image)

(a) Two dimensional periodic scatterer, (b) General incident plane wave.
\[ k_{z}^{m,n} = \sqrt{k^2 - \left(k_{x}^{m,n}\right)^2 - \left(k_{y}^{m,n}\right)^2}. \]  

(4.7)

\( k_{z}^{m,n} \) is real for propagating modes and imaginary for non-propagating modes. Each element of a scattering matrix in (4.2) is a scattering parameter, either a reflection coefficient or a transmission coefficient, that gives the linear relationship between the amplitude of a scattered harmonic \( \hat{A}_{m,n} \) and one of the incident harmonics that excites it \( \hat{A}_{i,j} \) [25].

To illustrate the above procedure, analyzing a periodic layer while taking into account only two modes (the dominant mode and the first harmonic) is considered. The same procedure used with the co- and cross-polarized components is used, so the S-parameters are calculated as follows:

\[
\begin{align*}
S_{11} &= \frac{E_{r}^{\text{Dom.}}}{E_{i}^{\text{(top)}}}, \quad S_{21} = \frac{E_{r}^{\text{Harm.1}}}{E_{i}^{\text{(top)}}}, \quad S_{31} = \frac{E_{i}^{\text{Dom.}}}{E_{i}^{\text{(top)}}}, \quad S_{41} = \frac{E_{i}^{\text{Harm.1}}}{E_{i}^{\text{(top)}}}, \\
S_{12} &= \frac{E_{r}^{\text{Dom.}}}{E_{i}^{\text{Harm.1}}}, \quad S_{22} = \frac{E_{r}^{\text{Harm.1}}}{E_{i}^{\text{Harm.1}}}, \quad S_{32} = \frac{E_{i}^{\text{Dom.}}}{E_{i}^{\text{Harm.1}}}, \quad S_{42} = \frac{E_{i}^{\text{Harm.1}}}{E_{i}^{\text{Harm.1}}},
\end{align*}
\]

(4.8a)

For the rest of the S-parameters the plane wave excitation is placed below the layer:

\[
\begin{align*}
S_{13} &= \frac{E_{r}^{\text{Dom.}}}{E_{i}^{\text{(bottom)}}}, \quad S_{23} = \frac{E_{r}^{\text{Harm.1}}}{E_{i}^{\text{(bottom)}}}, \quad S_{33} = \frac{E_{i}^{\text{Dom.}}}{E_{i}^{\text{(bottom)}}}, \quad S_{43} = \frac{E_{i}^{\text{Harm.1}}}{E_{i}^{\text{(bottom)}}}, \\
S_{14} &= \frac{E_{r}^{\text{Dom.}}}{E_{i}^{\text{Harm.1}}}, \quad S_{24} = \frac{E_{r}^{\text{Harm.1}}}{E_{i}^{\text{Harm.1}}}, \quad S_{34} = \frac{E_{i}^{\text{Dom.}}}{E_{i}^{\text{Harm.1}}}, \quad S_{44} = \frac{E_{i}^{\text{Harm.1}}}{E_{i}^{\text{Harm.1}}},
\end{align*}
\]

(4.8b)
where $E_{\text{dom./Harm.}}^{i/r/t}$ are the complex amplitudes of the frequency-domain electric fields for both the dominant mode and first harmonic (incident or reflected or transmitted). Calculating these complex amplitudes is described in detail in the next section.

### 4.4 FDTD/PBC Floquet Harmonic Analysis of Periodic Structures

In this section, a procedure is developed to extract all the harmonics from the FDTD/PBC simulation and study their frequency behavior. In addition, another procedure is developed based on the geometric properties of the multilayered periodic structure and based on the frequency-domain harmonic behavior to determine the proper gap size after which higher harmonic effects can be neglected. This procedure is also used as a guideline to select the proper harmonics to be considered in the analysis for a certain gap size.

#### 4.4.1 Evanescent and Propagating Harmonics in Periodic Structures

The presence of periodicity in the scatterer can lead to the appearance of far-field transmission and reflection at additional angles, often referred to as Floquet harmonics [18]. In this dissertation the periodicity is in the $x$- and $y$-directions, and the generated harmonics will have wavenumbers as follows:

$$
    k_x^{m,n} = k_x^i + \frac{2\pi m}{P_x}, \quad k_y^{m,n} = k_y^i + \frac{2\pi n}{P_y},
$$

(4.9)

where $m$ and $n$ are the harmonic indices in the $x$- and $y$-directions, respectively.
In this analysis, the harmonics are named using the following convention:

\[ M_{m,n}, \quad m = 0, \pm 1, \pm 2, \ldots, n = 0, \pm 1, \pm 2, \ldots, \]  

(4.10)

For example, take the basic (dominant) mode and two different harmonics as follows:

\[ m = 0, n = 0 \rightarrow M_{0,0} \left( k_{x}^{0,0} = k_{x}^{i}, k_{y}^{0,0} = k_{y}^{i} \right), \]

\[ m = 1, n = -1 \rightarrow M_{1,-1} \left\{ k_{x}^{1,-1} = k_{x}^{i} + \frac{2\pi}{P_{x}}, k_{y}^{1,-1} = k_{y}^{i} - \frac{2\pi}{P_{y}} \right\}, \]  

(4.11)

\[ m = -2, n = 4 \rightarrow M_{-2,4} \left\{ k_{x}^{-2,4} = k_{x}^{i} - \frac{4\pi}{P_{x}}, k_{y}^{-2,4} = k_{y}^{i} + \frac{8\pi}{P_{y}} \right\}. \]

These harmonics have cut-off frequencies, after which the harmonics start to propagate and are no longer evanescent harmonics. To determine the cut-off frequencies of different harmonics, consider the case of normal incidence where \( k_{x}^{i} = k_{y}^{i} = 0 \), and consider a periodic structure with 15 mm \( \times \) 15 mm. Using this information, the cut-off frequencies of the first five modes can be calculated as follows:
At $k^2 = (k_x^m)^2 + (k_y^m)^2$, the cut-off frequency occurs, which can be calculated as follows for different modes:

$$k = \frac{2\pi f}{c} \text{ for free space where } c \text{ is the speed of light in free space.}$$

$$m = 0, n = 0 \rightarrow k = \sqrt{(0)^2 + (0)^2} = 0 \rightarrow f_{\text{cut-off}}^{0,0} = 0 \text{GHz},$$

$$m = 0, n = 1 \rightarrow k = \sqrt{(0)^2 + (418.879)^2} = 418.879 \rightarrow f_{\text{cut-off}}^{0,1} = 20 \text{GHz},$$

$$m = 0, n = -1 \rightarrow k = \sqrt{(0)^2 + (-418.879)^2} = 418.879 \rightarrow f_{\text{cut-off}}^{0,-1} = 20 \text{GHz},$$

$$m = 1, n = 0 \rightarrow k = \sqrt{(418.879)^2 + (0)^2} = 418.879 \rightarrow f_{\text{cut-off}}^{1,0} = 20 \text{GHz},$$

$$m = -1, n = 0 \rightarrow k = \sqrt{(-418.879)^2 + (0)^2} = 418.879 \rightarrow f_{\text{cut-off}}^{-1,0} = 20 \text{GHz}. $$

To study the frequency behavior of the electric field for these harmonics, the same previous assumptions (periodicity of 15 mm × 15 mm and normal incidence) will be considered, and the electric field of any mode can be generally written as (assume the $y$-component):

$$\vec{E} = E_0 e^{-j(k_x^m x + k_y^m y + k_z^{m,n})z} \hat{a}_y. \quad (4.12)$$

Assuming that the magnitude of the incident electric field of each mode is unity and observing the electric field magnitude at a distance of 15 mm from the excitation plane, the attenuation of the magnitude of the electric field versus frequency can be plotted as shown in
Fig. 4.9. It can be noticed from the figure that the cut-off frequency for the \((M_{1,0})\) harmonic is 20 GHz, as it was calculated analytically. Also, after that cut-off frequency, the harmonic starts to propagate. In addition, it can be noticed that the \((M_{1,1})\) harmonic cut-off frequency is almost 28.3 GHz. Moreover, it can be noticed that the effect of the harmonics increase for frequencies near the cut-off frequency. For the real case of periodic structure, the magnitude of the harmonics \(E_0\) in (4.12) will not be unity, but it will be of a certain value depending on the angle of incidence and the geometry of the periodic structure. To calculate the actual magnitude of different harmonics, the expression for the magnitude of the harmonic related to the total field can be stated as follows:

\[
E_{m,n}(\omega) = \frac{1}{P_x P_y} \int_0^{P_x} \int_0^{P_y} E(\omega, x, y) e^{i k_x m x} e^{i k_y n y} \, dx \, dy.
\]  

(4.13)

where \(k_x^{m,n}, k_y^{m,n}\) are given by equation (4.9), \(E(\omega, x, y)\) is the total frequency-domain field, and \(x, y\) are the position of this electric field. Equation (4.13) can be re-written in the discretized form as

\[
E_{m,n}(\omega) = \frac{1}{N_x N_y} \sum_{u=0}^{N_x} \sum_{v=0}^{N_y} E(\omega, u \Delta x, v \Delta y) e^{i k_x^{m,n} (u \Delta x)} e^{i k_y^{n,n} (v \Delta y)},
\]

(4.14)

where \(N_x\) and \(N_y\) are the total number of cells in the \(x\)- and \(y\)-directions, respectively, and \(\Delta x\) and \(\Delta y\) are the cell size in the \(x\)- and \(y\)-directions, respectively.
Fig. 4.9 The magnitude of the electric field at 15 mm from the excitation plan for \((M_{1,0})\) and \((M_{1,1})\) harmonics.

The electric field \(E(\omega, u\Delta x, v\Delta y)\) is calculated using the DFT to transform the time-domain electric field at each cell into the frequency-domain. This process requires saving all the time-domain components of electric fields at each cell. For instance, if the simulation is done using 30 \(\times\) 30 cells and 2,500 time steps, for every time step, at least two matrices \((E_x, E_y)\) of the size 30 \(\times\) 30 have to be stored. These matrices are then transformed to the frequency-domain, and the magnitude of different harmonics can be calculated using (4.14), which requires huge memory usage. However, if the constant horizontal wavenumber approach is used, then \(k_x^{m,n}, k_y^{m,n}\) are constant and (4.14) can be directly transformed to the time-domain as

\[
E^{m,n}(t) = \frac{1}{N_x N_y} \sum_{u=0}^{N_x} \sum_{v=0}^{N_y} E(t, u\Delta x, v\Delta y) e^{i k_x^{m,n}(u\Delta x)} e^{i k_y^{m,n}(v\Delta y)}.
\] (4.15)

Using (4.15), the time-domain magnitude of each harmonic can be easily calculated in the FDTD/PBC simulation. Then this time-domain data is transformed to the frequency-domain.
using the DFT, which does not require any extra memory compared to the conventional FDTD technique, due to the fact that the fields are captured in the code using (4.15). This feature of the constant horizontal wavenumber FDTD/PBC approach is considered as an important advantage due to the reduction in memory usage.

**FDTD Harmonic Analysis Procedure:**

1. Use constant horizontal wavenumber approach to calculate $E(t, u\Delta x, v\Delta y)$.

2. Use (4.15) to calculate the time-domain magnitude of different harmonics in the FDTD/PBC simulation.

3. Repeat steps 1 and 2 until all time steps in the FDTD simulation are completed.

4. Use the DFT to calculate the frequency-domain magnitude of different harmonics.

5. Use the data from step 4 to calculate the distribution of the fields for different harmonics as $E^{m,n}(\omega, u\Delta x, v\Delta y) = E^{m,n}(\omega) \times e^{-jkx^m,\Delta x} \times e^{jk\rho_n,\Delta y}$.

The above procedure can be used with any periodic structure to completely study the effect of different harmonics on the cascading configuration.

### 4.4.2 Guideline for Harmonic Selection

In this section a procedure for determining the proper gap size (for neglecting the higher harmonics effects) is described. The procedure can also be used to determine which harmonics to be considered for specific gap size.
Fig. 4.10 The flow chart of gap determination procedure.

**FDTD Gap Determination Procedure:**

1. Specify the periodicity, the order, and the geometry of each layer: The periodicity and geometry of the layer are important to determine the cut-off frequencies and magnitudes of different harmonics. As for the layers order, it determines if the reflected or transmitted harmonics are to be considered.

2. Specify the frequency range of interest. The frequency range of interest is important to determine whether the harmonics are propagating or evanescent harmonics in this frequency range.
(3) Specify the incident wave parameters \((k_x^i, k_y^i)\). Use \(k_x^i\) and \(k_y^i\) to determine the cut-off frequencies of different harmonics. Any propagating harmonics in the frequency range of interest should be considered whatever the gap size is.

(4) Use the harmonic analysis procedure to determine the magnitudes of the evanescent harmonics: Calculate \(k_z^{m,n}\) and use it together with the harmonic magnitudes to study the decaying behavior of the evanescent harmonics with distance.

(5) The gap size for neglecting the harmonic effect is calculated as the distance after which all evanescent harmonics magnitudes reach -40dB compared to the excitation electric field magnitude. The -40 dB threshold was concluded from different test cases for error less than 5%. Any other accuracy can be achieved by changing the threshold value. If the gap size is less than that determined by the algorithm, all the evanescent harmonics that have magnitudes larger than the threshold (-40 dB from excitation magnitude) should be included in the cascading process for accurate results.

4.5 Numerical Results

In this section, numerical examples are provided to prove the validity of the proposed algorithm. The test plan is shown in Table 1; this test plan is based on testing different multilayer categories described in Section 4.2 with different types of plane wave incidence (normal and oblique). In all the test cases, the results of the cascading technique are compared with the FDTD simulation of the entire structure. The FDTD code was developed in MATLAB programming language and run on a computer with an Intel Core 2 CPU 6700, 2.66 GHz with 2 GB RAM.
Table 4.1 Multilayered periodic structure code verification test plan

<table>
<thead>
<tr>
<th>Test Case number</th>
<th>Periodicity / Gap size</th>
<th>Incidence</th>
<th>Cross-polarization</th>
<th>Higher harmonics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Dielectric Slab</td>
<td>Normal/Obl</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>1:1 /Large</td>
<td>Normal</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>1:1 /Small</td>
<td>Normal</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>4</td>
<td>1:1 /Large</td>
<td>Oblique</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>1:1 /Small</td>
<td>Oblique</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>6</td>
<td>n:m/Large</td>
<td>Normal</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>n:m/Small</td>
<td>Normal</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>8</td>
<td>n:m/Large</td>
<td>Oblique</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

4.5.1 Test Case 1 (Infinite Dielectric Slab)

Due to the homogeneity of the dielectric slab, it is considered a good verification case. In addition, the results can be compared with the analytical solution. The code is used to analyze an infinite dielectric slab with thickness $h = 9.375$ mm and relative permittivity $\varepsilon_r = 2.56$. The slab is illuminated by TM$^z$ and TE$^z$ plane waves, respectively. The plane wave is incident normally ($k_x = k_y = 0$ m$^{-1}$) and obliquely ($k_x = 104.8$ m$^{-1}$, $k_y = 0$ m$^{-1}$ for min frequency of 5 GHz).

![Dielectric slab simulation using cascading technique.](image)

(a) (b) (c)

Fig. 4.11 Dielectric slab simulation using cascading technique.
In this test case, a dielectric slab with half the thickness of the original slab was simulated, and the cascading technique was used to simulate the original dielectric slab. As shown in Fig. 4.11, (a) the dielectric slab is analyzed analytically with different excitation polarizations and angles of incidence; (b) half the dielectric slab is analyzed using the FDTD/PBC technique and the scattering parameters are extracted as previously described; and (c) the cascading technique is used to get the scattering parameters of the whole dielectric slab from the scattering parameters of half of the original slab. The slab is excited using a cosine-modulated Gaussian pulse centered at 10 GHz with 20 GHz bandwidth. The FDTD grid cell size is \( \Delta x = \Delta y = \Delta z = 0.3125 \) mm, and the slab is represented by 5x5 cells. In the FDTD code, 2,500 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries at the top and the bottom of the computational domain. The results are compared with analytical results in Figs. 4.12, 4.13, and 4.14. It should also be noticed that due to the homogeneity of the dielectric slab, the harmonics effects will be neglected even for a very small gap (zero gap), and only the dominant mode will be considered in the analysis.

From Figs. 4.12, 4.13, and 4.14, it should be noticed that the cascading technique is very accurate in calculating the S-parameters of the entire structure. In addition, good agreement can be noticed between the proposed technique and the analytical solution for both magnitude and phase of the reflection and transmission coefficients, with both oblique and normal incidence TE\( ^z \) and TM\( ^z \) cases.
Fig. 4.12 Reflection and transmission coefficients of infinite dielectric slab with normal incidence TE\(^z\) and TM\(^z\), (a) Magnitude, (b) Phase.

Fig. 4.13 Reflection and transmission coefficients of infinite dielectric slab with oblique incidence \(k_x = 104.8 \text{ m}^{-1}\) TE\(^z\), (a) Magnitude, (b) Phase.
Fig. 4.14 Reflection and transmission of coefficients infinite dielectric slab with oblique incidence \( k_x = 104.8 \, \text{m}^{-1} \, \text{TM}^z \), (a) Magnitude, (b) Phase.

4.5.2 Test Case 2 (1:1 case, Normal incidence and large gap)

In this test case, the multilayer geometry consists of two identical FSS structures consisting of dipole elements (1:1 case) separated by an air gap of width \( d \). The dipole length is 12 mm and width is 3 mm. The periodicity is 15 mm in both \( x \)- and \( y \)-directions. The substrate has a thickness of 6 mm and relative permittivity \( \varepsilon_r = 2.2 \), as shown in Fig. 4.15. The structure is illuminated by a \( \text{TE}^z \) normally incident plane wave (with polarization along \( y \)-axis). The frequency range of interest is 0-16 GHz. The FDTD grid cell size is \( \Delta x = \Delta y = \Delta z = 0.5 \, \text{mm} \) and 2,500 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries at the top and the bottom of the computational domain. The goal is to determine the distance \( d \) after which all the harmonics reach -40 dB from the magnitude of the incident electric field. Using the gap determination procedure:
(1) The two layers are identical; analyzing the harmonics of one layer is enough. The reflection and transmission harmonics must be calculated.

(2) The frequency range of interest as specified by the problem is 0-16GHz (as shown in Fig. 4.9, at the highest frequency the effect of harmonics is maximum).

(3) $k_x$ and $k_y$ are equal to zero (normal incidence). Determine the cut-off frequencies for the first eight harmonics as follows:

$$M_{0,1}, M_{0,-1} \rightarrow f_{\text{cut-off}}^{0,1} = f_{\text{cut-off}}^{0,-1} = 20\, \text{GHz}$$

$$M_{1,0}, M_{-1,0} \rightarrow f_{\text{cut-off}}^{1,0} = f_{\text{cut-off}}^{-1,0} = 20\, \text{GHz}$$

$$M_{1,1}, M_{1,-1} \rightarrow f_{\text{cut-off}}^{1,1} = f_{\text{cut-off}}^{1,-1} = 28.3\, \text{GHz}$$

$$M_{-1,1}, M_{-1,-1} \rightarrow f_{\text{cut-off}}^{-1,1} = f_{\text{cut-off}}^{-1,-1} = 28.3\, \text{GHz}$$

(4) Use the harmonic analysis to calculate the magnitude coefficient of the eight harmonics and plot the behavior of these harmonics versus frequency, as shown in Figs. 4.16 and 4.17.

Fig. 4.15 Two identical dipole FSS geometry (all dimensions are in mm).
Fig. 4.16 The eight transmitted harmonics at 16 GHz (a) Magnitude compared to incident electric field, (b) The decaying behavior of the harmonics with distance.

Fig. 4.17 The eight reflected harmonics at 16 GHz (a) Magnitude compared to the incident electric field, (b) The decaying with distance.

As can be noticed from Figs. 4.16 and 4.17, almost 95% of the dominant mode will be transmitted. In addition, a distance $d = 15.5\text{mm}$ between the two layers for this range of
frequencies is considered enough to neglect all the higher harmonics effects (the magnitude of all higher harmonics are less than -40 dB compared to the incident filed magnitude). To validate the cascading technique and the gap determination procedure, several air gap distance are analyzed and compared with the FDTD simulation of the entire structure, as shown in Fig. 4.18.

Fig. 4.18 Reflection coefficients of two identical dipole FSS with normal incidence TE\(_z\) case for
(a) \(d = 4\) mm, (b) \(d = 7\) mm, (c) \(d = 17\) mm.
It should be noticed from Fig. 4.19, that when the gap size \(d\) is less than 15.5 mm, the cascading technique using only the dominant mode is not accurate, especially at high frequency, which validates the gap determination procedure. The relative error was calculated as follows:

\[
error(f) = \frac{\| \Gamma_{\text{entire}}(f) - |\Gamma_{\text{cascaded}}(f)| \|}{\max(|\Gamma_{\text{entire}}(f)|)} \times 100\%.
\] (4.16)

The maximum error in case of a 4 mm gap is about 52%, and for \(d = 7\) mm it is about 23% due to neglecting the higher harmonics effects which cause the frequency shift noticed in Fig. 4.19 (a) and (b). However, for the case of a gap size of 17 mm, the relative error is about 0.4%. The computational time using the cascading technique is less than the computational time for the entire structure, especially with large gaps (which require a large number of time steps to generate stable results). The computational time for the cascading case for \(d = 17\) mm is 6 minutes (for calculating the S-parameters of the FSS layer and air gap and calculating the total GSM), while the entire simulation for the same case takes 35 minutes, which illustrates the efficiency of the hybrid FDTD/GSM technique. In addition, the domain size for the cascading case is equal to 43,200 cells (\(30 \times 30 \times 48\)), while for the entire structure, the domain size is 73,800 cells (\(30 \times 30 \times 82\)), which illustrate the efficiency of the hybrid FDTD/GSM algorithm with respect to memory usage. Moreover, the scattering parameters generated for this layer can be saved and reused in any other cascading structure that uses the same layer with the same angle of incidence and frequency range (so the same S-parameters for the layer were used with the three gap sizes only the S-parameters of air gap where changed, while for the entire structure the whole simulation had to be repeated for each case).
To study the effect of geometry on harmonic frequency behavior, a test case is shown in Appendix A.2, where the two layers of the multilayered periodic structure have the same periodicity as test case 2, but the elements are square patches instead of dipoles. In addition, another test case is shown in Appendix A.3, where the two layers of the multilayered periodic structure have the same periodicity as test case 2, but the elements are L-shaped dipoles to study the effect of cross-polarized components.

4.5.3 Test Case 3 (1:1 case, Normal incidence and small gap)

To analyze the same structure shown in Fig. 4.15 accurately with a gap size less than 15.5 mm, the cascading technique should include all the harmonics that have a magnitude greater than -40 dB compared to the incident (to achieve the required accuracy). For example, the case of gap size \( d = 7 \) mm is considered. From Figs. 4.16 and 4.17, it should be noticed that for a gap size of 7 mm, only two harmonics need to be added in the analysis to get accurate results (\( M_{1,0} \) and \( M_{-1,0} \)). These two harmonics have a magnitude higher than -40 dB compared to the incident field at 7 mm. The S-parameters of these harmonics can be calculated from (4.8). Figure 4.19 compares the results of the cascading technique while using only the dominant mode and while using the dominant mode and the first two harmonics (\( M_{1,0} \) and \( M_{-1,0} \)). It should be noticed that including the two harmonics in the cascading analysis enhances the results. The small gap case can be easily analyzed after using harmonic analysis to determine exactly which harmonics should be considered in the analysis. The maximum relative error in the case of cascading technique with dominant mode and the two harmonics included is 0.5%.
Fig. 4.19 The reflection coefficient of two identical dipole FSS normal incident TE$_z$ case with $d = 7$ mm.

4.5.4 Test Case 4 (1:1 case, Oblique incidence and large gap)

To study the effect of cross-polarization components, the algorithm is used to analyze the same structure shown in Fig. 4.15 with a general obliquely incident plane wave $k_x = 20$ m$^{-1}$ and $k_y = 10$ m$^{-1}$ (general oblique incidence for minimum frequency of almost 1 GHz and angle $\phi = 26.65^\circ$). The frequency range of interest is 5-15 GHz. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.5$ mm, 3,000 time steps and a Courant factor of 0.9 are used. Using the procedure of gap determination used in Section 4.4.2, different harmonics can be plotted versus distance at the highest frequency (15 GHz) in the frequency range of interest, as shown Fig. 4.20.
From Fig. 4.20, it can be concluded that $d = 16.45 \text{ mm}$ is enough to neglect the effect of all the harmonics. In addition, it should be noticed that the case of oblique incidence required a larger gap to neglect the harmonics compared to the case of normal incidence. The reflection and transmission coefficients of the whole structure are calculated using the cascading technique for different values of $d$, and the results are compared with the FDTD simulation of the entire structure, as shown in Fig. 4.21. It should be noticed from the figure that when $d$ is less than 16.45 mm, inaccurate results are obtained from the cascading technique due to the effect of the harmonics, while when $d$ is larger than 16.45 mm, accurate results are obtained. In addition, the oblique incidence will generate cross-polarized components, and these components must be considered in the analysis using equation (4.4) as described in Section 4.3.2. The maximum relative error in the case of $d = 10 \text{ mm}$ is about 8.2%, while it is about 1.2% in the case of $d = 18 \text{ mm}$. The computational time using the cascading technique is much less than the computational time for the entire structure, especially with large gaps.
Fig. 4.21 Reflection and transmission coefficients of two identical dipole FSS with oblique incidence TE\textsuperscript{z} case ($k_x = 20 \text{ m}^{-1}, k_y = 10 \text{ m}^{-1}$), (a) $d = 10 \text{ mm}$, (b) $d = 18 \text{ mm}$.

4.5.5 Test Case 5 (1:1 case, Oblique incidence and small gap)

The algorithm is used to analyze the same structure shown in Fig. 4.15. The structure is illuminated by an obliquely incident plane wave $k_x = 40 \text{ m}^{-1}$ and $k_y = 0 \text{ m}^{-1}$ (for minimum frequency of almost 1.9 GHz); the frequency range of interest is 5-15 GHz, and $d = 10\text{mm}$. The structure is to be simulated using the cascading technique; the same procedure used in test case 4 was used, and it was found that for a gap of 10 mm at frequency of 15 GHz, only one harmonic needs to be added in the analysis to get accurate results from the cascading technique ($M_{1,0}$). Figure 4.22 shows the results of the co-polarized reflection coefficient using the cascading technique with the dominant mode only and with the dominant mode plus the harmonic ($M_{1,0}$). The results are compared with the FDTD simulation of the entire structure.
Fig. 4.22 The reflection coefficient of two identical dipole FSS oblique incident \(k_x = 40 \text{ m}^{-1}, k_y = 0 \text{ m}^{-1}\) TE\(_z\) case with \(d = 10\text{mm}\).

It should be noticed from the Fig. 4.22 that when the effect of the \((M_{1,0})\) harmonic is taken into consideration, accurate results are obtained. The maximum relative error in the case of cascading technique with only the dominant mode was calculated using (4.16) to be 38\% (due to the frequency shift), while for the case in which the \((M_{1,0})\) harmonic is included a maximum relative error of 0.6\% is obtained.

4.5.6 Test Case 6 (n:m case, Normal incidence and large gap)

As shown in Fig. 4.23, in this test case, the multilayer geometry consists of two different FSS layers. The first FSS structure consists of square patch elements with a size of 6 mm. The periodicity is 10 mm in both the \(x\)- and \(y\)-directions. The substrate has a thickness of 6 mm and relative permittivity \(\varepsilon_r = 2.2\). The second FSS structure is the same as the FSS structure used in test case 2 (Fig. 4.15) (general case n:m). The structure is illuminated by a normally incident plane wave \((k_x = k_y = 0 \text{ m}^{-1})\) and the frequency range of interest is 0-16 GHz. The FDTD grid cell
size is \( \Delta x = \Delta y = \Delta z = 0.5 \text{ mm} \). 2,500 time steps and a Courant factor of 0.9 are used. The goal is to determine the distance \( d \) after which all the harmonics reach -40 dB from the magnitude of the incident electric field. Using the gap determination procedure described in Section 4.4.2 this distance can be easily determined. For the first layer only, the transmitted harmonics will affect the cascaded structure. As for the second layer, only the reflected harmonics will affect the cascaded structure.

(1) The frequency range of interest as specified by the problem is 0-16GHz.

(2) \( k_x \) and \( k_y \) are equal zero (normal incidence).

(3) Determine the cut-off frequencies for the first eight harmonics of the first layer as follows:

\[
M_{0,1}, M_{0,-1}, M_{1,0}, M_{-1,0} \left( f_{\text{cut-off}} = 30GHz \right) \\
M_{1,1}, M_{1,-1}, M_{-1,1}, M_{-1,-1} \left( f_{\text{cut-off}} = 42.42GHz \right)
\]

The harmonics of the second layer are the same as in test case 2.

We use the harmonic analysis to calculate the magnitude coefficient of the first eight harmonics of layers 1 and 2 and plot the behavior of these harmonics with frequency as shown in Figs. 4.24 and 4.17. Figure 4.24 describes the transmitted harmonics from layer 1 at 16 GHz, while Fig. 4.17 describes the reflected harmonics from second layer. It should be noticed from Fig. 24 that only 57\% of the dominant mode will be transmitted from the first layer. In addition, due to the smaller periodicity compared to the second layer, the harmonics generated at the first layer will decay faster than the harmonics generated at the second layer. Using this information, it can be concluded that the second layer harmonics control the gap size.
Fig. 4.23 Square FSS and dipole FSS geometry n:m case (all dimensions are in mm).

Fig. 4.24 The first four transmitted harmonics from layer 1 at 16 GHz, (a) Magnitude compared to incident electric field, (b) The decaying with distance.

To calculate the proper gap size after which the harmonics for both layers decay below -40 dB, the reflected harmonics shown in Fig. 4.17 should be multiplied by 0.57. A gap of 13.11 mm was found to be enough to neglect the higher harmonics effects.
Fig. 4.25 The reflection coefficient of square patch FSS and dipole FSS with normal incidence TE$^z$ case, (a) $d = 3.5$ mm, and (b) 15 mm.

To validate the cascading technique and the gap determination procedure, two air gaps were analyzed using the cascading technique (in the cascading technique only one unit cell from each layer is analyzed) and compared with the FDTD simulation of the entire structure, as shown in Fig. 4.25. The maximum relative error in the case of $d = 3.5$ mm is 3%, while in the case of $d = 15$ mm, it is less than 0.3%. This test case is less sensitive for the harmonic effect, which might be due to the high cut-off frequencies of the harmonics generated from the first layer compared to the second layer. The computational time using the cascading technique is less than the computational time for the entire structure, especially with large gaps. In addition, to simulate the entire structure, many unit cells are needed for each layer. However, by using the cascading technique, only one unit cell is simulated for each layer, which reduces the computational time dramatically. The computational time for the cascading case is 8 minutes (for calculating S-parameters of the FSS layers and the air gap and calculating the total GSM), while for the simulation of the entire structure, it takes 130 minutes due to the large domain simulated.
Moreover, the domain size for the cascading case is equal to 43,200 cells \((30 \times 30 \times 48)\), while for the entire structure, the domain size is 280,800 cells \((60 \times 60 \times 78)\), which illustrates the efficiency of the hybrid FDTD/GSM algorithm with respect to memory usage. In addition, the entire structure simulation requires a large number of time steps to generate stable results.

4.5.7 Test Case 7 \((n:m\) case, Normal incidence and small gap) 

To study the same structure shown in Fig. 4.23 with a small gap, the algorithm is used to analyze the structure with a gap size equal to 3.5 mm. From Fig. 4.24, it should be noticed that all the higher harmonics transmitted from the first layer will reach -40 dB at a distance of 2.5 mm, so for the gap size of 3.5 mm, the harmonics of the first layer can be neglected. As for the second layer, all the harmonics of Fig. 4.17 (b) should be multiplied by 0.57. It was found that for a gap size of 3.5 mm, only two harmonics of the second layer are required to be added in the analysis to get accurate results from the cascading technique \((M_{1,0}, M_{-1,0}\) of the second layer). As long as three modes are included in the analysis, the S-matrix of each layer will be of the size \(6 \times 6\). To calculate the S-parameters of each layer, equation (4.8) is used with the following parameters: 

- \(E_{Dom.}\) is related to the dominant mode \((k_x = k_y = 0 \text{ m}^{-1})\), 
- \(E_{Harm1}\) is related to the first harmonic of the second layer \((M_{1,0}, k_x = 418.879 \text{ m}^{-1} \text{ and } k_y = 0 \text{ m}^{-1})\), and 
- \(E_{Harm2}\) is related to the second harmonic of the second layer \((M_{1,0}, k_x = -418.879 \text{ m}^{-1} \text{ and } k_y = 0 \text{ m}^{-1})\). So, to calculate \(S_{12}\) of the first layer, for example, the layer should be excited with the first harmonic of the second layer \((M_{1,0})\). Similarly, all other S-parameters of the two layers can be calculated.
Fig. 4.26 The reflection coefficient of square patch FSS and dipole FSS with normal incidence TE\(^z\) case \(d = 3.5\) mm.

Figure 4.26 shows the results of the co-polarized reflection coefficient using the cascading technique with only the dominant mode and with the dominant mode plus the harmonics \((M_{1,0})\) and \((M_{-1,0})\) of the second layer. The results are compared with the FDTD simulation of the entire structure. It should be noticed from Fig. 4.26 that when the effect of the \((M_{1,0})\) and \((M_{-1,0})\) harmonics are taken into consideration, accurate results are obtained. The maximum relative error in the case of the cascading technique with only the dominant mode was calculated using (4.16) to be 3\%, while the case of the harmonics \((M_{1,0})\) and \((M_{-1,0})\) included results in a maximum relative error of 0.3\%.

4.5.8 **Test Case 8 (n:m case, Oblique incidence and large gap)**

The algorithm is used to analyze the same structure shown in Fig. 4.23. The structure is illuminated by an obliquely incidence plane wave \(k_x = 20\) m\(^{-1}\) and \(k_y = 10\) m\(^{-1}\) (general oblique incident for minimum frequency of almost 1 GHz and angle \(\varphi = 26.65^\circ\)), and the frequency range of interest is 5-15 GHz. Using the procedure of gap determination, the goal is to determine the...
distance $d$ after which all the harmonics reach -40dB from the magnitude of the incident electric field. For the first layer, only the transmitted harmonics will affect the cascaded structure, as for the second layer, only the reflected harmonics will affect the cascaded structure. Using the gap determination procedure:

(1) The frequency range of interest as specified by the problem is 5-15GHz.

(2) $k_x^i = 20 \text{ m}^{-1}$ and $k_y^i = 10 \text{ m}^{-1}$ (General oblique incidence).

(3) Determine the cut-off frequencies for the first four harmonics for the first layer and second layer as follows:

\[
\begin{align*}
S_1: f_{\text{cut-off}}^{1,0} &= 30.9 \text{ GHz}, \quad f_{\text{cut-off}}^{-1,0} = 29 \text{ GHz}, \quad f_{\text{cut-off}}^{0,1} = 30.5 \text{ GHz}, \quad f_{\text{cut-off}}^{0,-1} = 29.5 \text{ GHz}, \\
S_2: f_{\text{cut-off}}^{1,0} &= 20.9 \text{ GHz}, \quad f_{\text{cut-off}}^{-1,0} = 19.1 \text{ GHz}, \quad f_{\text{cut-off}}^{0,1} = 20.5 \text{ GHz}, \quad f_{\text{cut-off}}^{0,-1} = 19.5 \text{ GHz}.
\end{align*}
\]

(4) Use the harmonic analysis to calculate the magnitude coefficient of the first eight harmonics of layers 1 and 2. Plot the behavior of these harmonics with frequency as shown in Figs. 4.27 and 4.28 ($E_x$ and $E_y$ component).

(5) Set -40dB from the excitation electric field magnitude as threshold for neglecting the effect of the harmonic effect.
Fig. 4.27 The transmitted harmonics from first layer at 15 GHz, (a) Magnitude of first eight harmonics compared to incident electric field, (b) The decaying of first four harmonics with distance.
Fig. 4.28 The first eight reflected harmonics from second layer at 15 GHz, (a) Magnitude compared to incident electric field (b) The decaying with distance.

Figure 4.27 describes the transmitted harmonics from the first layer at 15 GHz, while Fig. 4.28 describes the reflected harmonics from the second layer. A distance of $d = 14.95$ mm was found to be large enough to neglect all the higher harmonics effect.
Fig. 4.29 Reflection and transmission coefficients of square patch FSS and dipole FSS with oblique incidence ($k_x = 20 \text{ m}^{-1}, k_y = 10 \text{ m}^{-1}$) TE$^z$ case for $d = 15 \text{ mm}$.

The structure is analyzed using the cascading technique (only one unit cell from each layer is analyzed) with $d = 15 \text{ mm}$ and compared with the FDTD simulation of the entire structure as shown in Fig. 4.29. The maximum error in the case of $d = 15 \text{ mm}$ is about 0.47%. The computational time using the cascading technique is less than the computational time for the entire structure.

### 4.6 Summary

In this chapter, an efficient hybrid FDTD/GSM technique is described. In this technique, the constant horizontal wavenumber FDTD/PBC approach is used to compute the scattering parameters of each layer, after which the scattering matrix of the entire structure is calculated using the cascading technique. In addition, two procedures were described; one is used to study the behavior of different harmonics (evanescent and propagating) using the constant horizontal wavenumber FDTD/PBC approach, which dramatically reduces memory usage. The other
procedure is used to determine the proper gap size (for neglecting the harmonics effects), and it can also be used to select proper harmonics for specific gap size. The validity of the algorithm was verified through several numerical examples including FSS structures with different periodicities and under different incident angles. The numerical results of the developed approach show good agreement with the results obtained from the direct FDTD simulation of the entire structure, while the proposed procedure saves computational time and memory usage.
CHAPTER V

5 DISPERSE PERIODIC STRUCTURES

5.1 Introduction

Electromagnetic simulation of dispersive media is essential in many applications such as medical telemetries, metamaterials designs, nanoplasmonic solar cells, shielding materials, etc. Debye media, Lorentz media, and Drude media are three important classes of dispersive materials and reflect the frequency-dependent behavior of the materials. FDTD provides an efficient means to simulate these media and various methods have been developed to model the frequency dependence of the material parameters in the FDTD. The recursive convolution (RC) method [34]-[39] and the auxiliary differential equation (ADE) method [40]-[41] are the two most well known approaches. Piecewise linear recursive convolution [42] and the Z-transform [43]-[45] are also used to model dispersive media.

It’s worthwhile to point out that most previous PBCs for the FDTD technique were developed to analyze periodic structures with dispersive media not located on the boundary of the unit cells. However, there are numerous applications where periodic structures with dispersive media on the boundaries of the unit cell must be used. In this chapter, a new dispersive periodic boundary condition (DPBC) for the FDTD technique is developed to solve the above challenge. The algorithm utilizes the ADE technique with a two-term Debye relaxation equation to simulate the general dispersive property in the medium. In addition, the constant horizontal wavenumber approach is modified accordingly to implement the periodic boundary conditions. The new algorithm offers many advantages such as implementation simplicity,
stability condition and numerical errors similar to the conventional FDTD, and computational efficiency.

The chapter is organized as follows: In Section 5.2, the description of ADE technique is provided. In Section 5.3, the FDTD updating equations are derived and the DPBC is described. In Section 5.4, several numerical examples proving the validity of the new approach are presented, including an infinite dispersive slab, nanoplasmonic solar cells, and a sandwiched composite frequency selective surface (FSS) structure. Various incident angles and polarizations have been tested in these examples, and the numerical results show good agreement with the analytical results or other numerical results obtained from frequency-domain methods. Section 5.5 provides summary.

5.1.1 Type of Dispersive Media

Debye media, Lorentz media, and Drude media are three important classes of dispersive materials and reflect the frequency-dependent behavior of the materials [46]. If $\chi$ is defined such that

$$\varepsilon_{\infty} = \varepsilon(\infty) = \varepsilon_{\infty} + \chi$$

then Debye media are characterized by a complex-valued frequency-domain susceptibility function $\chi(\omega)$ that has one or more real poles at separate frequencies. Here $\varepsilon_{\infty}$ is the relative permittivity at infinite frequency. For a single-pole Debye medium (with $e^{j\omega t}$ time harmonic convention),

$$\chi_p(\omega) = \frac{\varepsilon_s - \varepsilon_{\infty}}{1 + j\omega\tau} = \frac{\Delta\varepsilon}{1 + j\omega\tau},$$

where $\varepsilon_s$ is the static or zero frequency relative permittivity and $\tau$ is the relaxation time. For a Debye medium having $N$-poles the relative permittivity is given by
\[
\epsilon(\omega) = \varepsilon_\infty + \sum_{i=1}^{N} \frac{\Delta \varepsilon_i}{1 + j\omega\tau_i}.
\] (5.2)

Lorentz media are characterized by a complex-valued, frequency-domain susceptibility function \( \chi(\omega) \) that has one or more pairs of complex-conjugate poles. For a single-pole Lorentz medium (with \( e^{j\omega t} \) time harmonic convention),

\[
\chi_p(\omega) = \frac{(\epsilon_{s,p} - \epsilon_{\infty,p})\omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} \equiv \frac{\Delta \varepsilon_p \omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2},
\] (5.3)

where \( \omega_p \) is the frequency of the pole pair and \( \delta_p \) is the damping coefficient. For a Lorentz medium having \( N \)-poles the relative permittivity is:

\[
\epsilon(\omega) = \varepsilon_\infty + \sum_{i=1}^{N} \frac{\Delta \varepsilon_i \omega_i^2}{\omega_i^2 + 2j\omega\delta_i - \omega^2}.
\] (5.4)

For a single-pole Drude medium [46]

\[
\chi_p(\omega) = -\frac{\omega_p^2}{(\omega^2 - j\omega\gamma_p)}.
\] (5.5)

where \( \omega_p \) is the Drude pole frequency and \( \gamma_p \) is the inverse of the pole relaxation time. For a Drude medium having \( N \)-poles the relative permittivity is

\[
\epsilon(\omega) = \varepsilon_\infty - \sum_{i=1}^{N} \frac{\omega_i^2}{(\omega^2 - j\omega\gamma_i)}.
\] (5.6)

In this chapter the Debye model will be used to simulate the dispersive media.
5.1.2 The Recursive Convolution Method

Generally the constitutive relations for complex media are given in the frequency-domain as

\[ \tilde{D} = \varepsilon(\omega)\tilde{E}, \]  
(5.7a)\[ \tilde{B} = \mu(\omega)\tilde{H}, \]  
(5.7b)

with frequency-dependent complex permeability and permittivity. In order to construct the FDTD updating equations, time-domain forms of the constitutive relations are needed, together with Maxwell’s curl equations. The product in (5.7a) will turn into a convolution as

\[ \tilde{D}(t) = \varepsilon_0\varepsilon_\infty \tilde{E}(t) + \varepsilon_0 \int_{\tau=0}^{t} \tilde{E}(t-\tau)\chi_\varepsilon(\tau)d\tau. \]  
(5.8)

Evaluation of a convolution integral will, in general, require storing a large number of past time values of \( E \) for each of the cells, which consumes the computer memory. The discrete time-domain convolution may be updated recursively for some rational forms of complex permittivity, which removes the need to store the time history of the fields and makes the method feasible [34]. In the piecewise linear recursive convolution method the electric field is considered a piecewise linear function of time, instead of constant at each time step. Updating equations based on this assumption lead to more accurate FDTD calculations.

5.1.3 The Z-transform Method

The Z-transform is typically used in digital filtering and signal processing problems. The time discrete nature of the FDTD method makes it possible to use the Z-transform in implementing the FDTD method where complicated dispersive or non-linear materials are involved [44]. One of the most important properties of the Z-transform is that convolution in the
time-domain becomes multiplication in the Z-domain, which is similar to both the Fourier
transform and Laplace transform convolution theorems.

Consider Maxwell’s time-domain curl equations together with the constitutive relations in
(5.7) for the frequency-domain with $e^{j\omega t}$ time harmonic convention. At this point the Z-transform
method can be used to simplify the solution. The product of two frequency-dependent terms in
the frequency-domain turns out to be a multiplication in the Z-domain, which is simpler than a
convolution in the time-domain. Then (5.7) can be written in the Z-domain as

$$
\tilde{D}(z) = \varepsilon_0 \varepsilon(z) \tilde{E}(z) T, \quad \tilde{B}(z) = \mu_0 \mu(z) \tilde{H}(z) T,
$$

(5.9)

where $T$ is the time interval. The Z-transform method can be used to solve the same type of
problem that can be solved by the recursive convolution method. However it is easier to
construct an FDTD algorithm by the Z-transform method than by the recursive convolution
method.

### 5.2 Auxiliary Differential Equation Method

In the auxiliary differential equation (ADE) method a differential equation relating the
electric displacement vector $\mathbf{D}$ to the electric field vector $\mathbf{E}$ is added. Solving this new equation
simultaneously with the standard FDTD equations will lead to simulating the dispersive property
of the medium [47]-[48]. The time-domain Maxwell’s equations can be stated as in (2.1). For
dispersive material the electric displacement vector and the magnetic flux density vector are
described using (5.7). Assuming in this dissertation that only $\varepsilon$ depends on the frequency, (5.7b)
can be written as $\tilde{B} = \mu \tilde{H}$. The dispersive characteristics of $\varepsilon(\omega)$ can be described by a two-term
Debye relaxation equation as
\[
\varepsilon(\omega) = \varepsilon_o \left[ \frac{\varepsilon_s + \varepsilon_{s1} - \varepsilon_s + \varepsilon_{s2} - \varepsilon_{s0}}{1 + j \omega \tau_1} + \frac{\varepsilon_s - \varepsilon_{s2}}{1 + j \omega \tau_2} \right].
\] (5.10)

From (5.7a) and (5.10) \( \tilde{D}(\omega) \) can be written as follows:

\[
\tilde{D}(\omega) = \varepsilon_o \frac{\varepsilon_s + j \omega (\varepsilon_{s1} \tau_2 + \varepsilon_{s2} \tau_1) - \omega^3 \tau_1 \tau_2 \varepsilon_s}{1 + j \omega (\tau_1 + \tau_2) - \omega^2 \tau_1 \tau_2} \tilde{E}(\omega),
\] (5.11)

where the zero (static) frequency dielectric constant \( \varepsilon_s \) is given by

\[
\varepsilon_s = \varepsilon_{s1} + \varepsilon_{s2} - \varepsilon_{s0}.
\] (5.12)

For time harmonic fields (sinusoidal fields), (5.11) can be re-written into the differential time-domain form using the relations \( j \omega \rightarrow \frac{\partial}{\partial t}, -\omega^2 \rightarrow \frac{\partial^2}{\partial t^2} \) as follows:

\[
\tilde{D}(t) + (\tau_1 + \tau_2) \frac{\partial \tilde{D}(t)}{\partial t} + \tau_1 \tau_2 \frac{\partial^2 \tilde{D}(t)}{\partial t^2} = \varepsilon_o \varepsilon_s \tilde{E}(t) + \varepsilon_o (\varepsilon_{s1} \tau_2 + \varepsilon_{s2} \tau_1) \frac{\partial \tilde{E}(t)}{\partial t} + \tau_1 \tau_2 \varepsilon_s \frac{\partial^2 \tilde{E}(t)}{\partial t^2}.
\] (5.13)

Using equation (2.1a), (2.1b), and (5.13), each vector equation can be decomposed to three scalar equations for three dimensional space. Therefore, Maxwell’s curl equations can be represented with nine scalar equations in the Cartesian coordinate system \((x, y, z)\) relating \( H \) to \( E \) and \( E \) to \( D \) as follows (the conduction and displacement currents are combined in the definition of the complex permittivity \( \varepsilon(\omega) \)):

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu_x} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma_x m H_x - M_x \right),
\] (5.14a)

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu_y} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \sigma_y m H_y - M_y \right),
\] (5.14b)

100
\[ \frac{\partial H_z}{\partial t} = \frac{1}{\mu_z} \left( \frac{\partial E_y}{\partial y} - \frac{\partial E_x}{\partial x} - \sigma_z^w H_z - M_{iz} \right). \] (5.14c)

\[ \frac{\partial D_x}{\partial t} = \left( \frac{\partial H_y}{\partial y} - \frac{\partial H_z}{\partial z} - J_{ix} \right), \] (5.14d)

\[ \frac{\partial D_y}{\partial t} = \left( \frac{\partial H_z}{\partial z} - \frac{\partial H_x}{\partial x} - J_{iy} \right), \] (5.14e)

\[ \frac{\partial D_z}{\partial t} = \left( \frac{\partial H_x}{\partial x} - \frac{\partial H_y}{\partial y} - J_{iz} \right), \] (5.14f)

\[ D_x + (\tau_1 + \tau_2) \frac{\partial D_x}{\partial t} + \tau_1 \tau_2 \frac{\partial^2 D_x}{\partial t^2} = \varepsilon_o \varepsilon_r E_x + \varepsilon_o (\varepsilon_s \tau_2 + \varepsilon_s \tau_1) \frac{\partial E_{ix}}{\partial t} + \tau_1 \tau_2 \varepsilon_o \varepsilon_r \frac{\partial^2 E_{ix}}{\partial t^2}, \] (5.14g)

\[ D_y + (\tau_1 + \tau_2) \frac{\partial D_y}{\partial t} + \tau_1 \tau_2 \frac{\partial^2 D_y}{\partial t^2} = \varepsilon_o \varepsilon_r E_y + \varepsilon_o (\varepsilon_s \tau_2 + \varepsilon_s \tau_1) \frac{\partial E_{iy}}{\partial t} + \tau_1 \tau_2 \varepsilon_o \varepsilon_r \frac{\partial^2 E_{iy}}{\partial t^2}, \] (5.14h)

\[ D_z + (\tau_1 + \tau_2) \frac{\partial D_z}{\partial t} + \tau_1 \tau_2 \frac{\partial^2 D_z}{\partial t^2} = \varepsilon_o \varepsilon_r E_z + \varepsilon_o (\varepsilon_s \tau_2 + \varepsilon_s \tau_1) \frac{\partial E_{iz}}{\partial t} + \tau_1 \tau_2 \varepsilon_o \varepsilon_r \frac{\partial^2 E_{iz}}{\partial t^2}. \] (5.14i)

Re-arranging the above 9 equations, the recursive FDTD algorithm can be easily constructed, starting with \( H_x, E_x \), and \( D_x \). As long as the \( \mu \) (permeability) of the material is independent of the frequency, the updating equations for the magnetic field will be similar to the conventional FDTD. To obtain the updating equations of the electric displacement vector \( D \), we start by updating \( D_x \) as follows:
\[ \frac{D_x^{n+1}(i, j, k) - D_x^n(i, j, k)}{\Delta t} + \left( H_x^{n+1/2}(i, j, k) - H_x^n(i, j - 1, k) \right) \frac{\Delta y}{\Delta t} + \left( H_y^{n+1/2}(i, j, k) - H_y^n(i, j, k - 1) \right) \frac{\Delta z}{\Delta t} - J_{xt}^{n+1/2}(i, j, k), \]

\[ D_x^{n+1}(i, j, k) = D_x^n(i, j, k) + \left[ H_x^{n+1/2}(i, j, k) - H_x^n(i, j - 1, k) \right] \Delta t + J_{xt}^{n+1/2}(i, j, k), \]

\[ D_x^{n+1}(i, j, k) = C_{dxn}(i, j, k) \times D_x^n(i, j, k) + C_{dch}(i, j, k) \times \left[ H_x^{n+1/2}(i, j, k) - H_x^n(i, j - 1, k) \right] \]

\[ + C_{dhn}(i, j, k) \times \left[ H_x^{n+1/2}(i, j, k) - H_x^n(i, j, k - 1) \right] + C_{dhy}(i, j, k) \times J_{xt}^{n+1/2}(i, j, k), \]

where

\[ C_{dxn}(i, j, k) = 1, \quad C_{dch}(i, j, k) = \frac{\Delta t}{\Delta y}, \quad C_{dhn}(i, j, k) = \frac{-\Delta t}{\Delta z}, \quad C_{dhy}(i, j, k) = -\Delta t. \]

Similarly for \( D_y \):

\[ D_y^{n+1}(i, j, k) = C_{dyd}(i, j, k) \times D_y^n(i, j, k) + C_{dyh}(i, j, k) \times \left[ H_y^{n+1/2}(i, j, k) - H_y^n(i, j, k - 1) \right] \]

\[ + C_{dyz}(i, j, k) \times \left[ H_y^{n+1/2}(i, j, k) - H_y^n(i, j - 1, k) \right] + C_{dyz}(i, j, k) \times J_{yt}^{n+1/2}(i, j, k), \]

where

\[ C_{dyd}(i, j, k) = 1, \quad C_{dyh}(i, j, k) = \frac{\Delta t}{\Delta z}, \quad C_{dyz}(i, j, k) = \frac{-\Delta t}{\Delta x}, \quad C_{dyz}(i, j, k) = -\Delta t. \]

Similarly for \( D_z \):

\[ D_z^{n+1}(i, j, k) = C_{dzd}(i, j, k) \times D_z^n(i, j, k) + C_{dzh}(i, j, k) \times \left[ H_z^{n+1/2}(i, j, k) - H_z^n(i, j - 1, k) \right] \]

\[ + C_{dzh}(i, j, k) \times \left[ H_z^{n+1/2}(i, j, k) - H_z^n(i, j - 1, k) \right] + C_{dzz}(i, j, k) \times J_{zt}^{n+1/2}(i, j, k), \]

\[ (5.15) \]

\[ (5.16) \]

\[ (5.17) \]
where

\[ C_{dx} = 1, \; C_{dy} = \frac{\Delta t}{\Delta x}, \; C_{dz} = \frac{-\Delta t}{\Delta y}, \; C_{dj} = -\Delta t \]

To obtain the updating equations for the electric field vector \( \mathbf{E} \), starting by updating the \( E_x \) as follows:

\[
D_x + (\tau_1^x + \tau_2^x) \frac{\partial \mathbf{D}}{\partial t} + \tau_1^x \tau_2^x \frac{\partial^2 \mathbf{D}}{\partial t^2} = \varepsilon_0 \varepsilon_s E_x + \varepsilon_0 \left( \varepsilon_s^x \frac{\partial E_x}{\partial t} + \tau_1^x \varepsilon_s e_x ^x \frac{\partial^2 E_x}{\partial t^2} \right),
\]

Using central differences centered at time step \((n + \frac{1}{2})\) the above equation can be written as

\[
\frac{D_x^{n+1} + D_x^n}{2} + (\tau_1^x + \tau_2^x) \frac{D_x^{n+1} - D_x^n}{\Delta t} + \tau_1^x \tau_2^x \frac{D_x^{n+1} - 2D_x^n + D_x^{n-1}}{(\Delta t)^2} = \\
\varepsilon_0 \varepsilon_s E_x^{n+1} + \varepsilon_0 \left( \varepsilon_s^x \frac{E_x^{n+1} - E_x^n}{\Delta t} + \tau_1^x \varepsilon_s e_x ^x E_x^{n+1} - 2E_x^n + E_x^{n-1} \right) \frac{\partial^2 E_x}{\partial t^2}
\]

Taking \( \beta_0^x = \frac{1}{2}, \beta_1^x = \frac{\tau_1^x + \tau_2^x}{\Delta t}, \beta_2^x = \frac{\tau_1^x \tau_2^x}{(\Delta t)^2}, \alpha_0^x = \frac{\varepsilon_0}{2}, \alpha_1^x = \frac{\tau_1^x \varepsilon_s e_x ^x}{\Delta t} \), and \( \alpha_2^x = \frac{\tau_1^x \tau_2^x \varepsilon_s e_x ^x}{(\Delta t)^2} \)

we have

\[
\beta_0^x (D_x^{n+1} + D_x^n) + \beta_1^x (D_x^{n+1} - D_x^n) + \beta_2^x (D_x^{n+1} - 2D_x^n + D_x^{n-1}) = \\
\alpha_0^x (E_x^{n+1} + E_x^n) + \alpha_1^x (E_x^{n+1} - E_x^n) + \alpha_2^x (E_x^{n+1} - 2E_x^n + E_x^{n-1})
\]

\[
[E_x^{n+1} + \alpha_0^x + \alpha_1^x + \alpha_2^x]E_x^n = [-\alpha_0^x + \alpha_1^x + 2\alpha_2^x]E_x^{n+1} + [-\alpha_2^x]E_x^{n-1} + \\
[\beta_0^x + \beta_1^x + \beta_2^x]D_x^{n+1} + [\beta_0^x - \beta_1^x - 2\beta_2^x]D_x^n + [\beta_2^x]D_x^{n-1}
\]

\[
E_x^{n+1}(i,j,k) = C_{ex1} \times E_x^n(i,j,k) + C_{ex2} \times E_x^{n-1}(i,j,k) + C_{ex3} \times D_x^{n+1}(i,j,k) \\
+ C_{ex4} \times D_x^n(i,j,k) + C_{ex5} \times D_x^{n-1}(i,j,k)
\]

(5.18)

where
\[ C_{e1} = \frac{-\alpha_0^x + \alpha_1^x + 2\alpha_2^x}{\alpha_0^x + \alpha_1^x + \alpha_2^x}, \quad C_{e2} = \frac{-\alpha_0^z}{\alpha_0^x + \alpha_1^x + \alpha_2^x}, \quad C_{e3} = \frac{\beta_0^x + \beta_1^x + \beta_2^x}{\alpha_0^x + \alpha_1^x + \alpha_2^x}, \]

\[ C_{e2} = \frac{\beta_0^x - \beta_1^x - 2\beta_2^x}{\alpha_0^x + \alpha_1^x + \alpha_2^x}, \quad C_{e3} = \frac{\beta_0^x}{\alpha_0^x + \alpha_1^x + \alpha_2^x}. \]

Similarly for \( E_y \):

\[ E_y^{n+1}(i, j, k) = C_{e1} \times E_y^n(i, j, k) + C_{e2} \times E_y^{n-1}(i, j, k) + C_{e3} \times D_y^{n+1}(i, j, k) + C_{e4} \times D_y^n(i, j, k) + C_{e5} \times D_y^{n-1}(i, j, k) \]

\[(5.19)\]

where

\[ C_{e1} = \frac{-\alpha_0^y + \alpha_1^y + 2\alpha_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{e2} = \frac{-\alpha_0^z}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{e3} = \frac{\beta_0^y + \beta_1^y + \beta_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \]

\[ C_{e2} = \frac{\beta_0^y - \beta_1^y - 2\beta_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{e3} = \frac{\beta_0^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}. \]

For \( E_z \):

\[ E_z^{n+1}(i, j, k) = C_{e1} \times E_z^n(i, j, k) + C_{e2} \times E_z^{n-1}(i, j, k) + C_{e3} \times D_z^{n+1}(i, j, k) + C_{e4} \times D_z^n(i, j, k) + C_{e5} \times D_z^{n-1}(i, j, k) \]

\[(5.20)\]

where

\[ C_{e1} = \frac{-\alpha_0^z + \alpha_1^z + 2\alpha_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{e2} = \frac{-\alpha_0^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{e3} = \frac{\beta_0^z + \beta_1^z + \beta_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \]

\[ C_{e2} = \frac{\beta_0^z - \beta_1^z - 2\beta_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{e3} = \frac{\beta_0^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}. \]
For the magnetic field components the traditional updating equations for $H_x$, $H_y$, and $H_z$ can be used as follows:

For the $H_x$ component:

$$H_x^{n+1}(i, j, k) = C_{hxh}(i, j, k) \times H_x^n(i, j, k)$$

$$+ C_{hxey}(i, j, k) \times \left( E_y^n(i, j, k + 1) - E_y^n(i, j, k) \right)$$

$$+ C_{hxex}(i, j, k) \times \left( E_x^n(i, j, k + 1) - E_x^n(i, j, k) \right)$$

$$+ C_{hxm}(i, j, k) \times M_x^n(i, j, k),$$

where

$$C_{hxh}(i, j, k) = \frac{2\mu_y(i, j, k) - \Delta t \sigma_x^m(i, j, k)}{2\mu_y(i, j, k) + \Delta t \sigma_x^m(i, j, k)}$$

$$C_{hxey}(i, j, k) = \frac{-2\Delta t}{(2\mu_y(i, j, k) + \Delta t \sigma_x^m(i, j, k))\Delta y},$$

$$C_{hxex}(i, j, k) = \frac{-2\Delta t}{(2\mu_y(i, j, k) + \Delta t \sigma_x^m(i, j, k))\Delta y},$$

$$C_{hxm}(i, j, k) = \frac{-2\Delta t}{2\mu_y(i, j, k) + \Delta t \sigma_x^m(i, j, k)}.$$

For the $H_y$ component:

$$H_y^{n+1}(i, j, k) = C_{hyy}(i, j, k) \times H_y^n(i, j, k)$$

$$+ C_{hyey}(i, j, k) \times \left( E_y^n(i + 1, j, k) - E_y^n(i, j, k) \right)$$

$$+ C_{hyex}(i, j, k) \times \left( E_x^n(i, j, k + 1) - E_x^n(i, j, k) \right)$$

$$+ C_{hyym}(i, j, k) \times M_y^n(i, j, k),$$

where

$$C_{hyy}(i, j, k) = \frac{2\mu_x(i, j, k) - \Delta t \sigma_y^m(i, j, k)}{2\mu_x(i, j, k) + \Delta t \sigma_y^m(i, j, k)}$$

$$C_{hyey}(i, j, k) = \frac{-2\Delta t}{(2\mu_x(i, j, k) + \Delta t \sigma_y^m(i, j, k))\Delta x},$$

$$C_{hyex}(i, j, k) = \frac{-2\Delta t}{(2\mu_x(i, j, k) + \Delta t \sigma_y^m(i, j, k))\Delta x},$$

$$C_{hyym}(i, j, k) = \frac{-2\Delta t}{2\mu_x(i, j, k) + \Delta t \sigma_y^m(i, j, k)}.$$

For the $H_z$ component:
\[ H_z^{n+1}(i, j, k) = C_{hzh}(i, j, k) \times H_z^{n+1}(i, j, k) + C_{hhe}(i, j, k) \times \left( E_x^n(i, j+1, k) - E_x^n(i, j, k) \right) + C_{hhey}(i, j, k) \times \left( E_y^n(i+1, j, k) - E_y^n(i, j, k) \right) + C_{hzm}(i, j, k) \times M_{iz}^n(i, j, k), \]  

(5.23)

where

\[
C_{hzh}(i, j, k) = \frac{2\mu_x(i, j, k) - \Delta t \sigma_z^m(i, j, k)}{2\mu_x(i, j, k) + \Delta t \sigma_z^m(i, j, k)}, \\
C_{hhe}(i, j, k) = \frac{2\Delta t}{(2\mu_x(i, j, k) + \Delta t \sigma_z^m(i, j, k))\Delta y}, \\
C_{hhey}(i, j, k) = \frac{-2\Delta t}{(2\mu_x(i, j, k) + \Delta t \sigma_z^m(i, j, k))\Delta x}, \\
C_{hzm}(i, j, k) = \frac{-2\Delta t}{2\mu_x(i, j, k) + \Delta t \sigma_z^m(i, j, k)}. 
\]

Using equations (5.15) – (5.23) a complete FDTD algorithm for dispersive materials with a frequency-dependent permittivity is constructed. As in the conventional (frequency-independent) FDTD method, the fields \(E\) and \(H\) are calculated in a time-stepping manner for a lattice of Yee cells. In this formulation the values of \(E\) are used to calculate \(H\) from (5.21), (5.22), and (5.23); the values of \(H\) are used to calculate \(D\) from (5.15), (5.16), and (5.17); and the values of \(D\) are used to calculate \(E\) from (5.18), (5.19), and (5.20), after which the process is repeated iteratively.

The dispersive material equation and the developed code should also be capable of implementing normal dielectric material. This can easily be done by substituting zeros for \(\tau_1\) and \(\tau_2\) in equation (5.3), hence the equation will be reduced to \(\varepsilon(\omega) = \varepsilon_0\varepsilon_s\), where \(\varepsilon_s\) is given by (5.5). By substituting zeros for \(\tau_1\) and \(\tau_2\) in equation (5.14) the parameters \(\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = 0\) and hence, the equation will be reduced to

\[
E_x^{n+1}(i, j, k) = \frac{1}{\varepsilon_x(i, j, k)} D_x^{n+1}(i, j, k). 
\]  

(5.24)
Equation (5.24) verifies that the material is a dielectric. The $y$- and $z$-components can be also treated similarly. For an FDTD scattered field formulation for dispersive media the updating equations are listed in Appendix B.1.

5.3 Dispersive Periodic Boundary Conditions

In this section a new DPBC is developed to implement periodic structures with dispersive media on the boundaries of the unit cell. The new algorithm utilizes the ADE technique to update the magnetic field components and the non-boundary electric field components. In addition, a modified version of the constant horizontal wavenumber approach is derived to update electric field components on the boundaries. The update version of the constant horizontal wavenumber approach is based on Floquet equation (2.12) for the electrical field vector as follows:

$$ E(x = 0, y, z, \omega) = E(x = P_x, y, z, \omega) \times e^{i k_x P_x}. $$ (5.25)

Multiplying both sides of equation (5.25) by the complex permittivity will result in the following equation:

$$ \varepsilon(\omega)E(x = 0, y, z, \omega) = \varepsilon(\omega)E(x = P_x, y, z, \omega) \times e^{i k_x P_x}. $$ (5.26)

This can be represented as follows:

$$ D(x = 0, y, z, \omega) = D(x = P_x, y, z, \omega) \times e^{i k_x P_x}. $$ (5.27)

Equation (5.27) represents the Floquet theory for the displacement electric field vector $D$. Using the constant horizontal wavenumber approach, equation (5.27) can be directly transformed to the time-domain as follows:

$$ D(x = 0, y, z, t) = D(x = P_x, y, z, t) \times e^{i k_x P_x}. $$ (5.28)
Using equation (5.28) and the ADE technique, the updating equations for the magnetic and electric field components can be easily derived. The magnetic field components are updated using the FDTD updating equations (5.21) – (5.23). The electric field components are updated using ADE FDTD updating equations (5.18) – (5.20). While the non-boundary components of the electric displacement field vectors are updated using the ADE FDTD updating equations (5.15) – (5.17). The components on the boundaries will be updated using DPBC equations based on the constant horizontal wavenumber approach. The updating equations for the boundary electric displacement field components are organized as follows:

- Updating $D_x$ at $y = 0$ and $y = P_y$.
- Updating $D_y$ at $x = 0$ and $x = P_x$.
- Updating $D_z$ at $y = 0$, $y = P_y$, $x = 0$, and $x = P_x$, without the corners.
- Updating $D_z$ at the corners.

To update the $D_x$ on the boundary $y = 0$, the magnetic field components $H_z$ outside the computational domain are needed as shown in Fig. 2.6. However, due to periodicity in the $y$-direction, one can use magnetic field components $H_z$ of interest inside the computational domains; to update these electric displacement field vectors a procedure similar to the procedure in Section 2.3 is used.

$$D_x^{n+1}(i,1,k) = C_{dxd}(i,1,k)D_x^n(i,1,k) + C_{dhz}(i,1,k)[H_z^{n+1/2}(i,1,k) - H_z^{n+1/2}(i,0,k)] + C_{dhy}(i,1,k)[H_y^{n+1/2}(i,1,k) - H_y^{n+1/2}(i,1,k-1)],$$  

(5.29)
where the coefficients are stated as in (5.15), and $H_x^{n+1/2}(i, 0, k) = H_x^{n+1/2}(i, n_x, k) \times e^{jk \cdot P_y}$ due to the periodicity in the $y$-direction as shown in Fig. 2.6. The term $e^{jk \cdot P_y}$ is used to compensate the phase shift due to general oblique incidence. Then the updating equation for $D_x$ on the boundary $y = 0$ can be written as

$$D_x^{n+1}(i, 1, k) = C_{dxd}(i, 1, k) \times D_x^n(i, 1, k) + C_{dhd}(i, 1, k) \times [H_x^{n+1/2}(i, 1, k) - H_x^{n+1/2}(i, n_y, k) \times e^{jk \cdot n_y \Delta y}] + C_{dhy}(i, 1, k) \times [H_y^{n+1/2}(i, 1, k) - H_y^{n+1/2}(i, 1, k - 1)],$$

(5.30)

where $n_y$ is the total number of FDTD cells in the $y$-direction, and $\Delta y$ is the FDTD cell size in the $y$-direction. For $D_x$ on the boundary $y = P_y$ the updating equation can be written as

$$D_x^{n+1}(i, n_y + 1, k) = D_x^{n+1}(i, 1, k) \times e^{-jk \cdot n_y \Delta y}.$$  

(5.31)

Due to periodicity in $x$-direction as shown in Fig 2.7, the updating equation for the $D_y$ component on the boundary $x = 0$ can be written as

$$D_y^{n+1}(1, j, k) = C_{dyd}(1, j, k) \times D_y^n(1, j, k) + C_{dyhx}(1, j, k) \times [H_y^{n+1/2}(1, j, k) - H_y^{n+1/2}(1, j, k - 1)] + C_{dyhz}(1, j, k) \times [H_z^{n+1/2}(1, j, k) - H_z^{n+1/2}(n_x, j, k) \times e^{jk \cdot n_x \Delta x}],$$

(5.32)

where $n_x$ is the total number of FDTD cells in the $x$-direction within the period $P_x$ and $\Delta x$ is the FDTD cell size in the $x$-direction. For $D_y$ on the boundary $x = P_x$ the updating equation can be written as

$$D_y^{n+1}(n_x + 1, j, k) = D_y^{n+1}(1, j, k) \times e^{-jk \cdot n_x \Delta x}.$$  

(5.33)
A similar procedure is used for updating the $D_z$ components, but corner components are updated separately due to the presence of periodicity in both the $x$- and $y$-directions.

For $D_z$ on the boundary $x = 0$ and $x = P_x$, the updating equation can be written for $j \neq 1$ and $j \neq n_y + 1$ (avoiding the corners) as

$$D_z^{n+1}(1, j, k) = C_{dzd}(1, j, k) \times D_z^n(1, j, k)$$

$$+ C_{dzy}(1, j, k) \times [H_y^{n+\frac{1}{2}}(1, j, k) - H_y^{n-\frac{1}{2}}(n_x, j, k) \times e^{jkx, n_y\Delta x}]$$

$$+ C_{dzx}(1, j, k) \times [H_x^{n+\frac{1}{2}}(1, j, k) - H_x^{n-\frac{1}{2}}(1, j-1, k)].$$

$$D_z^{n+1}(n_x + 1, j, k) = D_z^{n+1}(1, j, k) \times e^{-jkx, n_y\Delta y}. \quad (5.34)$$

The updating equation for the $D_z$ components on the boundaries $y = 0$, and $y = P_y$ can be written for $i \neq 1$ and $i \neq n_x + 1$ (avoiding the corners) as

$$D_z^{n+1}(i, 1, k) = C_{dzd}(i, 1, k) \times D_z^n(i, 1, k)$$

$$+ C_{dzy}(i, 1, k) \times [H_y^{n+\frac{1}{2}}(i, 1, k) - H_y^{n+\frac{1}{2}}(i-1, 1, k)]$$

$$+ C_{dzx}(i, 1, k) \times [H_x^{n+\frac{1}{2}}(i, 1, k) - H_x^{n+\frac{1}{2}}(i, n_y, k) \times e^{jkx, n_y\Delta y}].$$

$$D_z^{n+1}(i, n_y + 1, k) = D_z^{n+1}(i, 1, k) \times e^{-jkx, n_y\Delta y}. \quad (5.36)$$

The $D_z$ components at the corners are updated as follows:

At $x = 0$ and $y = 0$

$$D_z^{n+1}(1, 1, k) = C_{dzd}(1, 1, k) \times D_z^n(1, 1, k)$$

$$+ C_{dzy}(1, 1, k) \times [H_y^{n+\frac{1}{2}}(1, 1, k) - H_y^{n+\frac{1}{2}}(n_x, 1, k) \times e^{jkx, n_y\Delta x}]$$

$$+ C_{dzx}(1, 1, k) \times [H_x^{n+\frac{1}{2}}(1, 1, k) - H_x^{n+\frac{1}{2}}(1, n_y, k) \times e^{jkx, n_y\Delta y}]. \quad (5.38)$$
At $x = P_x$ and $y = 0$:

$$D_z^{n+1}(n_x + 1, 1, k) = D_z^{n+1}(1, 1, k) \times e^{-jk \sigma_x}. \quad (5.39)$$

At $x = 0$ and $y = P_y$:

$$D_z^{n+1}(1, n_y + 1, k) = D_z^{n+1}(1, 1, k) \times e^{-jk \sigma_y}. \quad (5.40)$$

At $x = P_x$ and $y = P_y$:

$$D_z^{n+1}(n_x + 1, n_y + 1, k) = D_z^{n+1}(1, 1, k) \times e^{-jk \sigma_y} \times e^{-jk \sigma_x}. \quad (5.41)$$

Equations (5.29) – (5.41) together with the equations (5.21) – (5.23) and (5.18) – (5.20) describe the new FDTD/DPBC. After deriving the updating equations, a time marching algorithm can be constructed, as shown in Fig. 5.1. The main difference between this algorithm and the conventional FDTD algorithm is that the computational domain is divided into four main regions, as shown in Fig. 5.2. The first region is the middle region where all components of $E$, $H$, and $D$ are updated. The second region consists of the two CPML regions where only $E$ and $H$ are updated using the CPML (the CPML is not modified to handle dispersive media). The third region is the middle region of the boundaries where $D$ is updated using the new DPBC. The fourth region consists of the boundaries of the CPML regions where only $E$ is updated using the conventional PBC.
Fig. 5.1 The flowchart of the new FDTD/DPBC code.

Fig. 5.2 The four different regions of the new FDTD/DPBC computational domain.
5.4 Numerical Results

In this section, numerical results generated using the new algorithm are presented. The FDTD code was developed in MATLAB programming language and run on a computer with an Intel Core 2 CPU 6700, 2.66 GHz with 2 GB RAM. These results demonstrate the validity of the new algorithm for determining reflection and transmission properties of periodic structures with general dispersive media. The results generated by the new formulation are compared with results obtained from analytical solutions, the FDTD method with conventional PBC, and Ansoft high frequency structural simulator (HFSS), which is based on finite element method (FEM) [50].

5.4.1 An Infinite Water Slab

The algorithm is first used to analyze an infinite water slab with thickness $h = 6$ mm. The slab is illuminated by TM$^z$ and TE$^z$ plane waves in two different simulations. The geometry of the slab is shown in Fig. 5.3. The parameters of water permittivity are obtained from [47] as $\varepsilon_{s1} = 81$, $\varepsilon_{s2} = 1.8$, $\varepsilon_{\infty} = 1.8$, $\tau_1 = 9.4 \times 10^{-12}$ and $\tau_2 = 0$. The permittivity of water versus frequency is shown in Fig. 5.4. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.125$ mm, and the slab is represented by $2 \times 2$ cells (due to the homogeneity of the infinite slab it could be considered as a periodic structure with any periodicity). In the FDTD code 10,000 time steps and a Courant factor of 0.9 were used. The CPML was used for the absorbing boundaries at the top and the bottom of the computational domain. The slab is excited using a cosine-modulated Gaussian pulse centered at 10 GHz with 20 GHz bandwidth for the normal incidence case ($k_x = 0$ m$^{-1}$), and it is excited using a cosine-modulated Gaussian pulse centered at 12.75 GHz with 14.5 GHz bandwidth for the oblique incidence case ($k_x = 104.8$ m$^{-1}$ for minimum frequency of 5 GHz). The results are compared with analytical results.
Fig. 5.3 Geometry of the simulated infinite water slab.

Fig. 5.4 Water dispersive property versus frequency, (a) Relative permittivity, (b) Loss tangent.
Fig. 5.5 Reflection coefficient for infinite water slab of thickness 6mm under normal incidence 

\( (k_x = 0 \text{ m}^{-1}). \)

Fig. 5.6 Reflection coefficients for infinite water slab of thickness 6mm TM\(^z\) and TE\(^z\) oblique incidence \( (k_x = 104.8 \text{ m}^{-1}). \)
From Figs. 5.5 and 5.6 good agreement between analytical solutions and results generated by the new algorithm for both TM\(^z\) and TE\(^z\) cases (normal and oblique incidence) can be noticed. The computational time is equal to 1.17 minutes.

5.4.2 Nanoplasmonic Solar Cell Structure

The algorithm is then used to analyze a nanoplasmonic solar cell structure. The nanoparticles are used to increase the optical absorption within semiconductor solar cells, and hence enhance its performance [52]. The structure consists of cuboids elements of silver particles (dispersive media). The cuboids have length of 20 nm, width of 20 nm, and height of 10 nm. These cuboids are mounted over an SiO\(_2\) (silicon dioxide) substrate of thickness 30 nm and \(\varepsilon_r = 3.9\), and the structure has periodicity of 30 \(\times\) 30 nm in both the \(x\)- and \(y\)-directions, as shown in Fig. 5.7. The permittivity of the silver particles is described by a single-pole Lorentz medium using the parameters in [53]-[54]. Using these parameters and equation (5.10), the parameters for a two-term Debye relaxation model were derived (details are provided in Appendix B.4) as follows: \(\varepsilon_{s1} = 4.8233 \times 10^7\), \(\varepsilon_{s2} = -2.50721 \times 10^5\), \(\varepsilon_\infty = 4.391\), \(\tau_1 = 6.8479 \times 10^{-12}\) and \(\tau_2 = 3.5597 \times 10^{-14}\). The dispersive properties of the silver versus frequency are shown in Fig. 5.8.
Fig. 5.7 Geometry of the nanoplasmonic solar cell (all dimensions are in nm).

Fig. 5.8 Silver dispersive property versus frequency, (a) Relative permittivity, (b) Loss tangent.
As shown in Fig. 5.7, the structure can be simulated using unit cell A or unit cell B. If the structure is simulated using unit cell A there is no need to modify the PBC, the conventional PBC can be used since all the boundaries of the unit cell A are dielectric and there are no dispersive media on the boundaries (but the non-boundary field components still need to be handled using ADE technique). However, if the structure is to be simulated using unit cell B the new DPBC must be used due to the presence of dispersive media on the boundaries. Figure 5.9 shows the simulation domains used in both cases. The structure is illuminated by a normally incident plane wave \( (k_x = 0 \text{ m}^{-1}) \), using a cosine-modulated Gaussian pulse centered at 500 THz with a bandwidth of 500 THz. The structure is simulated using an FDTD grid cell size \( \Delta x = \Delta y = \Delta z = 1.25 \text{ nm} \), 50,000 time steps, and a Courant factor of 0.9; the CPML is used for the absorbing boundaries at the top and the bottom of the computational domain.
The results of case 1 and case 2 are compared with results obtained from Ansoft HFSS in Fig. 5.10. Good agreement between the results generated using HFSS, FDTD case 1, and the new algorithm for normal incidence can be noticed. The computational time for FDTD case 1 is 120 minutes, and for case 2 is 121 minutes, while using HFSS for 40 frequency points requires 350 minutes. The good agreement between the results generated using FDTD case 1 (conventional constant horizontal wavenumber PBC) and results generated using FDTD case 2 (new DPBC) prove the validity of the new DPBC. In addition, it should be noticed that the presence of the nanoparticles enhances the absorption of the structure at the frequency range around 500THz.

### 5.4.3 Sandwiched Composite FSS

The algorithm is used to analyze a sandwich composite-FSS structure. The composite materials have been investigated for their potential applications as shielding materials to protect electronics system from electromagnetic pulses or electromagnetic interference. To enhance the
shielding effectiveness, one possible solution is to introduce an additional layer or layers of FSS structures between the interfaces of the composite material [55]. The sandwiched structure studied here is shown in Fig. 5.11.

![Diagram of sandwiched composite-FSS structure](image)

**Fig. 5.11** Geometry of the sandwiched composite-FSS structure (all dimensions are in mm).

![Graphs of relative permittivity and loss tangent](image)

**Fig. 5.12** Composite material dispersive property versus frequency, (a) Relative permittivity, (b) Loss tangent.
An infinite thin metal film is inserted between two composite material layers with a thickness of 2.5 mm each; the metal film has a periodic array of cross-shaped slots with a 2 mm periodicity in both the x- and y-directions. The parameters of the permittivity of the composite medium as given in [55] are: $\varepsilon_{s1} = 5.2$, $\varepsilon_{s2} = 3.7$, $\varepsilon_{\infty} = 3.7$, $\tau_1 = 5.27 \times 10^{-10}$, and $\tau_2 = 0$. The dispersive properties of the composite material versus frequency are shown in Fig. 5.12. The structure is simulated using an FDTD grid cell size $\Delta x = \Delta y = \Delta z = 0.1$ mm and a Courant factor of 0.9; the CPML is used for the absorbing boundaries at the top and the bottom of the computational domain. The structure is first illuminated by a normally incident plane wave ($\theta = 0^\circ$ and $\varphi = 0^\circ$), using a cosine-modulated Gaussian pulse centered at 5 GHz with 10 GHz bandwidth. Then the structure is illuminated by an obliquely incident plane wave ($\theta = 30^\circ$ and $\varphi = 60^\circ$). To study the shielding enhancement provided by adding the FSS at the interface of the composite media, the transmission coefficient without the presence of the FSS is provided as a reference.

![Graph](image)

Fig. 5.13 Transmission coefficient for sandwiched composite-FSS structure illuminated by a normally incident plane wave ($\theta = 0^\circ$, $\varphi = 0^\circ$).
Fig. 5.14 Transmission coefficient for sandwiched composite-FSS structure illuminated by an obliquely incident plane wave \((\theta = 30^\circ, \phi = 60^\circ)\).

Figure 5.13 provides results for a normal incidence plane wave \((\theta = 0^\circ \text{ and } \phi = 0^\circ)\) exciting the composite-FSS structure. Good agreement between results obtained from the new FDTD/DPBC algorithm and HFSS can be noticed, which proves efficiency and validity of the new algorithm. The computational time for FDTD is equal to 9.56 minutes while the computational time is 12.34 minutes using HFSS for 40 frequency points. Figure 5.14 provides results for an oblique incidence plane wave \((\theta = 30^\circ \text{ and } \phi = 60^\circ)\) exciting the composite-FSS structure. Good agreement between results obtained from the new FDTD/DPBC algorithm and HFSS can be noticed. The computational time for FDTD is equal to 13.6 minutes while the computational time is 14.8 minutes using HFSS for 40 frequency points. It should be noticed from Figs. 5.13 and 5.14 that the transmission coefficient is dramatically decreased due to the presence of the FSS, which enhance the shielding effectiveness.
5.5 Summary

This chapter introduces a new FDTD/DPBC to analyze the scattering properties of periodic structures with dispersive media on the boundaries. The approach is developed based on both the constant horizontal wavenumber technique and the auxiliary differential equation technique. The new procedure is simple to implement and efficient in terms of both computational time and memory usage. The algorithm is capable of calculating reflection and transmission coefficients for the cases of normal and oblique incidence for both TE^2 and TM^2 cases. Numerical examples for potential applications such as dispersive slabs, nanoplasmonic structures, and sandwiched composite-FSS were provided. The results show good agreement with results from the analytical solution for a dispersive slab, and with the frequency-domain solutions for different dispersive periodic structures.
CHAPTER VI

6 CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

Electromagnetic periodic structures are of great importance in electromagnetics due to their wide range of applications. In this dissertation different types of electromagnetic periodic structures were analyzed using the constant horizontal wavenumber FDTD/PBC technique. A full description of the FDTD/PBC constant horizontal wavenumber approach was provided in Chapter 2. The main advantages and disadvantages of the approach were discussed. The FDTD updating equations were derived, and numerical results were provided to verify the validity of the approach.

In Chapter 3, a new FDTD approach was introduced to analyze the scattering properties of general skewed grid periodic structures. The approach is simple to implement and efficient in terms of both computational time and memory usage. In addition, the stability criterion is angle-independent. Therefore, it is efficient in implementing incidence with angles close to grazing ($\theta = 90^\circ$) as well as normal incidence ($\theta = 0^\circ$). The algorithm is capable of calculating the co- and cross-polarization reflection coefficients for normal and oblique incidence with either TE$^\parallel$ or TM$^\parallel$ cases, and for different skewed grid periodic structures. The numerical results showed good agreement with results from the analytical solution for a dielectric slab, and results from the MoM solutions for dipole and JC FSSs. The new algorithm is faster than many commercial software packages such as Ansoft Designer. In addition, to its ability to implement circuit components such as resistors, capacitors, inductors, diodes and transistors.

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In Chapter 4, an efficient hybrid FDTD/GSM technique is described. In this technique the constant horizontal wavenumber FDTD/PBC approach is used to compute the scattering parameters of each layer, after which the scattering matrix of the entire structure is calculated using the cascading technique. In addition, two procedures were described; one is used to study the behavior of different harmonics (evanescent and propagating) using the constant horizontal wavenumber FDTD/PBC approach, which dramatically reduces the memory usage. The other procedure is used to determine the proper gap size (for neglecting the harmonics effects) and it can also be used to select the proper harmonics for a specific gap size. The validity of the algorithm was verified through several numerical examples including FSSs with different periodicities, and illuminated at different incident angles. The numerical results of the developed approach show good agreement with the results obtained from the direct FDTD simulation of the entire structure, while the proposed procedure saves computational time and memory usage. This dissertation provides a complete study for determining the proper gap size for neglecting the higher harmonics effects. In addition, it provides a means to select the proper harmonics for the small gap case. Thirdly, it provides results for multilayered periodic structures with different periodicities which increases the degree of freedom in designing these structures.

In Chapter 5, a new FDTD/DPBC approach to analyze the scattering properties of general dispersive periodic structures was introduced. The approach is developed based on both the constant horizontal wavenumber and the auxiliary differential equation techniques. It is simple to implement and efficient in terms of both computational time and memory usage. It is capable of calculating the co- and cross-polarization reflection and transmission coefficients, for the case of normal and oblique incidence, and for both TE$^z$ and TM$^z$ cases. The numerical results show good agreement with results from the analytical solution for a water dispersive slab, and results from
the frequency-domain solutions for dispersive periodic structures. The new algorithm is much faster than HFSS, and it can be used to implement embedded circuit elements.

The algorithms developed in this dissertation were implemented using the MATLAB programming language. These algorithms provide a complete software tool that is capable of analyzing efficiently and accurately almost any kind of electromagnetic periodic structure using the FDTD technique. This software package could be used in many applications such as the design of reconfigurable FSS using lumped elements or studying the effect of skew angle on the performance of periodic structures. Various multilayered periodic structures can be analyzed or designed. In addition, the algorithm can be used to study or design different dispersive periodic structures. Moreover, this software package is capable of simulating different linear and non-linear circuit elements such as resistors, inductors, capacitors, diodes, and transistors with their full wave simulation models, which provide very accurate modeling for such elements.

6.2 Future Work

The work presented in this dissertation triggers quite a few interesting future research topics, among which are applying the FDTD/PBC constant horizontal wavenumber approach to arbitrary geometries such as hexagonal or triangular unit cells, instead of rectangular or square unit cells. In addition, the skewed grid approach described in Chapter 3 and the new FDTD/DPBC described in Chapter 5 may be combined to develop a new algorithm capable of analyzing dispersive skewed grid periodic structure. Furthermore, the algorithm described in Chapter 4 can be extended using the skewed grid approach to analyze multilayered periodic structures with arbitrary skewed grids. Designing and simulating different reconfigurable FSS
structures using linear and non-linear circuit elements might also be a very interesting future research topic.


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APPENDICES
A  Appendix A

A.1  General S- to T-parameters Transformation

To prove equation (4.3) for the general case matrix, a partitioning technique should be used as follows:

\[
\begin{bmatrix}
    b_1 \\
    b_2 \\
    \ldots \\
    b_4
\end{bmatrix}
= \begin{bmatrix}
    S_{11} & S_{12} & \cdots & S_{13} & S_{14} \\
    S_{21} & S_{22} & \cdots & S_{23} & S_{24} \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    S_{41} & S_{42} & \cdots & S_{43} & S_{44}
\end{bmatrix}
\begin{bmatrix}
    a_1 \\
    a_2 \\
    \ldots \\
    a_4
\end{bmatrix}
\begin{bmatrix}
    b_1 \\
    b_2 \\
    \ldots \\
    b_4
\end{bmatrix}
\begin{bmatrix}
    T_{11} & T_{12} & \cdots & T_{13} & T_{14} \\
    T_{21} & T_{22} & \cdots & T_{23} & T_{24} \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    T_{41} & T_{42} & \cdots & T_{43} & T_{44}
\end{bmatrix}
\begin{bmatrix}
    a_1 \\
    a_2 \\
    \ldots \\
    a_4
\end{bmatrix}
\]

(A.1)

\[
|B_1| = \begin{bmatrix}
    b_1 \\
    b_2 \\
    \ldots \\
    b_4
\end{bmatrix},
|B_2| = \begin{bmatrix}
    b_3 \\
    b_4 \\
    \ldots \\
    b_4
\end{bmatrix},
|A_1| = \begin{bmatrix}
    a_1 \\
    a_2 \\
    \ldots \\
    a_4
\end{bmatrix},
|A_2| = \begin{bmatrix}
    a_3 \\
    a_4 \\
    \ldots \\
    a_4
\end{bmatrix},
\]

\[
S_{11} = \begin{bmatrix}
    S_{11} & S_{12} \\
    S_{21} & S_{22}
\end{bmatrix},
S_{12} = \begin{bmatrix}
    S_{13} & S_{14} \\
    S_{23} & S_{24}
\end{bmatrix},
S_{21} = \begin{bmatrix}
    S_{31} & S_{32} \\
    S_{41} & S_{42}
\end{bmatrix},
S_{22} = \begin{bmatrix}
    S_{33} & S_{34} \\
    S_{43} & S_{44}
\end{bmatrix},
\]

\[
T_{11} = \begin{bmatrix}
    T_{11} & T_{12} \\
    T_{21} & T_{22}
\end{bmatrix},
T_{12} = \begin{bmatrix}
    T_{13} & T_{14} \\
    T_{23} & T_{24}
\end{bmatrix},
T_{21} = \begin{bmatrix}
    T_{31} & T_{32} \\
    T_{41} & T_{42}
\end{bmatrix},
T_{22} = \begin{bmatrix}
    T_{33} & T_{34} \\
    T_{43} & T_{44}
\end{bmatrix}.
\]

(A.2)

\[
\begin{bmatrix}
    |B_1| \\
    |B_2|
\end{bmatrix} = \begin{bmatrix}
    S_{11} & S_{12} \\
    S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
    |A_1| \\
    |A_2|
\end{bmatrix},
\begin{bmatrix}
    |B_1| \\
    |A_1|
\end{bmatrix} = \begin{bmatrix}
    T_{11} & T_{12} \\
    T_{21} & T_{22}
\end{bmatrix}
\begin{bmatrix}
    |A_2| \\
    |B_2|
\end{bmatrix}.
\]

(A.3)

From equation (A.3), four equations can be stated as follows:

\[
|B_1| = S_{11} |A_1| + S_{12} |A_2|,
|B_2| = S_{21} |A_1| + S_{22} |A_2|,
|B_1| = T_{11} |A_2| + T_{12} |B_2|,
|A_1| = T_{21} |A_2| + T_{22} |B_2|.
\]

(A.4)
To convert from S- to T-parameters we multiply equation (A.4b) by $S_{21}^{-1}$ from the left hand side, and then the equation will reduce to

$$S_{21}^{-1} | B_2 >=| A_1 > + S_{21}^{-1} S_{22} | A_2 >,$$

$$| A_1 >= -S_{21}^{-1} S_{22} | A_2 > + S_{21}^{-1} | B_2 >.$$  \hspace{1cm} (A.5)

From this equation, two T-parameters can be calculated as

$$T_{21} = -S_{21}^{-1} S_{22}, \ T_{22} = S_{21}^{-1}.$$ \hspace{1cm} (A.6)

By substituting (A.5) in (A.4a) the following equation will be obtained

$$| B_1 >= (S_{12} - S_{11} S_{21}^{-1} S_{22}) | A_2 > + S_{11} S_{21}^{-1} | B_2 >.$$ \hspace{1cm} (A.7)

From (A.7), the other two T-parameters can be calculated as

$$T_{41} = S_{12} - S_{11} S_{21}^{-1} S_{22}, \ T_{42} = S_{11} S_{21}^{-1}.$$ \hspace{1cm} (A.8)

To convert from T- to S-parameters we multiply equation (A.4d) by $T_{22}^{-1}$ from the left hand side, and then the equation will reduce to

$$T_{22}^{-1} | A_1 >= T_{22}^{-1} T_{21} | A_2 > + | B_2 >,$$

$$| B_2 >= T_{22}^{-1} | A_1 > - T_{22}^{-1} T_{21} | A_2 >.$$ \hspace{1cm} (A.9)

From this equation, two S-parameters can be calculated as

$$S_{21} = T_{22}^{-1}, \ S_{22} = -T_{22}^{-1} T_{21}.$$ \hspace{1cm} (A.10)

By substituting (A.9) in (A.4c) the following equation will be obtained

$$| B_1 >= T_{42} T_{22}^{-1} | A_1 > + (T_{41} - T_{42} T_{22}^{-1} T_{21}) | A_2 >.$$ \hspace{1cm} (A.11)
From (A.11), the other two $S$- parameters can be calculated as

$$S_{11} = T_{12} T_{22}^{-1}, \quad S_{12} = (T_{11} - T_{12} T_{22}^{-1} T_{21}).$$  

(A.12)

The general result is then given by

$$\begin{bmatrix}
T_{12} - S_{12} S_{22}^{-1} S_{21} \\
-S_{21}^{-1} S_{22} & S_{21}^{-1}
\end{bmatrix},$$  

(A.13a)

$$\begin{bmatrix}
T_{12} T_{22}^{-1} \\
T_{22}^{-1}
\end{bmatrix},$$  

(A.13b)
A.2 Square Patch Multilayered FSS

To study the effect of the geometry on the harmonic frequency behavior, a test case with two identical square patch FSS layers is studied. In this test case the multilayer geometry consists of two identical FSS structures consisting of square patch elements (1:1 case). The square patch has a side length of 10 mm. The periodicity is 15 mm in both the $x$- and $y$-directions. The substrate has a thickness of 6 mm and relative permittivity $\varepsilon_r = 2.2$, as shown in Fig. A.1. The structure is illuminated by a normally incident plane wave and the frequency range of interest is 0-16 GHz.

The goal is to determine the distance $d$ after which all the higher harmonics magnitudes reach -40dB from the magnitude of the incident electric field. Using the gap determination procedure:

1. The two layers are identical, so analyzing the harmonics of one layer is enough. The reflection and transmission harmonics must be calculated.

2. The frequency range of interest as specified by the problem is 0-16GHz (as shown in Fig. 4.9 the highest frequency will have the strongest effect).

3. $k_x^i$ and $k_y^i$ are equal to zero (normal incidence).

4. Determine the cut-off frequencies for the first eight harmonics as follows:

\[ M_{01}, M_{0-1} \rightarrow k = \sqrt{(0)^2 + (\pm 418.9)^2} = 418.9 \rightarrow f_{turn-on}^{01} = f_{turn-on}^{0-1} = 20GHz, \]
\[ M_{10}, M_{-10} \rightarrow k = \sqrt{(\pm 418.9)^2 + (0)^2} = 418.9 \rightarrow f_{turn-on}^{10} = f_{turn-on}^{-10} = 20GHz, \]
\[ M_{11}, M_{1-1} \rightarrow k = \sqrt{(418.9)^2 + (\pm 418.9)^2} = 592.4 \rightarrow f_{turn-on}^{11} = f_{turn-on}^{-11} = 28.3GHz, \]
\[ M_{-11}, M_{-1-1} \rightarrow k = \sqrt{(-418.9)^2 + (\pm 418.9)^2} = 592.4 \rightarrow f_{turn-on}^{-11} = f_{turn-on}^{1-1} = 28.3GHz. \]

5. Use the harmonic analysis to calculate the magnitude coefficient of the first eight harmonics, and plot the behavior of these harmonics with frequency as shown in Figs. A.2 and A.3.
Fig. A.1 The geometry of two identical square patch FSS structures.

Fig. A.2 The first eight transmitted harmonics at 16 GHz, (a) Magnitude compared to incident electric field, (b) The decaying behavior with distance.
Fig. A.3 The first eight reflected harmonics at 16 GHz, (a) Magnitude compared to incident electric field, (b) The decaying behavior with distance.

It should be noticed from Figs. A.2 and A.3 that a distance $d = 17.26$ mm between the two layers for this range of frequencies is enough to neglect all the harmonics. In addition, it should be noticed that the effect of the harmonics is stronger for the square-patch case compared to the dipole-FSS, which indicates the effect of the geometry on the harmonic behavior for the same periodicity (so both the geometry and periodicity controls the harmonics behavior).
A.3 L-Shaped Multilayered FSS

To study the effect of cross-polarized fields, a test case with two identical L-shaped FSS structures is studied. In this test case the multilayer geometry consists of two identical FSS structures consisting of L-shaped elements (1:1 case). The L-shaped element consists of two perpendicular dipoles of length 12 mm and width 3 mm. The periodicity is 15 mm in both x- and y-directions. The substrate has thickness of 6 mm and relative permittivity $\varepsilon_r = 2.2$, as shown in Fig. A.4. The structure is illuminated by a normally incident plane wave and the frequency range of interest is 0-15 GHz. This structure is used to study the effect of cross-polarization components. The structure generates cross-polarization components with normal incidence and the reflection and transmission co- and cross-polarization coefficients are shown in Fig. A.5. Using the harmonic analysis, the proper distance for ignoring the harmonics was found to be 13.34 mm. The structure is simulated using the cascaded technique with $d = 15$ mm. The results are compared to the FDTD simulation of the entire structure, as shown is Fig. A.6.

Fig. A.4 Two identical L-shaped FSS geometry.
Fig. A.5 Reflection and transmission coefficients for co- and cross-polarized components for single layer L-shaped FSS structure.

Fig. A.6 Reflection and transmission coefficients for co- and cross-polarized components for two identical L-shaped FSS structures with $d = 15\text{mm}$.
B  Appendix B

B.1  Auxiliary Differential Equation Scattered Field Formulation

For an FDTD scattered field formulation for dispersive media, the equations are as follows for plane wave excitation [49]:

\[
\begin{align*}
\frac{\partial \tilde{D}(t)}{\partial t} + (\tau_1 + \tau_2) \frac{\partial \tilde{D}(t)}{\partial t} + \tau_1 \tau_2 \frac{\partial^2 \tilde{D}(t)}{\partial t^2} &= \varepsilon_0 \left[ \varepsilon_s \tilde{E}_s(t) + (\varepsilon_{s1} \tau_2 + \varepsilon_{s2} \tau_1) \frac{\partial \tilde{E}_s(t)}{\partial t} + \tau_1 \tau_2 \varepsilon_\infty \frac{\partial^2 \tilde{E}_s(t)}{\partial t^2} \right] \\
+ &\varepsilon_0 \left[ \varepsilon_s \tilde{E}_s(t) + (\varepsilon_{s1} \tau_2 + \varepsilon_{s2} \tau_1) \frac{\partial \tilde{E}_s(t)}{\partial t} + \tau_1 \tau_2 \varepsilon_\infty \frac{\partial^2 \tilde{E}_s(t)}{\partial t^2} \right],
\end{align*}
\]  

\[\frac{\partial \tilde{H}_s(t)}{\partial t} = -\frac{1}{\mu} \nabla \times \tilde{E}_s,\]  

\[\frac{\partial \tilde{D}(t)}{\partial t} = \nabla \times \tilde{H}_s + \varepsilon_0 \frac{\partial \tilde{E}_s(t)}{\partial t}, \text{ where } \nabla \times \tilde{H}_s \rightarrow \varepsilon_0 \frac{\partial \tilde{E}_s(t)}{\partial t}. \]  

Now it is obvious that the vector differential equations (B.1) – (B.3) are expressed in terms of incident and scattered fields. The incident field and its derivatives are usually defined analytically. Using the central difference approximation for the derivatives in equations (B.1) – (B.3), the updating equations for the components of the field vectors \( \mathbf{E}_s, \mathbf{H}_s, \) and the auxiliary displacement vector \( \mathbf{D} \) can be easily obtained.

Similar to the total field formulation, the updating equations can be written in the same manner as [1], assuming \( \sigma^m \) and \( M_i = 0 \):

\[
\frac{\partial H^s_x}{\partial t} = \frac{1}{\mu_s} \left( \frac{\partial E^s_y}{\partial z} - \frac{\partial E^s_z}{\partial y} \right), \]  

\[\text{B.4a}\]
By re-arranging the above nine equations the recursive FDTD algorithm can be easily written, starting with $H_x$, $E_x$, and $D_x$ as follows [1]:
For the $H_x$ component:

\[
H_x^{n+1}(i, j, k) = C_{hxx}(i, j, k) \times H_x^n(i, j, k) \\
+ C_{hxy}(i, j, k) \times \left( E_y^n(i, j, k + 1) - E_y^n(i, j, k) \right) \\
+ C_{hxx}(i, j, k) \times \left( E_z^n(i, j, k + 1) - E_z^n(i, j, k) \right),
\]

where

\[
C_{hxx}(i, j, k) = 1, C_{hxy}(i, j, k) = \frac{\Delta t}{(\mu_x(i, j, k))\Delta z}, C_{hxx}(i, j, k) = \frac{-\Delta t}{(\mu_x(i, j, k))\Delta y}.
\]

For the $H_y$ component:

\[
H_y^{n+1}(i, j, k) = C_{hyh}(i, j, k) \times H_y^n(i, j, k) \\
+ C_{hye}(i, j, k) \times \left( E_z^n(i + 1, j, k) - E_z^n(i, j, k) \right) \\
+ C_{hye}(i, j, k) \times \left( E_x^n(i, j, k + 1) - E_x^n(i, j, k) \right),
\]

where

\[
C_{hyh}(i, j, k) = 1, C_{hye}(i, j, k) = \frac{\Delta t}{(\mu_y(i, j, k))\Delta x}, C_{hye}(i, j, k) = \frac{-\Delta t}{(\mu_y(i, j, k))\Delta z}.
\]

For the $H_z$ component:

\[
H_z^{n+1}(i, j, k) = C_{hzh}(i, j, k) \times H_z^n(i, j, k) \\
+ C_{hzx}(i, j, k) \times \left( E_y^n(i, j + 1, k) - E_y^n(i, j, k) \right) \\
+ C_{hzy}(i, j, k) \times \left( E_x^n(i + 1, j, k) - E_x^n(i, j, k) \right),
\]

where
\[ C_{hzh}(i, j, k) = 1, C_{hze}(i, j, k) = \frac{\Delta t}{(\mu_{i}(i, j, k))\Delta y}, C_{hzy}(i, j, k) = \frac{-\Delta t}{(\mu_{j}(i, j, k))\Delta x}. \]

As long as the \( \mu \) (permeability) of the material is independent of the frequency the updating equations for the magnetic field will be similar to the conventional FDTD updating equation. For updating the displacement field vector \( \mathbf{D} \), we start by updating the \( D_x \) as follows:

\[
D_{x}^{n+1}(i, j, k) = C_{dxd}(i, j, k) \times D_{x}^{n}(i, j, k) \\
+ C_{dxh}(i, j, k) \times \left[ H_{z}^{n+\frac{1}{2}}(i, j, k) - H_{z}^{n-\frac{1}{2}}(i, j-1, k) \right] \\
+ C_{dhy}(i, j, k) \times \left[ H_{y}^{n+\frac{1}{2}}(i, j, k) - H_{y}^{n-\frac{1}{2}}(i, j, k-1) \right] \\
+ C_{dexe}(i, j, k) \times \left[ E_{inc,x}^{n+1}(i, j, k) - E_{inc,x}^{n}(i, j, k) \right],
\]  

where

\[ C_{dxd}(i, j, k) = 1, C_{dxh}(i, j, k) = \frac{\Delta t}{\Delta y}, C_{dhy}(i, j, k) = \frac{-\Delta t}{\Delta x}, C_{dexe}(i, j, k) = \varepsilon_{0} \]

Similarly, for the \( D_y \):

\[
D_{y}^{n+1}(i, j, k) = C_{dyd}(i, j, k) \times D_{y}^{n}(i, j, k) \\
+ C_{dyh}(i, j, k) \times \left[ H_{x}^{n+\frac{1}{2}}(i, j, k) - H_{x}^{n-\frac{1}{2}}(i, j, k-1) \right] \\
+ C_{dye}(i, j, k) \times \left[ H_{z}^{n+\frac{1}{2}}(i, j, k) - H_{z}^{n-\frac{1}{2}}(i-1, j, k) \right] \\
+ C_{dye}(i, j, k) \times \left[ E_{inc,y}^{n+1}(i, j, k) - E_{inc,y}^{n}(i, j, k) \right],
\]  

where

\[ C_{dyd}(i, j, k) = 1, C_{dyh}(i, j, k) = \frac{\Delta t}{\Delta z}, C_{dye}(i, j, k) = \frac{-\Delta t}{\Delta y}, C_{dye}(i, j, k) = \varepsilon_{0} \]

Similarly, for the \( D_z \):
\[ D_{z}^{n+1}(i, j, k) = C_{dd}(i, j, k) \times D_{z}^{n}(i, j, k) \\
+ C_{dsh}(i, j, k) \times [H_{y}^{\alpha+1/2}(i, j, k) - H_{y}^{\alpha+1/2}(i-1, j, k)] \\
+ C_{dht}(i, j, k) \times [H_{x}^{\alpha+1/2}(i, j, k) - H_{x}^{\alpha+1/2}(i, j-1, k)] \\
+ C_{dse}(i, j, k) \times [E_{inc,x}^{n+1}(i, j, k) - E_{inc,x}^{n}(i, j, k)], \tag{B.10} \]

where

\[ C_{dd}(i, j, k) = 1, C_{dsh}(i, j, k) = \frac{\Delta t}{\Delta x}, C_{dht}(i, j, k) = -\frac{\Delta t}{\Delta y}, C_{dse}(i, j, k) = \varepsilon_{0} \]

To update the electric field vector \( E \), we start by updating \( E_{x} \) as follows:

\[
\frac{1}{2}(D_{x}^{n+1} + D_{x}^{n}) + \frac{\tau_{1} + \tau_{2}}{\Delta t}(D_{x}^{n+1} - D_{x}^{n}) + \frac{\tau_{1} \tau_{2}}{(\Delta t)^{2}}(D_{x}^{n+1} - 2D_{x}^{n} + D_{x}^{n-1}) = \\
\frac{\varepsilon_{0}E_{x}^{n+1}}{2}(E_{x}^{n+1} + E_{x}^{n}) + \frac{\varepsilon_{0}(E_{x}^{n} + E_{x}^{n})}{\Delta t}(E_{x}^{n+1} - E_{x}^{n}) + \frac{\varepsilon_{0}E_{x}^{n+1} \tau_{2}}{(\Delta t)^{2}}(E_{inc,x}^{n+1} - 2E_{inc,x}^{n} + E_{inc,x}^{n-1}) + \\
\frac{\varepsilon_{0}E_{x}^{n}}{2}(E_{inc,x}^{n+1} + E_{inc,x}^{n}) + \frac{\varepsilon_{0}(E_{inc,x}^{n} + E_{inc,x}^{n})}{\Delta t}(E_{inc,x}^{n+1} - E_{inc,x}^{n}) + \frac{\varepsilon_{0}E_{x}^{n+1} \tau_{2}}{(\Delta t)^{2}}(E_{inc,x}^{n+1} - 2E_{inc,x}^{n} + E_{inc,x}^{n-1})
\]

Then

\[
\begin{align*}
[\alpha_{0}^{x} + \alpha_{1}^{x} + \alpha_{2}^{x}]E_{x}^{n+1} &= [-\alpha_{0}^{x} + \alpha_{1}^{x} + 2\alpha_{2}^{x}]E_{x}^{n} + [-\alpha_{2}^{x}]E_{x}^{n-1} \\
- [\alpha_{0}^{x} + \alpha_{1}^{x} + \alpha_{2}^{x}]E_{inc,x}^{n+1} &= [-\alpha_{0}^{x} + \alpha_{1}^{x} + 2\alpha_{2}^{x}]E_{inc,x}^{n} + [-\alpha_{2}^{x}]E_{inc,x}^{n-1} \\
+ [\beta_{0}^{x} + \beta_{1}^{x} + \beta_{2}^{x}]D_{x}^{n+1} &= [\beta_{0}^{x} - \beta_{1}^{x} - 2\beta_{2}^{x}]D_{x}^{n} + [\beta_{2}^{x}]D_{x}^{n-1}
\end{align*}
\]

\[ E_{x}^{n+1}(i, j, k) = -E_{inc,x}^{n+1}(i, j, k) + C_{exc}\times[E_{x}^{n}(i, j, k) + E_{inc,x}^{n}(i, j, k)] \\
+ C_{exc}\times[E_{inc,x}^{n+1}(i, j, k) + E_{inc,x}^{n}(i, j, k)] + C_{exc1}\times D_{x}^{n+1}(i, j, k) \\
+ C_{exc2}\times D_{x}^{n}(i, j, k) + C_{exc3}\times D_{x}^{n-1}(i, j, k) \tag{B.11} \]

\[ C_{exc1} = \frac{[-\alpha_{0}^{x} + \alpha_{1}^{x} + 2\alpha_{2}^{x}]}{[\alpha_{0}^{x} + \alpha_{1}^{x} + \alpha_{2}^{x}]}, \quad C_{exc2} = \frac{[-\alpha_{2}^{x}]}{[\alpha_{0}^{x} + \alpha_{1}^{x} + \alpha_{2}^{x}]}, \quad C_{exc1} = \frac{[\beta_{0}^{x} + \beta_{1}^{x} + \beta_{2}^{x}]}{[\alpha_{0}^{x} + \alpha_{1}^{x} + \alpha_{2}^{x}]} \]
Similarly, for the $E_y$:

\[
E_y^{n+1}(i, j, k) = -E_{\text{inc},y}^n(i, j, k) + C_{\text{eyl}} \times [E_y^n(i, j, k) + E_{\text{inc},y}^n(i, j, k)]
\]

\[
+ C_{\text{eyl}2} \times [E_y^{n-1}(i, j, k) + E_{\text{inc},y}^{n-1}(i, j, k)] + C_{\text{eyl}1} \times D_y^{n+1}(i, j, k)
\]

\[
+ C_{\text{eyl}3} \times D_y^n(i, j, k) + C_{\text{eyl}4} \times D_y^{n-1}(i, j, k)
\]

(B.12)

\[
C_{\text{eyl}} = \frac{-\alpha_0^y + \alpha_1^y + 2\alpha_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{\text{eyl}2} = \frac{-\alpha_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{\text{eyl}1} = \frac{\beta_0^y + \beta_1^y + \beta_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}, \quad C_{\text{eyl}3} = \frac{\beta_2^y}{\alpha_0^y + \alpha_1^y + \alpha_2^y}
\]

Similarly, for the $E_z$:

\[
E_z^{n+1}(i, j, k) = -E_{\text{inc},z}^n(i, j, k) + C_{\text{ezl}} \times [E_z^n(i, j, k) + E_{\text{inc},z}^n(i, j, k)]
\]

\[
+ C_{\text{ezl}2} \times [E_z^{n-1}(i, j, k) + E_{\text{inc},z}^{n-1}(i, j, k)] + C_{\text{ezl}1} \times D_z^{n+1}(i, j, k)
\]

\[
+ C_{\text{ezl}3} \times D_z^n(i, j, k) + C_{\text{ezl}4} \times D_z^{n-1}(i, j, k)
\]

(B.13)

\[
C_{\text{ezl}} = \frac{-\alpha_0^z + \alpha_1^z + 2\alpha_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{\text{ezl}2} = \frac{-\alpha_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{\text{ezl}1} = \frac{\beta_0^z + \beta_1^z + \beta_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}, \quad C_{\text{ezl}3} = \frac{\beta_2^z}{\alpha_0^z + \alpha_1^z + \alpha_2^z}
\]
B.2 Scattering from 3-D Dispersive Objects

To check the validity of the ADE scattered field formulation, the formulation was developed using MATLAB code and two test cases were executed. In the first test case, the bistatic radar cross section (RCS) of a water dispersive cube was calculated, where the cube has a side length of 16 cm.

The parameters for water permittivity are obtained from [45] as $\varepsilon_{s1} = 81$, $\varepsilon_{s2} = 1.8$, $\varepsilon_\infty = 1.8$, $\tau_1 = 9.4 \times 10^{-12}$ and $\tau_2 = 0$. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.5$ cm. In the FDTD code 20,000 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries of the computational domain, as shown in Fig. B.1, and the cube is excited using a Gaussian pulse. The results were compared with results obtained from HFSS, as shown in Fig. B.2. Good agreement should be noticed between results generated by the FDTD method and the results generated using the HFSS package, which proves the validity of the scattered field formulation.

![Fig. B.1 Water dispersive cube computational domain.](image)
Fig. B.2 Water dispersive cube bistatic RCS at 1 GHz, (a) FDTD, (b) HFSS.

Fig. B.3 Water dispersive sphere computational domain.
In the second test case, the bistatic RCS of a water dispersive sphere was calculated, where the sphere has a radius of 10 cm. The parameters for water permittivity are obtained from [45] as $\varepsilon_s^1 = 81$, $\varepsilon_s^2 = 1.8$, $\varepsilon_\infty = 1.8$, $\tau_1 = 9.4 \times 10^{-12}$ and $\tau_2 = 0$. The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.75$ cm. In the FDTD code 20,000 time steps and a Courant factor of 0.9 are used. The CPML is used for the absorbing boundaries of the computational domain, as shown in Fig. B.3, and the cube is excited using a Gaussian pulse. The results are compared with results obtained from HFSS, as shown in Fig. B.4. Good agreement should be noticed between results generated by the FDTD method and the results generated using the HFSS package, which proves the validity of the scattered field formulation.

Fig. B.4 Water dispersive sphere bistatic RCS at 1 GHz, (a) FDTD, (b) HFSS.
B.3 Analysis of RFID Tags Mounted over Human Body

Radio frequency identification (RFID) is becoming one of the most used systems in today's societies. A practical application for the RFID tags could be to use them to track animals or sometimes people (children or seniors), but mounting these tags on human tissues might affect their performance due to the dispersive nature of the human tissues. In this section, three test cases are conducted to study the effect of the human tissues on the performance of RFID tags. The geometry of the tag is shown in Fig. B.5, and the tag is designed to operate at 2.45 GHz. The details of the three test cases are shown in Table B.1.

![Diagram of RFID tag geometry](image)

Fig. B.5 Geometry of RFID tag mounted over a three medium substrate, (a) Side view, (b) Top view (all dimensions are in mm).
The parameters of dry skin permittivity as stated in [51] are $\varepsilon_{s1} = 37.161$, $\varepsilon_{s2} = 70.171$, $\varepsilon_\infty = 4.391$, $\tau_1 = 7.42 \times 10^{-12}$ and $\tau_2 = 5.736 \times 10^{-10}$, while for the muscles the parameters as stated in [51] are $\varepsilon_{s1} = 54.193$, $\varepsilon_{s2} = 192.873$, $\varepsilon_\infty = 6.473$, $\tau_1 = 6.796 \times 10^{-12}$ and $\tau_2 = 1.827 \times 10^{-9}$. The three test case are simulated using the FDTD code with a two-term Debye relaxation model and the results were compared to study the effect of the dispersive material on the matching of the RFID tag antenna. The chip used in this analysis has an impedance of $Z_c = (17.422-67.402j) \, \Omega$.

In the FDTD simulation a cell of size $\Delta x = \Delta y = \Delta z = 0.8$ mm, a Courant factor of 0.95, and 5,000 time steps are used. The results are shown in Fig. B.6.

![Reflection coefficient magnitude of the RFID tag for the three test cases](image_url)
It should be noticed from Fig. B.6, that there exists good matching for the tag before being mounted over any human tissue, but after mounting the tag over 5 mm of dry skin the matching is degraded, which will degrade the performance of the tag significantly. However, when the tag is mounted over 5 mm of dry skin and 5 mm of muscles the matching is enhanced, which will enhance the performance of such tag. As a rule of thumb for designing a good RFID tag, the application for which this tag is going to be used must be known. This will help the designer to know exactly the kind of substrate over which this tag will be mounted, so he could design an optimum tag for the application.
B.4. Lorentz to Debye Model Transformation for Gold and Silver Media

In this section the transformation from a single-term Lorentz model to a two-term Debye model is derived. The single-term Lorentz model can be stated as

\[
\varepsilon_{rL}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 + 2j\omega\delta_0 - \omega^2},
\]

which can be reduced to:

\[
\varepsilon_{rL}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)}{1 + j\omega\left(\frac{2\delta_0}{\omega_0^2}\right) - \omega^2\left(\frac{\varepsilon_\infty}{\omega_0^2}\right)},
\]

\[
\varepsilon_{rL}(\omega) = \varepsilon_s + j\omega\left(\frac{2\delta_0}{\omega_0^2}\right) - \omega^2\left(\frac{\varepsilon_\infty}{\omega_0^2}\right),
\]

The two-term Debye model can be stated as

\[
\varepsilon_{rD}(\omega) = \frac{\varepsilon_s + j\omega(\varepsilon_{s2}\tau_2 + \varepsilon_{s1}\tau_1) - \omega^2(\tau_1\tau_2\varepsilon_\infty)}{1 + j\omega(\tau_1 + \tau_2) - \omega^2(\tau_1\tau_2)}. \tag{B.17}
\]

From (B.16) and (B.17), the following equations can be obtained:

\[
\tau_1 + \tau_2 = \frac{2\delta_0}{\omega_0^2}, \quad \tau_1\tau_2 = \frac{1}{\omega_0^2}. \tag{B.18}
\]

Solving these two equations simultaneously, the following relation will be obtained:

\[
\tau_1 = \frac{2\delta_0 - 1}{\omega_0^2}, \quad \tau_2 = \frac{1}{2\delta_0 - 1}. \tag{B.19}
\]
In addition, from (B.16) and (B.17), the following equations can be obtained:

\[ \varepsilon_{s1} \tau_2 + \varepsilon_{s2} \tau_1 = \frac{2 \delta_0}{\omega_0^2} \varepsilon_\infty, \]  
(B.20)

\[ \varepsilon_{s1} + \varepsilon_{s2} - \varepsilon_\infty = \varepsilon_s. \]  
(B.21)

Solving these two equations simultaneously, one obtains:

\[ \varepsilon_{s1} = \varepsilon_s + \varepsilon_\infty - \varepsilon_{s2} \]  
(B.22)

\[ \varepsilon_{s2} = \frac{2 \delta_0}{\omega_0^2} \varepsilon_\infty - \left( \varepsilon_s + \varepsilon_\infty \right) \tau_2 \quad \left( \tau_1 - \tau_2 \right). \]  
(B.23)

Using equations (B.19), (B.22), and (B.23), if the Lorentz model parameters are known the Debye model parameters can be easily calculated.
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