A Dissertation by

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Submitted to the Department of Aerospace Engineering and the faculty of the Graduate School of Wichita State University in partial fulfillment of the requirements for the degree of Doctor of Philosophy

May 2020
NUMERICAL SOLUTION OF MAXWELL’S EQUATIONS ON TRANSFORMED COORDINATES FOR NON-RECTANGULAR ELECTROMAGNETIC APPLICATIONS

The following faculty members have examined the final copy of this dissertation for form and content and recommend that it may be accepted in partial fulfillment of the requirement for the degree of Doctor of Philosophy, with a major in Aerospace Engineering.

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DEDICATION

To my parents, my wife, my brother, my daughter, my in-laws, and my dear friends
ACKNOWLEDGEMENT

It would not have been possible to finish my Ph.D. without the support and guidance that I have received from many people in different walks of my life. Everyone has played their roles in their own capacity to make sure that I fulfill my ambition. I would like to thank my adviser and mentor, Dr. Klaus A. Hoffmann for accepting me to work under his supervision in his research group. His support and encouragement along with the thoughtful and patient guidance and continuous feedback has been instrumental during these many years that I have spent at Wichita State University. He motivates and inspires confidence in his students to develop the ability within themselves to grow as an independent researcher. Without him, I would not have become a researcher that I am today. I extend my gratitude to my committee members, Dr. Charles Yang, Dr. Roy Myose, Dr. Nicholas Smith and Dr. Hamid Lankarani for their constructive feedback and suggestions.

I greatly appreciate my managers and supervisors at the University Libraries, especially Ms. Cynorra Jackson, Ms. Angela Beatie and Ms. Sara Baldwin, who have been very supportive to me and always appreciated my professional ethics. I gratefully acknowledge the funding received through the graduate assistantship positions at the Department of Aerospace Engineering and at the Wichita State University Libraries to support my education and research. I also thank the Graduate School and the Student Government Association for the travel grants to present my research at the 2020 AIAA SciTech Forum, Orlando FL.

I am thankful to Dr. Raymond Rumpf from University of Texas at El Paso for his YouTube video lessons on computational electromagnetics. His videos lectures were extremely easy and thorough to understand the fundamental concepts in electromagnetics for students like me who are coming from a Fluid Dynamics background and have no prior coursework in electromagnetics.

To my fellow graduate students, thank you for offering your advice, brainstorming new ideas with me and for all those endless discussions. To my friends, thank you for always being there with me, for supporting me during my rough times and celebrating with me during my achievements.
Of course, no words can express my indebtedness to my family in the success of my Ph.D. research. I thank my wife and parents for providing me enormous support, emotional as well as financial. Without their support, I would not have been able to pursue my dreams. Additionally, I acknowledge my wife’s help in the final formatting and proofreading of my dissertation report. I would like to say a heartfelt thank you to my parent wife, parents, in-laws and all the family members for staying patient with me and continuously encouraging me to follow my dreams. They inspire strength, motivation and positivity, no matter what challenge may come, which is also reflected in my approach.
ABSTRACT

The utilization of a fourth-order Modified Runge-Kutta (MRK) scheme on a transformed coordinate system for simulating electromagnetic applications that involve non-rectangular domains are presented. The model equations were obtained by writing the governing Maxwell’s equations in the curvilinear coordinate system. Therefore, by transforming the arbitrary-shaped structures to a uniform rectangular grid, numerical schemes and boundary conditions can be easily implemented. The time advancement of fields in the computational space is performed by leapfrogging the stages of explicit fourth-order MRK method. The one-dimensional traveling wave simulation results indicate that the leapfrogging of MRK stages reduces the dissipation errors associated with the MRK solution of wave propagation. The computer algorithms based on this technique have been developed for near-field and far-field scattering applications. Several classes of problems have been investigated in the dissertation. In the initial stage, accuracy of the scheme has been established by simulating two standing wave problems and comparing MRK results with the existing exact solution. The results for both cases are found to be in good agreement. In the second stage, the total field-scattered field (TF-SF) formulation is incorporated in the algorithm for the simulation of far-field scattering. The two-dimensional and three-dimensional computer codes developed based on this algorithm are used to perform qualitative analysis using planes waves and cylindrical waves as source. The diffraction and penetration of the waves are studied in the presence of dielectric or conducting materials having linear, non-dispersive, and homogeneous properties. The results are compared with the results from the benchmark method and indicates good agreement. The grid independence investigations revealed the dependence on the Courant number to obtain accurate results. Subsequently, scattering investigations are carried out on non-rectangular geometries with the clustered grid points. Finally, computer algorithm is modified to include the modeling of dispersive (frequency-dependent) material, and the absorption and reflection of electromagnetic waves by biological tissues is studied in one-dimension. The predicted reflection coefficient for two separate studies indicate excellent agreement with the exact reflection coefficients for a wideband frequency range.
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LIST OF SYMBOLS

\( A, B, C \) : Flux Jacobian matrices in \( x, y, z \) coordinate system, respectively

\( \bar{A}, \bar{B}, \bar{C} \) : Flux Jacobian matrices in \( \xi, \eta, \zeta \) coordinate system, respectively

\( \mathbf{B} = \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix} \) : Magnetic flux density vector

\( c \) : Speed of wave in a medium, (m/s)

\( c_0 \) : Speed of light or wave in free space, (m/s)

\( \mathbf{D} = \begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} \) : Electric flux density vector

\( \mathbf{E} = \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \) : Electric field intensity vector (V/m)

\( E_0 \) : Amplitude of source electric field

\( f \) : Frequency (Hz)

\( f_{\text{max}} \) : Maximum frequency (Hz)

\( f_0 \) : Peak frequency (Hz)

\( \mathbf{H} = \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix} \) : Magnetic field intensity vector

\( J \) : Jacobian of the transformation

\( \mathbf{J} = \begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} \) : Current density vector
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<tr>
<td>$J_e$</td>
<td>Eddy current density vector</td>
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<tr>
<td>$J_s$</td>
<td>Source current density vector</td>
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<td>$K_\sigma$</td>
<td>Non-dimensional number for conductivity in a medium, $K_\sigma = \frac{\sigma}{\sqrt{\mu_0/\varepsilon_0}}$</td>
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<td>$L$</td>
<td>Reference or characteristic length (m)</td>
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<tr>
<td>$n_0$</td>
<td>Integer time level for Gaussian pulse delay period</td>
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<tr>
<td>$t$</td>
<td>Time (s)</td>
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<td>$\Delta t$</td>
<td>Time step (s)</td>
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<td>$t_0$</td>
<td>Pulse delay time period ($= n_0 \Delta t$)</td>
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<td>$P = {P}_{s \times 1}$</td>
<td>Convective flux vector in $x$ direction, where $s = 2$ (in 1-D), 4 (in 2-D) or 6 (in 3-D)</td>
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<td>$\bar{P} = {\bar{P}}_{s \times 1}$</td>
<td>Convective flux vector in $\zeta$ direction, where $s = 2$ (in 1-D), 4 (in 2-D) or 6 (in 3-D)</td>
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<td>Unknown flux vector in physical coordinates, where $s = 2$ (in 1-D), 4 (in 2-D) or 6 (in 3-D)</td>
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<td>Unknown flux vector in computational coordinates, where $s = 2$ (in 1-D), 4 (in 2-D) or 6 (in 3-D)</td>
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<td>$x, y, z$</td>
<td>Cartesian coordinates (m)</td>
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LIST OF SYMBOLS (continued)

$\Delta x, \Delta y, \Delta z$ : Grid step in physical coordinates (m)

**Greek Symbols**

$\beta$ : Clustering density parameter

$\Gamma$ : Reflection coefficient

$\epsilon$ : Electrical permittivity of the medium

$\epsilon_{sp}$ : Static electrical permittivity of $p$-th pole

$\epsilon_\infty$ : Electric permittivity at infinite frequency

$\lambda_1A, \lambda_2A, \lambda_3A$ : Eigenvalues of flux Jacobian matrix $\bar{A}$

$\lambda_1B, \lambda_2B, \lambda_3B$ : Eigenvalues of flux Jacobian matrix $\bar{B}$

$\lambda_1C, \lambda_2C, \lambda_3C$ : Eigenvalues of flux Jacobian matrix $\bar{C}$

$\mu$ : Magnetic permeability of the medium

$\xi, \eta, \zeta$ : Computational coordinates

$\Delta \xi, \Delta \eta, \Delta \zeta$ : Grid step in physical coordinates

$\rho_v$ : Volume charge density

$\sigma$ : Electrical conductivity of the medium (S/m)

$\sigma_s$ : Static electric conductivity

$\tau$ : Time in computational coordinates (s), $\tau = t$

$\tau_p$ : Relaxation time constant of $p$-th pole (s)

$\tau_w$ : Gaussian pulse spread or width

$\Delta \tau$ : Time step in computational coordinates (s), $\Delta \tau = \Delta t$

$\chi_A, \chi_B, \chi_C$ : Eigenvector matrices of flux Jacobian matrices, $\bar{A}, \bar{B}, \bar{C}$ respectively

$\omega$ : Angular frequency ($2\pi f$)
### LIST OF SYMBOLS (continued)

#### Index Notations

- **i, j, k**: Integer indices notation for grid points on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **IM, JM, KM**: Integer indices notation for maximum grid points on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **f**: Integer index notation for frequency points
- **NM**: Integer index notation for maximum time level

#### Subscripts

- **0**: Reference quantities for non-dimensionalization of terms.
- **ia, ja, ka**: Integer indices for location of inlet TF-SF boundary on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **ib, jb, kb**: Integer indices for location of outlet TF-SF boundary on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **inc**: Incident or source field quantity
- **is, js, ks**: Integer indices for source location representation on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **p**: Integer index for poles in Debye equation, $p = 1, 2, \ldots, P$
- **ref**: Reflected fields
- **scat**: Scattered field quantity
- **sx, sy, sz**: Integer indices location for source specification on $\xi$, $\eta$, $\zeta$ coordinates, respectively
- **total**: Total field quantity

#### Superscripts

- *****: Non-dimensional quantity
- **n**: Integer time level
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<td>ABC</td>
<td>Absorbing Boundary Conditions</td>
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<tr>
<td>ADE</td>
<td>Auxiliary Differential Equation</td>
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<td>CFL</td>
<td>Courant-Friedrichs-Lewy</td>
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<td>EM</td>
<td>Electromagnetics</td>
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<td>FD</td>
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<td>FDTD</td>
<td>Finite Difference Time Domain</td>
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<td>FDFD</td>
<td>Frequency Dependent Finite Difference Frequency Domain</td>
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<td>FE</td>
<td>Finite Element</td>
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<td>FFT</td>
<td>Fast Fourier Transform</td>
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<td>FV</td>
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<td>MRI</td>
<td>Magnetic Resonance Imaging</td>
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<td>MRK</td>
<td>Modified Runge-Kutta</td>
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<td>PEC</td>
<td>Perfect Electrically Conducting</td>
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<td>PML</td>
<td>Perfectly Matched Layer</td>
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<td>RCS</td>
<td>Radar Cross Section</td>
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<td>SAR</td>
<td>Specific Absorption Ratio</td>
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<td>TE</td>
<td>Transverse Electric</td>
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<td>TEM</td>
<td>Transverse Electric and Magnetic</td>
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<td>TF-SF</td>
<td>Total Field-Scattered Field</td>
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CHAPTER 1

INTRODUCTION

1.1 Background

Electromagnetics (EM) is a branch of physics to study the interaction between electromagnetic waves, generated by the flow of time-varying electric and magnetic fields, and a radiating or scattering body depending on the application. The present-day technologies are heavily reliant on the application of electromagnetic fields. The range of applications involve everyday appliances to industrial and research applications. The examples of applications are communication devices such as cellular phones, hyperthermia treatment, non-destructive testing of big structures, satellite communication and navigation, radar cross-section, geophysics, and power transmission lines. The study of electromagnetic fields is, therefore, an important step in the designing process for such applications.

The theory of electromagnetism was first put forward by James C. Maxwell by unifying the Faraday’s law and Ampere’s law. The resulting set of equations are known as the Maxwell’s equations and are the governing equations for classical electromagnetic theory. In fact, the first theory that light is an electromagnetic wave was proposed by Maxwell using his classical equations.

Since the advent of supercomputers, the development of fast and accurate numerical methods to simulate physical phenomenon has grown exponentially. A fast and accurate numerical model helps a designer in analysis and prediction of performance of a design before even developing a prototype of it and hence minimize the time and cost in the product development. On the contrary, analytical methods to study physical phenomena are limited to simple geometries and the experimental testing on a prototype yields accurate results, however, it is a more time consuming and costly approach. All physical phenomena are governed by their corresponding governing equations specified by a combination of partial differential equations (PDE) such as the fluid flow is represented by the Navier-Stokes equations or the electromagnetic wave propagation is represented by the Maxwell’s equations. A branch of electromagnetics that utilizes computational approaches to investigate electromagnetic phenomena is known as computational...
electromagnetics (CEM). Generally, a computational model is required to obtain a numerical solution for a system of linear or non-linear mathematical equations, however, a computer processor cannot understand a PDE to solve them computationally, and therefore, the algebraic form of the PDEs are obtained. A numerical scheme utilizes the algebraic form of the governing equations in the discretized form, which is often called as the approximation of the exact equations, and it is solved on the grid points or within the small regions/volumes. The methods that solve the algebraic equations on the discretized grid points are known as the Finite-Difference (FD) approximation methods and similarly, when the equations are solved over small regions or volumes, the approach is known as the Finite Volume (FV) methods or the Finite Element (FE) methods.

An approximation of the PDE with a higher order of accuracy is required to obtain an accurate solution for the given application. The finite-difference approximations are by far the most robust and powerful tool to predict most physical phenomena. Consequently, a robust and efficient numerical method is required in order to perform investigations of electromagnetic waves in electrically large systems. The simplicity of the finite difference methods resides in the fact that the domain is discretized along the cartesian, cylindrical or spherical coordinate axes, separated by uniform small distances, known as grid step size and the solutions are obtained at those grid points. The finite difference methods yield accurate results for simple, rectangular structures where boundaries are aligned with the grid axes. However, for applications that involve curved boundaries, the finite-difference methods require approximation of curved structures which leads to inaccuracies or increased computational costs.

1.2 Objective

As discussed previously, an accurate representation of the boundaries on the finite-difference grid is required to obtain an accurate solution. However, due to the curvilinear nature of the object boundaries in most practical applications, an error is introduced in the solution when finite-difference methods are used. Such errors are commonly known as the staircasing errors that arise due to the approximations of the curved surfaces on a finite difference grid. The approximations of the curved surfaces results in the stair-stepped feature of the boundaries and hence, the inaccuracies that arise are referred to as staircasing errors.
As a result, the attractiveness of finite difference methods diminishes. Therefore, a numerical approach is required that can retain the benefits of the finite difference methods and predict accurate results for applications that involve non-rectangular geometries. To address this challenge, we propose to use the coordinate transformation of the grid points on the physical non-rectangular coordinates to a uniform rectangular curvilinear coordinate system and utilize the explicit, fourth-order accurate Modified Runge-Kutta scheme for time advancement of the solution. This approach is widely popular for fluid dynamics applications. A simple modification will be introduced here in the existing Modified Runge-Kutta scheme by leapfrogging the stages of the Runge-Kutta method. To investigate the efficiency of the given formulation for electromagnetic application, we will simulate several classes of problem using the developed computer solver. The studies cases can be segregated into two categories: far-field applications and the near-field applications.

The step-by-step plan utilized in this research to validate the proposed hypothesis is specified as under:

❖ Obtain the conservative form of the governing time-domain Maxwell’s equations in 2D and 3D curvilinear coordinates and subsequently, discretize the model equation using explicit, fourth-order Modified Runge-Kutta scheme;

❖ Develop computer codes to solve the discretized equations;

❖ Obtain results for two standing-wave problems and investigate the accuracy of the numerical method by comparing with the existing analytical solutions;

❖ Implement the Total Field-Scattered Field (TF-SF) formulation in the curvilinear coordinates and obtain solutions and perform qualitative analysis for the following applications.
  ➢ Scattering from a lossless dielectric square cylinder on uniform and clustered grid system,
  ➢ Scattering from a lossy dielectric square cylinder on uniform grid system,
  ➢ Scattering from a lossless circular cylinder on clustered grid system,
  ➢ Scattering from a conducting airfoil on clustered grid system, and
  ➢ Scattering from a lossless dielectric cube on clustered grid system.
Implement the dispersive modeling method in the developed codes to investigate absorption of electromagnetic waves by human tissues and validate numerical results with analytical results.

The objectives that will be accomplished by the proposed implementation are as under:

- The alignment of the curved boundaries with the grid lines by the implementation of coordinate transformation technique will result in the removal of errors that occurs due to the staircase approximation on the finite difference grid. Additionally, clustering of grid points in the regions where required can be included efficiently.

- The following benefits associated with the finite-difference methods are retained: simplicity, robustness, and intuitive nature.

- The application of the explicit Modified-Runge Kutta method will provide a better stability criteria and fast convergence, that leads to improved efficiency over the benchmark method.

- The accuracy order of centered differencing for spatial derivatives is preserved by transforming non-uniform, clustered grid to equally spaced uniform grid system.

- Simple structure of developed computer codes due to the finite-difference algorithm.

1.3 Dissertation Outline

This dissertation report includes seven Chapters with an Appendix and a Reference section. The literature survey related to the numerical methods in computational electromagnetics, and the far-field scattering with total field-scattered field formulation is presented in Chapter two. Chapter three covers the introduction to Electromagnetism, description of the governing Maxwell’s equations, and its formulation in the derivative form that will be used in the finite difference approximation. The assumptions, and some fundamental ‘need to know’ theory have also been included.

Subsequently in Chapter four, a detailed step-by-step numerical modeling is presented to derive the PDEs in the required finite-difference form for both two-dimensional and three-dimensional examples. The finite difference equations derived in this Chapter are used to develop several computer codes. A post-processing method has also been included to transform the time-domain fields to frequency-dependent data,
if desired. In order to investigate the far-field scattering examples, the incorporation of the total field-scattered field approach with the numerical model is presented in Chapter five.

The validation of the numerical approach using standing wave examples and subsequently, the far-field scattering investigations and analysis results are presented in Chapter six. The extension and validity of the proposed approach for bioelectromagnetic applications is demonstrated in Chapter seven.

Subsequently, the conclusion of the research is presented in Chapter eight along with limitations and future scope of this work. Some mathematical derivations such as the coordinate transformation technique, derivation of eigenvalues and eigenvectors are presented in the Appendices in the last.
CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

The advancement of computational systems and processors has provided the opportunity to develop numerical schemes that can accurately predict real world phenomena involved in electromagnetism, fluid dynamics, etc. Simulating electromagnetic wave scattering and radiation phenomenon is the subject of vast interest in computational sciences. The last several decades have seen the emergence of the new numerical methods or improvements over the existing numerical methods. Accordingly, the existing literature covers a wide range of such topics, however, to stay on track with the theme of this research, this review will focus on the literature relevant to the four topics. These topics are the historical background of finite difference methods in computational electromagnetics, the application of finite difference methods to two major subject, namely, far-field scattering and bioelectromagnetics, the various challenges associated with the finite difference methods and the improvements made to increase accuracy and efficiency of the finite difference method. The chapter is divided into three sections and each section covers the literature that focuses on the aforementioned topics.

2.2 The Finite Difference Methods

Initially, during 1960s the frequency-domain numerical schemes were more popular in electromagnetism. Due to the limitations of the frequency domain approach, the time domain form of the Maxwell’s curl equations began gaining popularity due to its simplicity and straightforward application. The numerical scheme to solve scattering problem in electromagnetism based on the time-domain Maxwell’s equations was first proposed by Yee [1] in 1966. Maxwell’s equations were replaced by finite difference equations in space and time. Yee’s numerical scheme employs the use of primary and secondary grid, spaced at half a cell distance in space and time. The components of electric fields were computed on primary grid points and the magnetic field components were computed on secondary grid points. This grid scheme has since been used in most of the research applications till date and it is famously known as Yee
grid among computational electromagnetism community. A similar approach used in computational fluid dynamics is known as staggered grid scheme. For electrically large systems, however, Yee’s [1] method is highly dispersive and therefore, not efficient. The introduction of the Yee scheme laid down the foundation for finite difference time domain (FDTD) schemes and the advancement of the finite difference schemes is continually the major topic of research. Engquist and Majda [2] proposed the method of absorbing boundary conditions (ABC) for limiting the size of the computational domain. The open and unbounded problems can be solved using absorbing boundary conditions and hence reducing the cost of computational memory requirements. These boundary conditions used with Yee’s numerical scheme increased the stability and accuracy of the solutions by reducing non-physical reflections of numerical waves from the boundaries. Mur [3] proposed an advanced version of the absorbing boundary conditions presented by Engquist and Majda [2]. It was demonstrated by Mur [3] that the proposed absorbing boundary conditions are second-order accurate and has better stability. The term finite difference time domain was first coined by Taflove [4] in 1980. The significant discovery to handle the artificial reflection from the boundaries was made by Berenger [5]. It is known as Perfectly Matched Layer (PML) and is a special type of absorbing boundary condition for solving two-dimensional problems. Katz et al. [6] extended application of PML to three-dimensional problems. It was demonstrated by Berenger [5] that the PML boundary conditions are highly effective in obtaining accurate numerical solution and are superior to most other ABCs. The various classes of ABCs as described in Ref. [7] are: Differential-Equation based ABCs, Other Nonmaterial ABCs, and Material ABCs. The finite difference solutions for generalized orthogonal coordinates has been discussed in Ref. [8] and for non-orthogonal coordinates in Ref. [9]. It has been demonstrated that if non-orthogonal coordinates are followed, Gauss’s law is violated which gives rise to errors [10]. Kim and Hoefer [11] presented a model for conservation of energy when using the finite difference time domain scheme and has suggested to exercise caution when choosing a particular finite-difference approximation for solving Maxwell’s equations because some of the schemes such as Lax-Wendroff scheme do not have non-dissipative property.
The numerical stability criteria for the Yee scheme was first presented by Taflove and Brodwin [12]. The stability criteria relate the physical time step to the spatial step size. Yee’s numerical scheme was highly dispersive in nature, that means as the numerical scheme moves further in time, the solution becomes inaccurate due to the growth of discretization errors. Since the introduction of the Yee’s scheme, several related numerical approximation methods have been investigated and published with the objective of reducing the dispersion errors. Usage of very fine mesh has also been proposed to reduce dispersion errors. Computational memory requirements and computation time increases exponentially by using fine mesh for large structures. Hence, it is not an efficient method to control dispersion. Another approach to control dispersion is to use higher-order differencing. Fang [13] proposed two higher-order FDTD approximation schemes; (2,4) scheme which is second-order accurate in time, fourth-order accurate in space and (4,4) scheme which is fourth-order accurate in both space and time. Deveze et al. [14] developed and demonstrated the application of absorbing boundary condition for the (2,4) scheme. Young et al. [15] developed a (4,4) scheme using four-stage Runge-Kutta scheme with an implicit, compact operator for space derivatives. Yefet and Petropoulos [16], Xie et al. [17], Fathy et al. [18] presented (2,4) and (4,4) schemes that is based on Fang’s [13] method but with slight modifications in their approach. Hesthaven and Warburton [19] developed unstructured, higher-order numerical scheme, and presented its validation and parallel performance. Shlager et al. [20] investigated the dispersion errors in several higher-order numerical schemes and presented their comparison. Liu [21] demonstrated that central differencing schemes are more precise and efficient as compared to forward or backward differencing schemes. Due to the enlarged grid stencil in higher order schemes, these schemes suffered a major disadvantage. Additionally, higher order schemes require special treatment at the material interfaces and therefore, are not an efficient approach in computational electromagnetics.

The extension of the computational fluid dynamics based methods to applications in CEM by casting the hyperbolic governing equations to conservative form was pioneered by Shankar et al. [22]. They developed a finite volume time domain (FVTD) method using Lax-Wendroff upwind scheme. Arbitrary shaped structures were addressed by coordinate transformation. The numerical results were presented and
validated for two dimensional cases. Shang [23,24] developed an FVTD scheme based on Steger and Warming flux vector splitting which was later validated by Sherer and Blake [25]. Sherer and Blake [25] presented the comparison of radar cross section (RCS) results of benchmark test cases specified by Electromagnetics Code Consortium with analytical and experimental results. The second-order accuracy in time was achieved by employing two-stage Runge-Kutta scheme for temporal integration. Multi-block grid approach was used for meshing. Parallel performance evaluation of a CEM solver developed by Blake [26] during their Ph.D. dissertation was carried out by Camberos and White [27]. Another study that utilized the Steger and Warming flux vector splitting scheme was presented by Chiu et al. [28]. They developed their numerical formulation based on fifth-order accurate, dual-compact scheme on non-staggered grid to reduce dissipation and dispersion errors. The results were found to be in good agreement with the semi-analytical results for the classical Mie scattering problem. Liao et al. [29] investigated a technique used in fluid dynamics of transforming conformal grid into cartesian coordinates for two-dimensional domain. The numerical scheme developed using such conformal grid technique was investigated in conjunction with the first-order ABC. An assessment of the advancement in numerical electromagnetics till year 1999 is presented in [30,31] and the review of the CFD techniques extended to CEM and computational magneto-aerodynamics is given in Ref. [32]. Various challenges encountered in CEM simulations for aerospace applications were discussed. Special emphasis in the review papers [30-32] was given to developments pertaining to the subject of magneto-aerodynamics, identified as a promising interdisciplinary field of research. Camberos [33] presented development of the EM solver by using the capabilities of the CFD based finite-volume code to solve time domain Maxwell’s equations and analyzed its parallel performance. The investigations pertaining to the development of unconditionally stable Alternating Direction Implicit scheme for electromagnetic applications are presented in Ref. [34-37].

The discretization of the domain is another important topic of research in numerical modelling of Maxwell’s equation. The exact representation of grid points of the arbitrary shaped structures has always been challenging. The accuracy of the numerical scheme also depends on the specification of grid points of complex shaped materials and capturing fine geometrical features. “Staircasing” is the most popular
technique for approximating surfaces that are not parallel to grid axes. The errors associated with the staircasing were investigated by Cangellaris and Wright [38] and Holland [39]. The difficulties in implementing staircase approximation arise when the structure to be modeled includes small geometric features such as a narrow slot. Schneider and Shlager [40] also investigated errors due to staircasing using a different test case and further laid down guidelines to minimize staircasing errors. Merewether [41] and Holland [42] specified the numerical approximation on orthogonal grid instead of Cartesian grid. The conformal grid technique to represent curved boundaries accurately were presented in two separate works by Jurgens et al. [43] and Yee et al. [44] and a comparison of these two methods is presented by Steeds et al. [45]. The other commonly used technique for non-rectangular applications is the averaging of material properties in cell area near the interface boundaries as described in [46-48]. This method is termed as the cell average method. The line average method was proposed by Liu and Chang [49] and they demonstrated that their technique is slightly accurate than cell average method and it requires less computational power. Another notable work to overcome the staircasing errors was presented by Dridi et al. [50]. This second-order accurate method was investigated for two-dimensional applications and it was demonstrated that it reduces the requirement of minimum number of points per wavelength as compared to classical Yee [1] FDTD method. Simulation using non-uniform grid system is, yet another approach used with finite difference approximations for enhancing accuracy and faster convergence. Clustered grid system was first used in electromagnetic applications by Kunz and Lee [51] to approximate the response of an aircraft to the electromagnetic pulse. Clustering is performed in the regions where large gradients exist within the domain. Using this technique, grid points can be minimized by using continuously varying grid size in the entire domain. In the clustered grid approach, the spatial step size varies in the entire domain. The dispersion errors analysis for clustered grid system was presented by Svigelj and Mittra [52]. Another discretization technique that was popular in the past investigations was subgridding. The investigations using their own subgrid approach have been presented by Yee [53], Kasher and Yee [54] to name a few. In this system, a combination of fine and coarse grid system is used within the solution domain. The accuracy of subgrids depends on the method used for interpolation of the grid points within the domain. The limitations of
subgridding have been investigated in several publications. Conformal grid technique is another topic in grid discretization that received some attraction from researchers.

To achieve better stability and higher order accuracy in temporal discretization, the Runge-Kutta methods are the ideal candidate. Several numerical formulations involving Runge-Kutta methods have been investigated in the past. A method based on five and six stage low-storage Runge-Kutta scheme coupled with a seven point spatial operator was developed by Jurgens and Zingg [55] and Zingg et al.[56,57]. This higher order Runge-Kutta method requires only two storage space of dependent variables per time step of computations. It was demonstrated through several examples that the simulation accuracy is maintained after wave has travelled large distance of the order of hundreds of wavelength. Cao et al. [58] presented the Runge-Kutta multiresolution time domain methods for obtaining efficient solution of electromagnetic waves. Zhu et al. [59] combined the strong stability preserving Runge-Kutta algorithm with the higher-order finite difference methods for fast convergence and low dispersion. A drawback associated with the Runge-Kutta method is the dissipation of the wave solution. This has been reported in [15] and a method to reduce dissipation of the acoustic waves by deriving the modified coefficients in the Runge-Kutta method are presented by Hu et al. [60]. Similarly, Zingg et. al. [56,57] have determined coefficients for the six stage Runge-Kutta that would reduce the phase and amplitude errors. However, using the standard coefficients retain the maximum level of order defined for a p-stage Runge-Kutta scheme. According to Young et al. [15], their formulation that involves compact Runge-Kutta method is 7.6 times more efficient than Yee’s scheme, however, low-storage Runge-Kutta requires more time step per time level and therefore, their efficiency may be less than predicted. Sheu et al. [61] presented a formulation that utilizes non-staggering approach for three-dimensional Maxwell’s equations. A second-order Runge-Kutta was used for temporal approximations with fourth-order central approximation for spatial derivatives. The explicit Runge-Kutta was specified in a partitioned form which solves for the magnetic field variables twice within the same time level, whereas, the electric field is solved once within that time level. This hypothesis was based on the fact presented that the Maxwell’s equations corresponds to the separable Hamiltonian model and can be solved accurately using partitioned two-stage R-K scheme.
Sanakaran’s [62] paper reviews the tools required in the accurate modeling for electromagnetic simulations. Additionally, it highlights the state-of-the-art developments in computational electromagnetics including other popular methods such as Finite element methods, Discontinuous Galerkin, Finite Volume methods and less popular but recently developed methods such as Algebraic Topological Method.

2.3 The Total Field – Scattered Field Technique

In addition to the numerical approximation methods of the partial differential equations, the accurate modeling of a physical phenomenon requires attention to accurate description of sources or the material parameters. One such physical phenomenon that requires special modeling technique is the plane wave scattering where the source and the receiver are separated by a large distance and hence the representation of such large distance within a computational grid is unrealistic. To address this challenge, the pure scattered field technique [41] was reported several decades ago. The limitations associated with the pure scattered field formulation has led to the development of the Total Field – Scattered Field method. The TF-SF formulation is a method of plane wave source introduction into the simulation domain. The TF-SF method is also known as the Huygens surface method and its formulation and implementation has been thoroughly investigated in the literature. This technique was first introduced in 1980 by Merewether et al. [63] and has been used extensively to simulate far-field applications. To implement the TF-SF technique generally, the simulation domain is divided into two regions by an imaginary boundary, wherein the region enclosed by the imaginary boundary is known as the total field region and the boundary is defined in such a manner that the scatterer is completely immersed within the total field region [63,64]. The area enclosed between the outer boundaries and the imaginary boundary is the scattered field region. In the absence of scatterer, the field values within the scattered field region will be zero. This technique is highly popular due to its robustness, and it is implemented in most softwares that are based on the FDTD approach. During the initial stages of the TF-SF development, a general approach was to define the TF-SF boundary within the free space region. However, with the research advancements, several researchers proposed the implementation of TF-SF in media other than free space such as within the ABCs and the PMLs. Taflove and Umashankar [64] used the total field-scattered field formulation to investigate scattering from arbitrary
shaped metal and transformed the simulated near scattered field data to far field for radar cross sections applications. Fusco [8] proposed an FDTD algorithm with TF-SF formulation in curvilinear coordinates to solve problems that involve complex shaped scatterers. To obtain the incident field at the imaginary Huygens surface, Taflove [65] presented a method that interpolates the incident field values specified on a separate one-dimensional grid to the field values on the Huygens surface. This separate grid is used for the propagation of the incident field and it is assumed to be inclined at any angle with respect to the finite difference grid. The propagation of the incident field on this separate grid is either obtained numerically or analytically.

A novel approach to specify the TF-SF within the PML region was presented by Anantha and Taflove [66] and they called it as generalized total-field/scattered-field (G-TF/SF) formulation. The application of this technique enables the modeling of the scatterer within the PML region and hence, it results in the small grid size required for simulation. Their validation results demonstrated excellent agreement with the analytical data.

All numerical formulations are prone to errors, and the TF-SF formulation is no stranger to such numerical errors. The artificial leakage of waves into the scattered field region is a matter of concern with TF-SF formulation. It is called artificial leakage because, ideally, in the absence of a scatterer or prior to wave impingement on the scatterer, the field values at all grid points within the scattered field region must be zero. This artificial leakage is due to the dispersion of numerical waves on the finite difference grid. The other source of errors in the TF-SF formulation is due to the phase mismatch between the source fields and total fields due to the inclined alignment of the source grid axis with the total field axis [67]. A simple method to reduce the leakage is by adopting a grid system for the source field having properties such as the spatial step, and time step similar to the properties of the grid system for the total fields. The 1-D source grid should be aligned parallel with one of the axis on the total-field grid. However, this may not be an ideal approach to model incident waves impinging on the scatterers at an angle. Several novel methods of TF-SF formulation have been presented to reduce the associated leakage errors. Schneider [67] and later, Schneider and Abdijalilov [68] presented approaches to compute the source fields at the required location without
performing the finite difference approximations and claimed that such analytical approach can minimize the TF-SF leakage errors. These approaches were specifically created for the Yee-FDTD approximation, however according to authors, the formulations for any other FDTD-based approximation methods can be derived by following a similar procedure. The other techniques to accurately model the TF-SF source are presented in [69].

2.4 Bioelectromagnetic Applications

Ever growing man-made technologies such as wireless communication devices, microwave ovens, power transmission and distribution lines are the continuous sources of electromagnetic energy in our ecosystem. This has posed serious concern among the public members about its negative impact on humans, which, subsequently, has led to the development of standard guidelines and imposition of regulations by concerned authorities. The devices emitting EM waves must be designed to operate under the regulatory standards. On the contrary, since the size requirement of mobile devices has continuously decreased over the years which requires the efficient designing of antennas, the early researches [70,71] were focused on the effect of humans on the performance of the antenna to gain knowledge about efficiency of the mobile communication devices. Some of the antenna performance studies are presented in Ref. [72-75].

Additionally, hyperthermia applications for cancer treatment as well as diagnostic imaging methods which utilizes the EM wave technology for the benefit of society cannot be overlooked. Therapeutic applications require the development of accurate antenna system that would radiate the waves within specified frequency limit for human absorption and therefore, requires careful designing of arrays of antenna that would function in a controlled manner and emit the energy for absorption by the human tissues. The absorbed energy gets converted into heat by lossy tissue material and subsequently kill or damage tumors cells [7]. The investigations pertaining to the temperature distribution within the biological tissues due to electromagnetic heat absorption are the quantity of interest for such applications [76]. A recent investigation was performed by Kodera and Hirata [77] in which they presented the comparison of thermal effect between the human and rat model. Such studies can be used as the base for extrapolation of results from animal studies on humans. Imaging methods such as Magnetic Resonance Imaging (MRI), which
utilizes the absorption property of dispersive materials to obtain relevant information, is useful in applications such as medical, security, non-destructive testing, etc. Such applications are generally known as diagnostic imaging. The applications discussed in the above paragraphs that involves EM wave interaction with the biological tissues are classified in the category of near-field applications where the source is located in the vicinity of the dispersive material.

Initially during the early stages of bioelectromagnetic studies, the investigations pertaining to the effect of electromagnetic waves on biological material were limited to analytical model. The introduction of computers, and the well-known limitations associated with the analytical model to provide detailed absorption data has led to the development of the numerical methods for simulation of EM wave absorption. The initial computational methods were based on the method of moments to investigate absorption rates and subsequently, the advancement in technology has served as the steppingstone for the development of robust finite-difference schemes and anatomically based human models with grid points on scale of millions for computational bioelectromagnetic applications [7].

Since the advent of mobile communication technology, finite-difference time-domain method, due to its robustness, has remained the most appealing method for researchers to investigate various bioelectromagnetic phenomenon. Several initial studies that utilizes the FDTD method to model EM wave exposure are reported in Ref. [78-82] for dosimetry, and Ref [83-85] for hyperthermia applications.

Based on the frequency ranges, the quantities of interest desired from simulation results differ. At very low frequencies (<100 kHz), the energy absorption is negligible and therefore induced currents are the quantity of interest. Such low frequency applications mean that the wavelength is too large and hence it poses the limitation to the accurate application of numerical methods. The human interaction with the EM waves generally falls in the range of Ultra-High Frequency spectrum (0.3 GHz – 3 GHz). The numerical simulation is generally carried out within this frequency band to obtain the specific absorption rate (SAR) which is calculated as the mass normalized rates of energy absorption by the biological material or tissues and is specified in W/kg.
Generally, the biological materials possess dispersive properties which means that their material parameters such as permittivity and/or permeability are dependent on frequency. Additionally, it is desired to obtain the response of the biological tissues at various frequencies to gain understanding about the useful frequency ranges for hyperthermia applications or learning about frequencies harmful or dangerous to human body. Some initial studies cited earlier in this section have demonstrated effective application of FDTD methods for computing SAR distributions within the human tissues. However, the FDTD methods are not adequate to address frequency dependent properties of the material. Moreover, FDTD methods are not suitable to obtain information about biological interaction at wideband frequencies of interest. The results, thus, obtained using FDTD methods with ultra-wide bandwidth may be highly inaccurate [86]. Such a limitation was overcome by the frequency-dependent finite-difference time domain method (FD-FDTD) or (FD)²TD which was introduced in early 1990 by Luebbers et al. [87]. The implementation of this method to biological applications was subsequently presented by Sullivan [88] and Gandhi et al. [89]. Within FD-FDTD approach, the constitutive relations are restored and defined as a function of frequency. Several methods have been developed to solve the frequency dependent equation on a discretized grid and to address the dispersive property of the material. One such approach for field computation within the dispersive media uses the convolution of the frequency domain equation to time domain by the time domain electric field using Fourier theorem. This method limits the additional storage requirement as the time history of the field values are not required to be stored by the use of recursive updation of electric fields. In our numerical modeling, this approach is implemented, and it is presented in detail in Section 7.2. This method has been successfully implemented in Ref. [86,87,90-92]. In the second approach, an Auxiliary Differential Equation (ADE) is introduced that relates electric flux density, \( \mathbf{D} \) with electric field intensity, \( \mathbf{E} \) in time-domain and discretized and solved along with the other two governing equations. This method has been successfully implemented in Ref. [85,88,93]. A third technique that uses the Z-transform method from theory of complex algebra to solve for the dispersive relation was proposed by Sullivan [94]. A comparison of accuracy of various approaches used in computing E- fields was presented in a recent study by Lin et al. [95]. It was concluded that the modified Z transform method has comparatively higher accuracy for modeling real term
in the complex permittivity, whereas, the bilinear transform method is accurate for imaginary term of permittivity. Additionally, the dispersion errors and the stability analysis of each method were analyzed in the presented study [95].

The frequency dependence of the dispersive material is governed by the definition of the electrical permittivity and/or magnetic permeability within the material. The complex electrical permittivity in biological tissues is generally considered to be the function of frequency, whereas the permeability is assumed to be non-dispersive. Hence, the complex electric permittivity within the biological tissues is required to be defined as a function of frequency. Several models have been proposed to define the dispersive property of the human tissues. For a long time, a single-pole or single-order Debye equation has been used to describe the complex permittivity. However, it was found by Sullivan [88] that the single-order Debye relaxation model can predict results accurately only within the narrow frequency ranges. The reason for such inaccuracies is the inability of the single pole and single relaxation parameter susceptibility function to accurately model the frequency dependence of the tissues at high frequencies. More accurate results may be obtained by using higher-order or multi-pole Debye model. Furse et al. [86] and, later, Gandhi and Furse [96] used the Debye equation with two relaxation constants in their studies for modeling complex permittivity of biological materials. The optimum values of the parameters in the Debye equation were obtained by non-linear least square method to fit with the experimental data for fat and muscles.

Later, it was demonstrated by Gabriel et al. [97] using experimental investigations that the second-order Debye model is not very accurate for describing frequency dependence of the human tissues over wideband frequency range. A Cole-Cole model is suggested to be a more accurate representation that describes human tissues over wideband spectrum. The application of Cole-Cole model in the FD-FDTD method was demonstrated by Schuster et al. [98] and Guo et al. [99]. Guo et al. [99] suggested that the Cole-Cole model has not been widely accepted because of the difficulty in the implementation with the finite difference approximation. They proposed a new formulation using Cole-Cole model and the Z-transform method to solve for E-fields from D-fields. For frequency of interest below 1 MHz, Cole-Cole interpolation is accurate [100]. Wuren et al. [101] formulated the two-pole Debye model using Gabriel’s
Cole-Cole experimental data to simulate EM absorption on whole body. Weedon and Rappaport [102] proposed a model instead of the Debye, Lorentz or Drude model to describe the complex permittivity of the medium. The resultant dispersive equation is a general equation which can be reduced to one of the algorithms as special cases. Mustafa et al. [103] formulated the fourth-order Debye equation for complex permittivity of human head tissues and demonstrated that the Debye model is more accurate than the multi-pole Cole-Cole method.

Several other finite difference schemes have been implemented for simulating dispersive media. Rouf et al. [104] presented the application of Crank-Nicolson implicit scheme for the frequency dependent media and validated that the method is unconditionally stable at larger time steps which is an intrinsic property of the Crank-Nicolson method. They used the ADE to solve the frequency dependent term specified by single pole Debye formulation. The implementation of alternating direction implicit scheme to simulate dispersive material was presented by Pereda et al. [105]. Chakarothai et al. [106] demonstrated a new approach for determining convergence of FDTD method in dosimetry applications. They presented results of a homogeneous sphere at single frequency with dielectric properties similar to that of a muscle. It was investigated that the convergence is dependent on permittivity, conductivity, and time step.

Another challenge in bioelectromagnetic simulation using the finite difference schemes is the modeling of human geometry. During the 1970s human spheroidal models were used, whereas, the anatomical cross sections in 1980s [107] were developed. The significant advancement in human model specification was the development of MRI based human body model in 1990s presented in Ref [108,109] to cite a few. The anatomical models of human are created by MRI in the form of fine blocks or voxels that can be represented on the finite difference grid. The process of obtaining anatomical data of human body using the MRI is highly specialized. Further details on human model using MRI are presented in Ref [77,97] for further reading.

Christ et al. [110] used a generic body model with three layer tissue. Water content greatly impacts the dielectric properties of the body tissue. Low water content tissues have low dielectric permittivity and conductivity and hence, results in increased wavelength of the absorbed EM wave within such tissues. To
demonstrate the reflections that would occur due to high water layer and low water layer, their body is modeled by placing a tissue layer with low water content in between two high water content tissue layer. The effect of the tissue thickness on the absorption and reflection cannot be accurately investigated using the existing anatomical computer models.

Till date, there are very few anatomical models available to describe the human model on FDTD grid. Since, the MRI-based human models requires specific skills, most studies utilize generic shapes such as sphere to represent head model to conduct their investigations. Based on the FDTD investigations [7], it was presented that SAR distribution is highly dependent on the shape of the model used in the study. Therefore, it is required to accurately represent the shape of the material on the discretized grid. The staircase approximation of the curved surfaces may lead to large errors because the absorption in human tissues is highly localized and hence significant quantity of fields may be present within a small region near the curved surfaces. A method is proposed by Laakso and Hirata [111] to reduce the staircasing errors.

The non-uniform grid approach for bioelectromagnetic applications are presented by Gao and Gandhi [112], Wiart et al. [113] and Tinniswood et al. [114]. The non-uniform grid implementation is beneficial for resolving regions in the vicinity of dispersive boundaries, such as in the modeling of hyperthermia application, an accurate modeling of shape and size of the tumor using non-uniform grid can be obtained. The expanding grid algorithm for bioelectromagnetic applications was first presented by Gao and Gandhi [112].

In conclusion, the methods based on the FDTD technique have been thoroughly investigated in the literature, of which the Yee-FDTD method remains the benchmark in the computational electromagnetics. Due to its robustness, the Yee-FDTD method is utilized in several commercial and non-commercial packages. Based on the literature, the FDTD methods have been applied to investigate various practical applications such as radar cross section analysis and absorption of EM waves by biological tissues and several approaches to increase the accuracy of the methods have been proposed. However, the demonstration of such methods to applications involving complex geometries is very limited. It is evident that the accurate representation of the curved boundaries yields accurate results. Additionally, the clustering
of grid is highly important in applications such as simulation of absorption by biological tissues where the penetration of EM waves into the tissue is minimal and therefore, finely resolved grid points are required near the material interfaces to capture essential data.

Considering the advantages of the coordinate transformation technique to accurately represent curved surfaces, very little attention has been paid for addressing non-rectangular applications using such technique. The past studies have been limited to canonical two dimensional geometries. Moreover, the simplicity with which the grid transformation can be used for incorporation of smoothly distributed clustered grid has been completely overlooked. In our knowledge, very little information is available regarding the applicability of the coordinate transformation technique to non-conventional shapes and three-dimensional studies. Therefore, the defined objective of this research is to utilize the Modified Runge-Kutta scheme with transformed coordinates in order to address applications with non-rectangular domain and having an option for clustering of the grid in regions where required.
Before we proceed further to the numerical algorithms, it is ideal to discuss briefly about the Maxwell’s equations, material characteristics and simulation set-up to develop understanding of the relevant topics. With this in mind, the subjects considered in this chapter are restricted only to the topics that are relevant to the simulation and investigation applications presented in this report.

3.1 Introduction to Electromagnetism

The fundamental concept of electromagnetic theory can be attributed to electric charges at rest and in motion. The static electric charges produce electrostatic fields while the charges moving with uniform velocity produces magneto-static fields. Additionally, time varying fields are produced due to charges with acceleration or time varying currents [115].

The theory of electromagnetism was first presented by James C. Maxwell and the set of equations known as Maxwell’s equations collectively are the governing equations in electromagnetism. Scientists have presented their independent theories related to electricity and magnetism which, subsequently, has led to the formation of Maxwell’s equations in electromagnetism. A brief discussion on the Gauss’ law, Ampere’s law and the Maxwell’s equations are presented in Sections 3.1.1 to 3.1.3.

3.1.1 Electrostatic Field

Electrostatic fields are governed by the Gauss’ law (divergence) and the law of conservation of electrostatic field, represented in integral form in equations (3.1) and (3.2) respectively.

\[ \oint D \cdot dS = \int \rho_e \, dv \]  \hspace{1cm} (3.1)

\[ \oint E \cdot d\ell = 0 \]  \hspace{1cm} (3.2)
Application of Gauss’ theorem and Stokes’ theorem to equations (3.1) and (3.2) results in the differential form of the equations

\[ \nabla \cdot D = \rho_v \tag{3.3} \]

\[ \nabla \times E = 0 \tag{3.4} \]

Electric flux density, \( D \) and electric field intensity, \( E \) are related through electrical permittivity as shown in equation (3.5).

\[ D = \varepsilon E \tag{3.5} \]

### 3.1.2 Magneto-static Fields

These fields are governed by the Ampere’s law (related to Biot-Savart law) and the Gauss’ law for magnetostatics, represented in integral form in equations (3.6) and (3.7), respectively.

\[ \oint L \cdot dI = \oint_S J \cdot dS \tag{3.6} \]

\[ \oint B \cdot dS = 0 \tag{3.7} \]

The differential form of the equations (3.6) and (3.7) can be easily obtained by the application of Gauss’ theorem and Stokes’ theorem.

\[ \nabla \times H = J \tag{3.8} \]

\[ \nabla \cdot B = 0 \tag{3.9} \]

Magnetic flux density, \( B \) and the magnetic field intensity, \( H \) are related through magnetic permeability, \( \mu \) of the medium as
Electric current density, \( \mathbf{J} \) and electric field intensity, \( \mathbf{E} \) are related through electric conductivity, \( \sigma \) as

\[
\mathbf{J} = \sigma \mathbf{E}
\]  
(3.11)

### 3.1.3 Time-Varying Fields

The time-varying fields are produced by accelerated charges and it results in the simultaneous flow of electric and magnetic fields. It is governed by first-order, linear, hyperbolic differential equations commonly known as Maxwell’s equations. They are represented in general form presented in equations (3.12) through (3.15). As observed, Maxwell’s equations consist of two divergence equations and two curl equations.

\[
\nabla \cdot \mathbf{D} = \rho_v
\]  
(3.12)

\[
\nabla \cdot \mathbf{B} = 0
\]  
(3.13)

\[
\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}
\]  
(3.14)

\[
\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}
\]  
(3.15)
The first term on the right-hand side of equation (3.15) represents the summation of source current density and eddy current density terms and the last term represents displacement current density. Hence, equation (3.15) can be re-written as equation (3.16) where $J_s$ is the source current density and $J_e$ is the eddy current density, also known as eddy current loss.

$$\nabla \times \mathbf{H} = J_s + J_e + \frac{\partial \mathbf{D}}{\partial t}$$ (3.16)

Equations (3.5), (3.10), and (3.11) are repeated here and they are the three medium dependent relations which are known as constitutive equations for the medium.

$$\mathbf{D} = \varepsilon \mathbf{E}$$ (3.17)

$$\mathbf{B} = \mu \mathbf{H}$$ (3.18)

$$J_e = \sigma \mathbf{E}$$ (3.19)

Equations (3.12) through (3.15) and equations (3.17) - (3.19) forms the seven foundational equations in the field of electromagnetic theory.

### 3.1.4 Assumptions

The following assumptions have been used in the numerical formulation of the governing equations. The explanation of assumptions regarding the material properties is presented in Section 3.3.4.

- Linear,
- Non-dispersive,
- Isotropic,
- No surface currents, and
- No surface charge density.
The method of excitation of the source waveform is presented later in Section 3.4. Accordingly, the source is not excited using the current source and therefore, it is assumed that the source current density term, \( J_s \) is zero. Based on the value of electrical conductivity, \( \sigma \), the material medium can be categorized as presented in Table 3.1. Ideally, there is no power loss within lossless conductors, whereas, in lossy material, the field variables decrease exponentially with distance which contributes to the loss of power. Therefore, \( J = \sigma E \) is a loss term and it is accounted only for lossy dielectric media.

**Table 3.1**

**Classification of the Material Medium**

<table>
<thead>
<tr>
<th>Material classification</th>
<th>Conductivity</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lossless</td>
<td>( \sigma = 0 )</td>
<td>Air or vacuum</td>
</tr>
<tr>
<td>Lossy</td>
<td>( \sigma &gt; 0 ), finite</td>
<td>Silicon</td>
</tr>
<tr>
<td>Conductors</td>
<td>( \sigma \gg 0 ), infinite</td>
<td>Silver, copper</td>
</tr>
</tbody>
</table>

### 3.2 Formulation of Governing Equations

Maxwell’s equations can be coupled using the constitutive relations given by equations (3.17) through (3.19). Substitute equations (3.17) and (3.19) in equation (3.15) and equation (3.18) in equation (3.14) to obtain two coupled partial differential equation in vector form, respectively as shown in equations (3.20) and (3.21).

\[
\epsilon \frac{\partial E}{\partial t} = \nabla \times H - \sigma E \tag{3.20}
\]

\[
\mu \frac{\partial H}{\partial t} = -\nabla \times E \tag{3.21}
\]

The resultant equations involve two unknown vectors, \( E \) and \( H \). The material parameters in the equations are the known values dependent on the type of material. Thus, the six scalar unknowns for \( E \) and \( H \) fields
can be calculated computationally using the six governing equations when expanded to scalar form. Expand equations (3.20) and (3.21) to obtain the expanded form of 3-D Maxwell’s equations presented in equations (3.22) and (3.23).

\[
\frac{\varepsilon}{\partial t} \frac{\partial E_x}{\partial t} \hat{i} + \frac{\varepsilon}{\partial t} \frac{\partial E_y}{\partial t} \hat{j} + \frac{\varepsilon}{\partial t} \frac{\partial E_z}{\partial t} \hat{k} = \left( \frac{\partial H_y}{\partial y} - \frac{\partial H_z}{\partial z} \right) \hat{i} - \left( \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right) \hat{j} + \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \hat{k} - \sigma E_x \hat{i} - \sigma E_y \hat{j} \quad (3.22)
\]

\[- \sigma E_z \hat{k} \]

\[
\mu \frac{\partial H_x}{\partial t} \hat{i} + \mu \frac{\partial H_y}{\partial t} \hat{j} + \mu \frac{\partial H_z}{\partial t} \hat{k} = - \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial z} \right) \hat{i} + \left( \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right) \hat{j} - \left( \frac{\partial E_x}{\partial x} - \frac{\partial E_z}{\partial y} \right) \hat{k} \quad (3.23)
\]

Separate the x, y, and z components of the equation to obtain six scalar partial differential equations;

\[ x: \quad \frac{\varepsilon}{\partial t} \frac{\partial E_x}{\partial t} = \left( \frac{\partial H_y}{\partial y} - \frac{\partial H_z}{\partial z} \right) - \sigma E_x \quad (3.24) \]

\[ y: \quad \frac{\varepsilon}{\partial t} \frac{\partial E_y}{\partial t} = - \left( \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right) - \sigma E_y \quad (3.25) \]

\[ z: \quad \frac{\varepsilon}{\partial t} \frac{\partial E_z}{\partial t} = \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) - \sigma E_z \quad (3.26) \]

\[ x: \quad \mu \frac{\partial H_x}{\partial t} = - \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial z} \right) \quad (3.27) \]

\[ y: \quad \mu \frac{\partial H_y}{\partial t} = \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial y} \right) \quad (3.28) \]

\[ z: \quad \mu \frac{\partial H_z}{\partial t} = - \left( \frac{\partial E_x}{\partial x} - \frac{\partial E_y}{\partial y} \right) \quad (3.29) \]

The six governing equations (3.24) through (3.29) are the full set of interdependent equations that can be discretized and solved on the grid system computationally using an appropriate approximation method.
3.3 Some Theoretical Aspects

It is important to evaluate some theoretical aspects from electromagnetics theory and numerical modeling which will be helpful during the numerical modeling and problem set-up for conducting numerical experiments. This section cover topics such as description of the electromagnetic spectrum, types of materials, the discussion on some popular numerical schemes, etc.

3.3.1 Physical Interpretation of EM Wave Equations

The rapid time varying electric and magnetic fields leads to the simultaneous flow of electric and magnetic fields with respect to both space and time. The flow of electric fields leads to rotational magnetic fields and subsequently, the magnetic fields results in the generation of rotational electric fields and hence, the two fields are coupled and are interdependent.

3.3.2 Classification of Applications

Bounded fields

The bounded application occurs when the solution region is enclosed within a solid boundary, similar to internal flow in fluid dynamics. An example of such an application is existence of fields within a waveguide.

Unbounded fields

Such applications are referred to problems where the region of interest is not surrounded by any physical boundaries or the outer boundaries may extend to infinity. It corresponds to external flow in fluid dynamics and the waves emitted from an antenna is an example of an unbounded application.

Far-Field Applications

When the distance between the transmitter and the receiver is very large, the applications are known as far-field and it requires special modeling features as it is not practically possible to incorporate such large distances in computer simulations. An example of far-field applications is radar cross-section (RCS).
Near-field Applications

The applications that involve the placement of the source and the receiver separated by a very small distance and can be represented within the discretized grid system, are known as near-field applications. The interaction between waves emitted by a mobile device and the human body is an example of near-field application.

3.3.3 The Electromagnetic Spectrum

The classification of EM waves based on the frequency ranges and their corresponding application examples are presented in Table 3.2 which has been reproduced from Ref [116]. The frequency spectrum given in the table consists of the range of frequencies that have been experimentally investigated which varies from 3 Hz classified as micropulsations, up to $10^{22}$ Hz. Considering the broad range of discovered frequencies, the spectrum visible to the human eye is very limited. The EM waves at each frequencies have been successfully utilized by humans for their benefit and hence the development of simulation tools for EM wave investigations is pivotal. It is worthwhile to know the frequency spectrum before developing a numerical model for a particular application.

<table>
<thead>
<tr>
<th>Frequency range</th>
<th>Classification</th>
<th>Application Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{18}$ to $10^{22}$ Hz</td>
<td>Gamma rays</td>
<td>Cancer therapy, astrophysics</td>
</tr>
<tr>
<td>$10^{16}$ to $10^{21}$ Hz</td>
<td>X-rays</td>
<td>Medical diagnosis</td>
</tr>
<tr>
<td>$10^{15}$ to $10^{28}$ Hz</td>
<td>Ultraviolet</td>
<td>Sterilization</td>
</tr>
<tr>
<td>$3.95 \times 10^{14}$ to $7.7 \times 10^{14}$ Hz</td>
<td>Visible spectrum</td>
<td>Vision, astronomy, optical communications</td>
</tr>
<tr>
<td>Frequency range</td>
<td>Classification</td>
<td>Application Examples</td>
</tr>
<tr>
<td>---------------------</td>
<td>---------------------</td>
<td>----------------------------------------------------------</td>
</tr>
<tr>
<td>$10^{12}$ to $10^{14}$ Hz</td>
<td>Infrared</td>
<td>Heating, night vision, optical communications</td>
</tr>
<tr>
<td>0.3 to 1 THz</td>
<td>Millimeter</td>
<td>Astronomy, meteorology</td>
</tr>
<tr>
<td>30 to 300 GHz</td>
<td>Extremely high frequency</td>
<td>Radar, remote sensing</td>
</tr>
<tr>
<td>3 to 30 GHz</td>
<td>Super high frequency</td>
<td>Radar, satellite communication</td>
</tr>
<tr>
<td>0.3 to 3 GHz</td>
<td>Ultra High frequency</td>
<td>Radar, TV, GPS, cellular phone</td>
</tr>
<tr>
<td>30 to 300 MHz</td>
<td>Very High Frequency</td>
<td>TV, FM, police</td>
</tr>
<tr>
<td>3 to 30 MHz</td>
<td>High frequency</td>
<td>Short-wave</td>
</tr>
<tr>
<td>0.3 to 3 MHz</td>
<td>Medium frequency</td>
<td>AM broadcasting</td>
</tr>
<tr>
<td>30 to 300 kHz</td>
<td>Low frequency</td>
<td>Navigation, radio beacons</td>
</tr>
<tr>
<td>3 to 30 kHz</td>
<td>Very low frequency</td>
<td>Navigation, positioning, naval communications</td>
</tr>
<tr>
<td>0.3 to 3 kHz</td>
<td>Ultra low frequency</td>
<td>Telephone, audio</td>
</tr>
<tr>
<td>30 to 300 Hz</td>
<td>Super low frequency</td>
<td>Power transmission, submarine communications</td>
</tr>
<tr>
<td>3 to 30 Hz</td>
<td>Extremely low frequency</td>
<td>Detection of buried metals</td>
</tr>
<tr>
<td>&lt; 3 Hz</td>
<td>Micropulsations</td>
<td>Geophysical prospecting</td>
</tr>
</tbody>
</table>
3.3.4 Types of Materials

The development and validation of a numerical model typically assumes material properties to be constants for simplicity. However, the materials used in practical applications are never simple. The electric permittivity, $\epsilon$, the magnetic permeability, $\mu$, and the electric conductivity, $\sigma$ together dictates the properties of the material and their classification. Several classes of materials have been discovered or invented and a brief discussion on material types is presented next in this section.

*Linear or non-linear*

The materials are classified as non-linear when the material properties $\epsilon$, and $\mu$ depends on the magnitude of $E$ and $H$ fields. The linear property of the materials results in the constant material coefficients, and thus, the development of the finite difference approximation becomes straightforward. Whereas, linearization of the non-linear model equations must be performed before obtaining the numerical approximation equations for non-linear applications.

*Homogenous or inhomogeneous*

The material media wherein the properties change along the coordinate locations are known as inhomogeneous or non-homogeneous materials. The values of $\epsilon$, $\mu$, and $\sigma$ are specified as inputs and assigned to each grid points within the domain at the start of the simulation and it stays same throughout the simulation. The simplest example of a non-homogeneous media is the dielectric device placed in free space. The material parameters for inhomogeneous medium are specified and stored at each grid points, however, for homogenous medium, the material properties can be specified as constants, hence only three storage spaces are required.

*Dispersive or non-dispersive*

The material is said to be dispersive when the material properties are a function of frequency. Generally, most practical materials are dispersive. The implementation of the numerical approximation to dispersive material requires additional equations to obtain the solution. These equations are obtained from the constitutive relations specified as a function of frequency and subsequently, solved using appropriate approach. Human muscle and space plasma are the examples of dispersive materials where permittivity is
a function of frequency. The additional vector equation for modeling human muscles is represented by equation (3.30).

\[ \mathbf{D}(\omega) = \epsilon(\omega)\mathbf{E}(\omega) \]  

(3.30)

**Isotropic or anisotropic**

The material parameters in the isotropic material are independent of the coordinate direction and therefore at one grid point only one value is assigned in an isotropic media. However, in an anisotropic media, the material properties vary with directional vectors and hence, at each grid points, the properties are defined as tensors. For example, the constitutive relation in an anisotropic medium is represented by the equation (3.31).

\[ \mathbf{D} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} \mathbf{E} \]  

(3.31)

### 3.3.5 Solution Methods

The methods that are used in electromagnetics for solving the governing equations can be categorized as the analytical methods, numerical methods, and the experimental methods. Experimental methods are by far the most accurate, however, not a cost-effective way of gathering scientific information, whereas the analytical methods are applicable only to applications involving simple geometries. However, since practical applications are far more complex than can be solved using analytical methods, hence there is a need for formulation of accurate and efficient numerical methods. The numerical methods are the approximation methods and yield results with acceptable accuracy. Some analytical and numerical methods are listed below.

- Analytical Methods (exact solution)
  - Separation of variables
  - Series Expansion
• Conformal Mapping
• Integral solutions, e.g., Laplace and Fourier transforms
• Perturbation Methods

• Numerical Methods (approximate solutions)
  • Finite difference methods
  • Finite Volume methods
  • Method of weighted residuals
  • Moment method
  • Finite element method
  • Transmission-line modeling
  • Monte Carlo method

The discussion on each of these methods is out of the scope of this report, and hence, a brief discussion is presented only for the finite difference method in Section 3.3.6.

3.3.6 Finite Difference Time Domain vs Finite Difference Frequency Domain (FDFD)

Since the introduction of the FDTD method by Yee [1], the method grew into popularity among researchers because of its inherent simplicity in application to the vast majority of problems. Finite difference frequency domain, however, was a preferred method before FDTD. FDFD method is very effective for performing broadband analysis wherein the frequency response is required for a wideband spectra. To obtain frequency response using FDTD method, additional post-processing implementation is required. Such implementation is discussed in Section 4.7. There are several advantages and disadvantages associated with both FDTD and FDFD schemes and based on the requirement and experience one may choose either of the method for simulation of EM wave propagation.

The FDTD methods utilizes the time-varying partial differential equations to obtain the solution, whereas, the complex governing equations based on frequency is used in FDFD method and the time dependence is implicit within the governing equations. When mentioning FDTD methods, it essentially includes all discretization methods that are developed based on the principles of staggering in time and
space method proposed by Yee [1]. The FDTD methods are intuitive in nature and can be developed within a short period of time. The explicit approach of FDTD schemes avoid large matrices calculations involved in implicit schemes. The FDTD methods suffers from staircasing errors as well as the dispersion errors. The staircasing errors arise when arbitrary shaped devices are involved in simulations and therefore, requires additional approximations of material properties to maintain accuracy. The application of FDTD to frequency dependent (dispersive) materials requires additional computational step. The FDFD methods, on the other hand, are the ideal candidate for simulating dispersive materials. However, this method is not a preferred one for solving Maxwell’s equations because the convergence rate for iteratively solving a system of linear equations is slow.

Time domain method requires only marginal efforts in computer programming as compared to frequency domain method for solving simple problems. Time domain analysis is comparatively much faster, does not require high amount of computer storage space, and a more accurate method. Moreover, the time domain analysis can be performed on a desktop computer with enormous amount of mesh cells necessary for studying complex structures that is not possible using frequency domain approach [117].

3.4 Incident Field Modeling

The modeling of sources is another fundamental topic for electromagnetic illumination of the simulation domain. Incident fields can be introduced in the computations through various approaches, primarily depending upon the problem of interest. Accurate representation of the problem under consideration requires knowledge of pros and cons of excitation sources and the method of introduction of selected source field, otherwise it may lead to undesired solution or additional computational costs. The first step in source modeling is the selection of an appropriate waveform and subsequently, based on the problem type, the method to introduce the selected sources is modeled. This section contains some of the frequently encountered source waveforms and the methods of realization of sources.
3.4.1 Types of Sources

3.4.1.1 Sinusoidal Wave

Continuous sinusoid, as shown in equation (3.31), can be specified at any single point or at number of points within the domain and it can be assigned to either \( E \) or \( H \) field.

\[
E_z = E_0 \sin(2\pi f_0 n \Delta t)
\]  
(3.31)

The sinusoidal wave is a function of frequency, \( f_0 \) and time level, \( t = n \Delta t \). The resultant field will propagate in both directions.

3.4.1.2 Gaussian Pulse

Like the sinusoidal waveform, the gaussian impulse function can be specified at a point or at number of points within the domain and it is given by equation (3.32). The gaussian field is a decaying function dependent on time, and the width of the pulse.

\[
E_z = E_0 \exp \left( -0.5 \left( \frac{t_0 - t}{\tau_w \Delta t} \right)^2 \right)
\]  
(3.32)

Where, \( t_0 = n_0 \Delta t \), is the pulse delay, and \( \tau_w \) is the spread or width of the pulse. The specification of \( n_0 \) in the pulse modeling ensures the smooth transition of the pulse into the domain starting from zero amplitude. This is demonstrated in Figure 3.1, where the gaussian function is plotted as a function of time step, \( n \) for different delay periods. When delay is zero (i.e. \( n_0 = 0 \)), the pulse is introduced in the simulation at its peak which may negatively impact the solution. Therefore, a good rule of thumb is to use the delay, \( n_0 \) equal to at least three times of the pulse spread, \( \tau_w \).
Different textbooks [118-120] have reported different formulations for modeling the Gaussian pulse based on the desired frequency, for example, according to Sheng and Song [120], the pulse spread, $\tau_w$ is calculated using the maximum frequency, $f_{max}$ for which the response of the object is required.

$$\tau_w = \frac{2}{f_{max}\Delta t}$$  \hfill (3.33)

### 3.4.1.3 Modulated Gaussian Pulse

It is specified as a function of sine wave and gaussian pulse as given in equation (3.34).

$$E_z = E_0 \exp \left(-0.5 \left(\frac{n_0 - n}{\tau_w}\right)^2 \right) \sin(2\pi f_0 (n - n_0)\Delta t)$$  \hfill (3.34)

The major benefit of using gaussian impulse and modulated gaussian pulse as a source field is that the single simulation can yield the spectral response over wide range of frequencies as compared to sine source which yields response of single frequency per simulation. Computing the frequency response of reflected and transmitted fields requires the application of Fast Fourier Transform (FFT) method to
transform the time domain solution at each time step to the frequency domain solution. In the case of sine waveform, solution is obtained after the attainment of sinusoidal steady state.

The snapshots of source field presented in Figure 3.2 demonstrates the major difference between the propagation characteristic of the sine wave, the gaussian pulse and the modulated gaussian pulse. The sinusoidal source continuously radiates the source field from the source location for extended time, whereas, the gaussian source is a short time impulse that decays with the time elapse.

![Figure 3.2. Modulated gaussian, sinusoidal and gaussian waveforms as a function of time.](image)

### 3.4.2 Source Specification

Depending upon the problem description, the sources are specified within the domain near the object such as in dosimetry applications or external to the domain such that the field appear to have generated away from the object such as in radar cross section calculations. Hence, the source specifications can be classified into two broad categories; internal specification and external specification.
3.4.2.1 Internal Source Specification

**Hard Source**

The hard sources are specified by assigning the hard-coded values to the \( E \) or \( H \) field at the desired locations within the domain at every time step after the execution of the finite difference approximations. This overwrites all the previously calculated values at those locations and therefore, this method is not suitable for practical applications as the source locations will act as a metal conductor and will reflect incoming fields, already reflected from the device, back towards the device and hence causing spurious reflections which may lead to inaccuracies. Hard source specification is not an advisable method for one-dimensional simulations, however, for two-dimensional and three-dimensional applications that involves waveguides, this is a very useful method \[65\]. The subscripts \((is, js)\) in equation (3.35) represents the index locations of \( x \) and \( y \) coordinates, respectively of the location of the source within the domain.

\[
E_{z,is,js} = \text{gaussian function} \tag{3.35}
\]

**Soft Sources**

Soft sources are modelled by adding the source field to the computed field at the prescribed locations to prevent artificial reflections from the source location.

\[
E_{z,is,js} = E_{z,is,js} + \text{gaussian function} \tag{3.36}
\]

**Current and Voltage Sources**

In such sources, the intrinsic components of the governing equations can be used to drive the simulations. The source current term, \( J_s \) appearing in the curl equation of \( E \) can be used to specify the source based on the problem where current is driving the fields.

\[
\varepsilon \frac{\partial E}{\partial t} = \nabla \times H - \sigma E - J_s
\]
Such source specification is similar to the soft source; however, the source term is an intrinsic part to the finite difference equation as compared to a soft source where the source field is added after the finite difference approximation. The other difference is that the soft source can either be $\mathbf{E}$ or $\mathbf{H}$ field, whereas the current density is the source in this formulation. Similarly, for applications involving wire antenna, the voltage source is specified in the finite difference equations.

*Thin-wire approximation*

Applications that involve low frequency simulations and relatively thin structures such as antennas, thin-wire approximation method for excitation is used. The detailed description pertaining to the thin-wire approximation is presented in Ref [65,116].

### 3.4.2.2 External Source Specification

For waves that may have generated at a far distance away from the scatterer, it is essential to model such waves appropriately. These types of problems occur in radar detection, antennas, satellite communications, etc. One approach is to increase the size of the computational domain to a large extent that represents the physical dimensions accurately. The cost of computing to run such a simulation will be incredible. A better approach is to approximate the incoming field as plane waves that may have been generated at a large distance because it is assumed that plane waves retain their properties over considerable distance. Total field-scattered field formulation and the pure scattered field formulation are popular methods for such applications. The brief introduction to these formulations is presented in the subsequent sub-sections and the detailed formulation is presented in Chapter 5 of this report.

*Total field-scattered field*

The linear nature of Maxwell’s equations is the underlying principle in the TF-SF formulation. For specifying this type of formulation, the simulation space is divided into two regions: an inner region containing the total field, which is the sum of scattered fields and incident fields and the outer region surrounding the total-field region containing the scattered field. The scattering device must be modeled in the total-field region.
Scattered field

This technique is based on the assumption that the scattered field quantities exist at all grid points within the domain and the finite difference approximations are derived for the scattered fields only. To obtain total-field values, additional post processing can be performed. Additionally, for applications that involve a device such as a perfect conductor, the specification of the fields inside the material is not straightforward using this approach.

The various source waveforms and the methods of their introduction that are frequently used to start the simulation were discussed in this section. However, this is not an exhaustive list of the methods for the source field excitation and some suggested literature for further reading are [65,116,119].
CHAPTER 4

NUMERICAL MODELING

The numerical method and the algorithm used to simulate the electromagnetic waves is presented in this Chapter. The finite difference approximation of the partial differential equation representing an underlying physical phenomenon is required to perform computational simulations. The finite difference approximation equations are the algebraic equations that are easily programmable into computer codes. Maxwell’s equations are the linear, first-order, hyperbolic system of equations that can be discretized using explicit Runge-Kutta approximation. The investigations presented in this paper utilized the explicit form of the fourth-order Modified Runge Kutta (MRK) method on the curvilinear coordinates to perform computational simulations. The description and the advantages of the MRK scheme is presented in next section, followed by the non-dimensionalization procedure. Subsequently, the partial differential equations on curvilinear coordinates and the MRK approximations are derived. The last section of this chapter discusses about the post-processing method for transformation of time-domain results to frequency-domain and the importance of such post-processing.

4.1 Fourth-Order Modified Runge Kutta Method

The Runge-Kutta method is a popular scheme within the computational fluid dynamics community. The scheme is based on obtaining several numerical solutions over a single time step, $\Delta t$. The number of solutions obtained within a single time step is determined by the employed number of stages, let us say $n$. This provides $n$-th order accuracy in time. The convective terms in the equation can be approximated by any appropriate approximation method. The solution at each stage are obtained sequentially and subsequently averaged at the final stage. Typically, a four-stage RK scheme with second-order central differencing of convective terms is used. The classical RK scheme, thus, requires additional storage space to store variables obtained during the four stages. The Modified Runge-Kutta scheme is an upgrade to RK schemes to overcome the storage limitations. In the MRK, a sequential solution is carried out in $n$-stages within the same time step, where computations at each subsequent stage requires known variable values.
computed from the previous stage until the final stage is reached. The solution obtained at the $n$-th stage is the final output from that time level. Therefore, the values are overwritten in the allocated memory space at each stage and consequently, the storage requirements are reduced.

The RK or MRK method is known to possess higher accuracy and better stability as compared to most explicit formulation scheme. The stability requirement for an MRK scheme with central differencing of spatial derivative is specified as $\text{CFL} \leq 2\sqrt{2}$ and for any other explicit scheme, the stability requirement is $\text{CFL} \leq 1$ [121]. We aim to utilize the four-stage MRK scheme for time stepping in the proposed algorithm and second-order central-differencing for the approximation of convective terms. The proven advantages of the MRK scheme can be summed up as; fourth-order accuracy, relaxed stability criteria, low storage requirements, and easily programmable.

4.2 Non-Dimensionalization

As we know that the free space electric permittivity and the magnetic permeability is $8.854\times10^{-12}$ F/m and $1.257\times10^{-6}$ H/m, respectively. Due to this large difference in the magnitudes of the material parameters, the computed values of the electric field intensity and the magnetic field intensity differs by several orders in magnitude. This may lead to unwanted numerical errors due to round-off during simulations. Therefore, the variables in the governing equations are scaled down to the same order by non-dimensionalizing them with respect to the reference variables using the appropriate relations obtained from Niegemann [122]. Such relations for performing non-dimensionalization of each variable are presented collectively as equation (4.1). The relations are usually modeled in such a manner that it ensures that the range of the non-dimensionalized variables remain between zero and one. Generally, the values of the reference variables are specified by the free space conditions or the characteristic dimensions.
\[ E^* = \frac{E}{E_0} \quad H^* = \frac{H}{E_0} \sqrt{\frac{\mu_0}{\epsilon_0}} \quad J^* = \frac{JL}{E_0} \sqrt{\frac{\mu_0}{\epsilon_0}} \]

\[ x^* = \frac{x}{L} \quad y^* = \frac{y}{L} \quad z^* = \frac{z}{L} \]  

\[ \sigma^* = \frac{\sigma}{\sigma_0} \quad \mu^* = \frac{\mu}{\mu_0} \quad \epsilon^* = \frac{\epsilon}{\epsilon_0} \]

\[ c_0^2 = \frac{1}{\epsilon_0 \mu_0} \quad t^* = \frac{tc_0}{L} \quad f^* = \frac{fL}{c_0} \]  

(4.1)

4.3 Maxwell’s Equation in Cartesian Coordinates

Next, the non-dimensional form of two-dimensional and the three-dimensional governing equations in the cartesian coordinates is derived.

4.3.1 Three-Dimensional Governing Equations

The six scalar PDEs from equations (3.24) through (3.29) presented previously in Section 3.2 are non-dimensionalized using the relations specified in equation (4.1). The expanded form of 3D Maxwell’s equations in non-dimensional form is provided in equations (4.2) through (4.7). It is to be noted that the asterisk ‘*’ has been dropped from the terms and all the quantities are non-dimensional unless otherwise stated.

\[ \epsilon \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - K_\sigma E_x \]  

(4.2)

\[ \epsilon \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} + \frac{\partial H_x}{\partial z} - K_\sigma E_y \]  

(4.3)

\[ \epsilon \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - K_\sigma E_z \]  

(4.4)
\[
\begin{align*}
\mu \frac{\partial H_x}{\partial t} &= -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z} \quad (4.5) \\
\mu \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \quad (4.6) \\
\mu \frac{\partial H_z}{\partial t} &= -\frac{\partial E_y}{\partial x} + \frac{\partial E_x}{\partial y} \quad (4.7)
\end{align*}
\]

In equations (4.2) - (4.4), a non-dimensional number \( K_\sigma \) has been introduced as a result of non-dimensionalization which is expressed as:

\[
K_\sigma = \frac{\sigma^* \sigma_0}{\epsilon_0 \mu_0} = \frac{\sigma}{\sqrt{\epsilon_0 / \mu_0}} \quad (4.8)
\]

Since \( \sigma = \sigma^* \sigma_0 \), the non-dimensional number \( K_\sigma \) is directly dependent on the dimensional value of material conductivity, \( \sigma \) and therefore, it is a representation of the lossy term in a lossy dielectric media, whereas this non-dimensional number will be zero for lossless dielectrics and perfect conductors.

### 4.3.2 Two-Dimensional Governing Equations

The two-dimensional form of the governing equations can be derived by assuming no changes in \( z \)-direction, \( \frac{\partial}{\partial z} = 0 \). (Asterisk has been dropped for convenience).

\[
\begin{align*}
\epsilon \frac{\partial E_x}{\partial t} &= \frac{\partial H_z}{\partial y} - K_\sigma E_x \quad (4.9) \\
\epsilon \frac{\partial E_y}{\partial t} &= -\frac{\partial H_z}{\partial x} - K_\sigma E_y \quad (4.10) \\
\epsilon \frac{\partial E_z}{\partial t} &= \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) - K_\sigma E_z \quad (4.11) \\
\mu \frac{\partial H_x}{\partial t} &= -\frac{\partial E_z}{\partial y} \quad (4.12)
\end{align*}
\]
\[ \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} \]  
(4.13)

\[ \mu \frac{\partial H_z}{\partial t} = -\left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \]  
(4.14)

The six equations presented in equations (4.9) through (4.14), can be categorized as two sets comprising three linear, first-order, coupled equations namely, the transverse electric (TE) mode and transverse magnetic (TM) mode. The brief description of the two modes is presented in the following sub-sections.

4.3.2.1 Transverse Electric Mode

In this mode, the component of electric field in z-direction is zero, \( E_z = 0 \), hence the electric components only exist in transverse direction. On the other hand, the component of magnetic field in z-direction is not equal to zero, \( H_z \neq 0 \). Using these assumptions, it can be seen in equations (4.15) – (4.17) that by knowing \( H_z \), the transverse components of electric field, \( E_x \) and \( E_y \) can be solved. Hence, in TE mode only three equations (4.15) - (4.17) are required to be solved computationally to find three relevant unknowns, \( E_x, E_y \) and \( H_z \).

\[ \frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \frac{\partial H_z}{\partial y} - \frac{K_\sigma}{\varepsilon} E_x \]  
(4.15)

\[ \frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon} \frac{\partial H_z}{\partial x} - \frac{K_\sigma}{\varepsilon} E_y \]  
(4.16)

\[ \frac{\partial H_z}{\partial t} = -\frac{1}{\mu} \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \]  
(4.17)

4.3.2.2 Transverse Magnetic Mode

Contrary to the TE mode, TM mode has magnetic field component in z-direction, \( H_z \) equals to zero, and \( E_z \neq 0 \). From equations (4.18) through (4.20), it is clear that \( H_x \) and \( H_y \) can be calculated using \( E_z \). Therefore, by solving equations (4.18), (4.19) and (4.20) computationally, three unknowns \( H_x, H_y, \) and \( E_z \) can be obtained.
\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) - \frac{K \sigma}{\varepsilon} E_z
\]  
(4.18)

\[
\frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \frac{\partial E_z}{\partial y}
\]  
(4.19)

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \frac{\partial E_z}{\partial x}
\]  
(4.20)

Finite difference time domain modeling in 2D can be done by using either of the two modes. Transverse Magnetic (TM) mode has been used in this work for solving the field unknowns computationally.

4.4 **Transformation of Maxwell’s Equations from Physical Space to Computational Space**

In this section, the arrangement of the governing equations in \((\xi, \eta, \zeta)\) coordinate is presented. Most applications involve complex-shaped structures, which are difficult to model using simple finite differencing approximations. By using the transformation technique, arbitrary-shaped structures can be mapped onto an equally spaced grid system known as a computational grid. The numerical schemes can be easily implemented on this transformed grid, and the specification of boundary conditions become simple and straightforward. Hence, the errors due to staircasing of material boundaries can be avoided and better accuracy is achieved. Additionally, the clustering of grid points in the vicinity of large gradients can be applied with much ease using transformed coordinates system.

An interpolation technique to perform such transformation is given in [123] for the governing equations in Fluid Dynamics and using a similar procedure, the transformation technique employed in our research is presented in Appendix A and Appendix B.

4.4.1 **2D Transverse Magnetic Mode**

The transformation of system of Maxwell’s equations from physical space to computational domain is presented in this section for two-dimensional applications. Consider the transverse magnetic mode presented in equations (4.18) – (4.20) and rearrange the terms to obtain expressions in equations (4.21) through (4.23).
\[
\frac{\partial E_z}{\partial t} - \frac{1}{\epsilon} \frac{\partial H_y}{\partial x} + \frac{1}{\epsilon} \frac{\partial H_x}{\partial y} + \frac{K_\sigma}{\epsilon} E_z = 0 \tag{4.21}
\]

\[
\frac{\partial H_x}{\partial t} + \frac{1}{\mu} \frac{\partial E_z}{\partial y} = 0 \tag{4.22}
\]

\[
\frac{\partial H_y}{\partial t} - \frac{1}{\mu} \frac{\partial E_z}{\partial x} = 0 \tag{4.23}
\]

The fourth term in left hand side of equation (4.21) represents the losses, as mentioned earlier. The non-dimensional 2D Maxwell’s equations are expressed in the flux vector form as

\[
\frac{\partial T}{\partial t} + X \frac{\partial P}{\partial x} + Y \frac{\partial Q}{\partial y} + J_\sigma = 0 \tag{4.24}
\]

Where \( T, P, \) and \( Q \) are known as the flux vectors in physical domain and the \( X \) and \( Y \) are the coefficient vectors that contains information about the material properties. The flux vectors are specified in equation (4.25) collectively as

\[
T = \begin{bmatrix} E_z \\ H_x \\ H_y \end{bmatrix}
\]

\[
P = \begin{bmatrix} -H_y \\ 0 \\ -E_z \end{bmatrix}
\]

\[
Q = \begin{bmatrix} H_x \\ E_z \\ 0 \end{bmatrix}
\]

\[
J_\sigma = \begin{bmatrix} K_\sigma E_z/\epsilon \\ 0 \\ 0 \end{bmatrix}
\]
And the coefficient vectors are presented in equation (4.26) as

\[
X = \begin{bmatrix}
1/\epsilon \\
0 \\
1/\mu
\end{bmatrix}
\]

\[
Y = \begin{bmatrix}
1/\epsilon \\
1/\mu \\
0
\end{bmatrix}
\] (4.26)

This governing equation in the flux vector form was subsequently transformed from physical space to computational domain using the process described in Appendix B and is expressed in equation (4.27) as

\[
\frac{\partial \bar{T}}{\partial \tau} + X \frac{\partial \bar{P}}{\partial \xi} + Y \frac{\partial \bar{Q}}{\partial \eta} + J_\sigma = 0
\] (4.27)

Where \(\bar{T}, \bar{P},\) and \(\bar{Q}\) are the flux vectors in computational domain and \(X\) and \(Y\) are the coefficient matrices obtained as a result of coordinate transformation and contains material data. The expressions that relate flux vectors in transformed coordinates to the flux vectors in physical domain and the corresponding primitive variables are presented in equation (4.28).

\[
\bar{T} = \frac{T}{J}
\]

\[
\bar{P} = \frac{1}{J}(\xi_x P + \xi_y Q)
\]

\[
\bar{Q} = \frac{1}{J}(\eta_x P + \eta_y Q)
\] (4.28)

\[
J_\sigma = \frac{1}{J}(J_\sigma)
\]

The expression for coefficient matrices is presented in equation (4.29).
Next, expand equation (4.27) and rearrange terms to obtain time derivatives of $\bar{T}_1$, $\bar{T}_2$, and $\bar{T}_3$.

$$\frac{\partial \bar{T}_1}{\partial \tau} = -\left( \bar{X}_{11} \frac{\partial \bar{P}_1}{\partial \xi} + \bar{Y}_{11} \frac{\partial \bar{Q}_1}{\partial \eta} + \bar{J}_{\sigma_1} \right)$$ \hspace{1cm} (4.30)

$$\frac{\partial \bar{T}_2}{\partial \tau} = -\left( \bar{X}_{22} \frac{\partial \bar{P}_2}{\partial \xi} + \bar{Y}_{22} \frac{\partial \bar{Q}_2}{\partial \eta} + \bar{J}_{\sigma_2} \right)$$ \hspace{1cm} (4.31)

$$\frac{\partial \bar{T}_3}{\partial \tau} = -\left( \bar{X}_{33} \frac{\partial \bar{P}_3}{\partial \xi} + \bar{Y}_{33} \frac{\partial \bar{Q}_3}{\partial \eta} + \bar{J}_{\sigma_3} \right)$$ \hspace{1cm} (4.32)

It is apparent that the first vector term of $\bar{J}_\sigma$ is non-zero and is dependent on $E_z$, and as we know that $\bar{T}_1$ is a representative term of $E_z$ in computational domain, the term $\bar{J}_{\sigma_1}$ in equation (4.30) is expressed in terms of $\bar{T}_1$ using the relation in equation (4.33).

$$\bar{J}_{\sigma_1} = \frac{1}{J} \left( \frac{K_\sigma}{\epsilon} E_z \right) = \left( \frac{K_\sigma}{\epsilon} \frac{T_1}{J} \right) = \frac{K_\sigma}{\epsilon} \bar{T}_1$$ \hspace{1cm} (4.33)

Substitute equation (4.33) in equation (4.30) to obtain the final form of the time derivative equation of $\bar{T}_1$ which will be used later in the finite difference approximation.

$$\frac{\partial \bar{T}_1}{\partial \tau} = -\left( \bar{X}_1 \frac{\partial \bar{P}_1}{\partial \xi} + \bar{Y}_1 \frac{\partial \bar{Q}_1}{\partial \eta} + \frac{K_\sigma}{\epsilon} \bar{T}_1 \right)$$ \hspace{1cm} (4.34)

For further simplification of the governing equations (4.31) and (4.32), substitute values of $\bar{J}_{\sigma_2}$ and $\bar{J}_{\sigma_3}$ that corresponds to zero from equation (4.25).

$$\frac{\partial \bar{T}_2}{\partial \tau} = -\left( \bar{X}_2 \frac{\partial \bar{P}_2}{\partial \xi} + \bar{Y}_2 \frac{\partial \bar{Q}_2}{\partial \eta} \right)$$ \hspace{1cm} (4.35)
\[
\frac{\partial \bar{T}_3}{\partial \tau} = - \left( \bar{X}_3 \frac{\partial \bar{P}_3}{\partial \xi} + \bar{Y}_3 \frac{\partial \bar{Q}_3}{\partial \eta} \right) \tag{4.36}
\]

Linearization of the governing equation (4.27) was performed assuming time-independent grid system and subsequently, the flux Jacobian matrices $\bar{A}$ and $\bar{B}$ were derived by following the procedure given in Ref. [123], and the derivation for the present applications is presented in Appendix D. Linearized form of the governing equations is shown in equation (4.37) where all flux vectors are expressed in terms of flux vector $\bar{T}$. Further modification is achieved by multiplication of the coefficient matrices and the final expression is shown in equation (4.38).

\[
\frac{\partial \bar{T}}{\partial \tau} + \bar{X} A \frac{\partial \bar{T}}{\partial \xi} + \bar{Y} B \frac{\partial \bar{T}}{\partial \eta} + \bar{J}_\sigma = 0 \tag{4.37}
\]

\[
\frac{\partial \bar{T}}{\partial \tau} + \bar{A} \frac{\partial \bar{T}}{\partial \xi} + \bar{B} \frac{\partial \bar{T}}{\partial \eta} + \bar{J}_\sigma = 0 \tag{4.38}
\]

Where, the coefficient matrices known as the flux Jacobian matrices are defined as

\[
\bar{A} = \frac{\partial \bar{P}}{\partial \bar{T}} = \begin{bmatrix}
0 & \frac{\xi_y}{\epsilon} & -\frac{\xi_x}{\epsilon} \\
\frac{\xi_y}{\mu} & 0 & 0 \\
-\frac{\xi_x}{\mu} & 0 & 0
\end{bmatrix}
\]

(4.39)

\[
\bar{B} = \frac{\partial \bar{Q}}{\partial \bar{T}} = \begin{bmatrix}
0 & \frac{\eta_y}{\epsilon} & -\frac{\eta_x}{\epsilon} \\
\frac{\eta_y}{\mu} & 0 & 0 \\
-\frac{\eta_x}{\mu} & 0 & 0
\end{bmatrix}
\]

The eigenvalues of the flux Jacobian matrices $\bar{A}$ and $\bar{B}$ are presented in equations (4.40) and (4.41), respectively. As demonstrated, the eigenvalues are real, with mixed positive and negative values, therefore,
the resulting form of Maxwell’s equations is classified as hyperbolic. The eigenvalues of $\tilde{A}$ and $\tilde{B}$ provide information about the direction of signal propagation. This knowledge is helpful in the development and application of the numerical model. Since the derived eigenvalues for the model equations are positive and negative, it suggests that the waves are forward travelling as well as backward travelling.

\[
\begin{align*}
\lambda_{1A} &= 0 \\
\lambda_{2A} &= -\frac{\sqrt{\xi_x^2 + \xi_y^2}}{\sqrt{\mu \varepsilon}} = -c \sqrt{\xi_x^2 + \xi_y^2} \\
\lambda_{3A} &= \frac{\sqrt{\xi_x^2 + \xi_y^2}}{\sqrt{\mu \varepsilon}} = c \sqrt{\xi_x^2 + \xi_y^2} \\
\lambda_{1B} &= 0 \\
\lambda_{2B} &= -\frac{\sqrt{\eta_x^2 + \eta_y^2}}{\sqrt{\mu \varepsilon}} = -c \sqrt{\eta_x^2 + \eta_y^2} \\
\lambda_{3B} &= \frac{\sqrt{\eta_x^2 + \eta_y^2}}{\sqrt{\mu \varepsilon}} = c \sqrt{\eta_x^2 + \eta_y^2}
\end{align*}
\]
The resultant eigenvector matrix of $A$ and $B$ are presented in equation (4.42).

$$
\chi_A = \begin{bmatrix}
\frac{\xi_x}{\xi_y} & \frac{\xi_y}{\xi_x} & -\frac{\xi_y}{\xi_x} \\
1 & 1 & 1
\end{bmatrix}
$$

$$
\chi_B = \begin{bmatrix}
\frac{\eta_x}{\eta_y} & \frac{\eta_y}{\eta_x} & -\frac{\eta_y}{\eta_x} \\
1 & 1 & 1
\end{bmatrix}
$$

4.4.2 Three-Dimensional Equations in Transformed Coordinates

The flux vector form of three-dimensional governing equation in physical space is obtained by first rearranging the terms in equation (4.2) through (4.9) to obtain equations (4.43) through (4.48), and subsequently, the vector form is presented in equation (4.49).

$$
\frac{\partial E_x}{\partial t} - \frac{1}{\epsilon} \frac{\partial H_z}{\partial y} + \frac{1}{\epsilon} \frac{\partial H_y}{\partial z} + \frac{K_\sigma}{\epsilon} E_x = 0
$$

$$
\frac{\partial E_y}{\partial t} + \frac{1}{\epsilon} \frac{\partial H_z}{\partial x} - \frac{1}{\epsilon} \frac{\partial H_x}{\partial z} + \frac{K_\sigma}{\epsilon} E_y = 0
$$

$$
\frac{\partial E_z}{\partial t} - \frac{1}{\epsilon} \frac{\partial H_y}{\partial x} + \frac{1}{\epsilon} \frac{\partial H_x}{\partial z} + \frac{K_\sigma}{\epsilon} E_z = 0
$$

$$
\frac{\partial H_x}{\partial t} + \frac{1}{\mu} \frac{\partial E_z}{\partial y} - \frac{1}{\mu} \frac{\partial E_y}{\partial z} = 0
$$
\[ \frac{\partial H_y}{\partial t} - \frac{1}{\mu} \frac{\partial E_z}{\partial x} + \frac{1}{\mu} \frac{\partial E_x}{\partial z} = 0 \]  \hspace{1cm} (4.47) \\

\[ \frac{\partial H_z}{\partial t} + \frac{1}{\mu} \frac{\partial E_y}{\partial x} - \frac{1}{\mu} \frac{\partial E_x}{\partial y} = 0 \]  \hspace{1cm} (4.48) \\

\[ \frac{\partial T}{\partial t} + X \frac{\partial P}{\partial x} + Y \frac{\partial Q}{\partial y} + Z \frac{\partial R}{\partial z} + J_\sigma = 0 \]  \hspace{1cm} (4.49)

Where $T$, $P$, $Q$, and $R$, are known as the flux vectors in physical domain and the $X$, $Y$, and $Z$ are the coefficient vectors that contains information about the material properties. The flux vectors in primitive variables are specified as

\[
T = \begin{bmatrix}
E_x \\
E_y \\
E_z \\
H_x \\
H_y \\
H_z \\
\end{bmatrix}
\]

\[
P = \begin{bmatrix}
0 \\
H_z \\
-H_y \\
0 \\
-E_z \\
E_y \\
\end{bmatrix}
\]

\[
Q = \begin{bmatrix}
-H_z \\
0 \\
H_x \\
E_z \\
0 \\
-E_x \\
\end{bmatrix}
\]
\[ R = \begin{bmatrix} H_y \\ -H_x \\ 0 \\ -E_y \\ E_x \\ 0 \end{bmatrix} \]

\[ J_\sigma = \begin{bmatrix} \frac{K_a E_x}{\epsilon} \\ \frac{K_a E_y}{\epsilon} \\ \frac{K_a E_z}{\epsilon} \\ 0 \\ 0 \\ 0 \end{bmatrix} \]

The coefficient matrices are specified as

\[ X = \begin{bmatrix} 0 \\ 1/\epsilon \\ 1/\epsilon \\ 0 \\ 1/\mu \\ 1/\mu \end{bmatrix} \]

\[ Y = \begin{bmatrix} 1/\epsilon \\ 0 \\ 1/\epsilon \\ 1/\mu \\ 0 \\ 1/\mu \end{bmatrix} \] (4.51)
This governing flux vector equation in the rectangular coordinates, shown in equation (4.52), is subsequently obtained by performing the transformation procedure described in Appendix A.

\[
\frac{\partial \vec{T}}{\partial \tau} + \vec{X} \frac{\partial \vec{P}}{\partial \xi} + \vec{Y} \frac{\partial \vec{Q}}{\partial \eta} + \vec{Z} \frac{\partial \vec{R}}{\partial \zeta} + \vec{J}_\sigma = 0
\]  

(4.52)

Where, the flux vectors $\vec{T}$, $\vec{P}$, $\vec{Q}$, and $\vec{R}$ in transformed coordinates are related to the flux vectors in physical coordinates as shown

\[
\vec{T} = \frac{T}{J}
\]

\[
\vec{P} = \frac{1}{J} (\xi_x P + \xi_y Q + \xi_z R)
\]

\[
\vec{Q} = \frac{1}{J} (\eta_x P + \eta_y Q + \eta_z R)
\]

(4.53)

\[
\vec{R} = \frac{1}{J} (\zeta_x P + \zeta_y Q + \zeta_z R)
\]

\[
\vec{J}_\sigma = \frac{1}{J} (J_\sigma)
\]
The coefficient matrices are given as

\[
\begin{bmatrix}
1/\epsilon & 0 & 0 & 0 & 0 & 0 \\
0 & 1/\epsilon & 0 & 0 & 0 & 0 \\
0 & 0 & 1/\epsilon & 0 & 0 & 0 \\
0 & 0 & 0 & 1/\mu & 0 & 0 \\
0 & 0 & 0 & 0 & 1/\mu & 0 \\
0 & 0 & 0 & 0 & 0 & 1/\mu
\end{bmatrix}
\]

(4.54)

Expand equation (4.52) and rearrange terms to obtain six differential equations for \(T_1, T_2, T_3, T_4, T_5,\) and \(T_6.\)

\[
\frac{\partial \vec{T}_1}{\partial \tau} = -\left( \vec{X}_{11} \frac{\partial p_1}{\partial \xi} + \vec{Y}_{11} \frac{\partial q_1}{\partial \eta} + \vec{Z}_{11} \frac{\partial r_1}{\partial \zeta} + \vec{J}_{\sigma 11} \right)
\]

(4.55)

\[
\frac{\partial \vec{T}_2}{\partial \tau} = -\left( \vec{X}_{22} \frac{\partial p_2}{\partial \xi} + \vec{Y}_{22} \frac{\partial q_2}{\partial \eta} + \vec{Z}_{22} \frac{\partial r_2}{\partial \zeta} + \vec{J}_{\sigma 2} \right)
\]

(4.56)

\[
\frac{\partial \vec{T}_3}{\partial \tau} = -\left( \vec{X}_{33} \frac{\partial p_3}{\partial \xi} + \vec{Y}_{33} \frac{\partial q_3}{\partial \eta} + \vec{Z}_{33} \frac{\partial r_3}{\partial \zeta} + \vec{J}_{\sigma 3} \right)
\]

(4.57)

\[
\frac{\partial \vec{T}_4}{\partial \tau} = -\left( \vec{X}_{44} \frac{\partial p_4}{\partial \xi} + \vec{Y}_{44} \frac{\partial q_4}{\partial \eta} + \vec{Z}_{44} \frac{\partial r_4}{\partial \zeta} + \vec{J}_{\sigma 4} \right)
\]

(4.58)

\[
\frac{\partial \vec{T}_5}{\partial \tau} = -\left( \vec{X}_{55} \frac{\partial p_5}{\partial \xi} + \vec{Y}_{55} \frac{\partial q_5}{\partial \eta} + \vec{Z}_{55} \frac{\partial r_5}{\partial \zeta} + \vec{J}_{\sigma 5} \right)
\]

(4.59)

\[
\frac{\partial \vec{T}_6}{\partial \tau} = -\left( \vec{X}_{66} \frac{\partial p_6}{\partial \xi} + \vec{Y}_{66} \frac{\partial q_6}{\partial \eta} + \vec{Z}_{66} \frac{\partial r_6}{\partial \zeta} + \vec{J}_{\sigma 6} \right)
\]

(4.60)
Using a similar procedure presented in Section 4.4.1, equations (4.55) through (4.60) are rewritten as

\[
\frac{\partial T_1}{\partial \tau} = - \left( x_{11} \frac{\partial p_1}{\partial \xi} + y_{11} \frac{\partial q_1}{\partial \eta} + z_{11} \frac{\partial r_1}{\partial \zeta} + \frac{K_\sigma}{\epsilon} T_1 \right) \quad (4.61)
\]

\[
\frac{\partial T_2}{\partial \tau} = - \left( x_{22} \frac{\partial p_2}{\partial \xi} + y_{22} \frac{\partial q_2}{\partial \eta} + z_{22} \frac{\partial r_2}{\partial \zeta} + \frac{K_\sigma}{\epsilon} T_2 \right) \quad (4.62)
\]

\[
\frac{\partial T_3}{\partial \tau} = - \left( x_{33} \frac{\partial p_3}{\partial \xi} + y_{33} \frac{\partial q_3}{\partial \eta} + z_{33} \frac{\partial r_3}{\partial \zeta} + \frac{K_\sigma}{\epsilon} T_3 \right) \quad (4.63)
\]

\[
\frac{\partial T_4}{\partial \tau} = - \left( x_{44} \frac{\partial p_4}{\partial \xi} + y_{44} \frac{\partial q_4}{\partial \eta} + z_{44} \frac{\partial r_4}{\partial \zeta} \right) \quad (4.64)
\]

\[
\frac{\partial T_5}{\partial \tau} = - \left( x_{55} \frac{\partial p_5}{\partial \xi} + y_{55} \frac{\partial q_5}{\partial \eta} + z_{55} \frac{\partial r_5}{\partial \zeta} \right) \quad (4.65)
\]

\[
\frac{\partial T_6}{\partial \tau} = - \left( x_{66} \frac{\partial p_6}{\partial \xi} + y_{66} \frac{\partial q_6}{\partial \eta} + z_{66} \frac{\partial r_6}{\partial \zeta} \right) \quad (4.66)
\]

Subsequently, using linearization procedure, the model equation is derived in terms of $\bar{T}$ and the flux Jacobian matrices $\bar{A}$, $\bar{B}$, and $\bar{C}$ are determined. The detailed derivation is presented in Appendix C.

\[
\frac{\partial \bar{T}}{\partial \tau} + \bar{A} \frac{\partial \bar{T}}{\partial \xi} + \bar{B} \frac{\partial \bar{T}}{\partial \eta} + \bar{C} \frac{\partial \bar{T}}{\partial \zeta} + \bar{J}_\sigma = 0 \quad (4.67)
\]

\[
\frac{\partial \bar{T}}{\partial \tau} + \tilde{A} \frac{\partial \bar{T}}{\partial \xi} + \tilde{B} \frac{\partial \bar{T}}{\partial \eta} + \tilde{C} \frac{\partial \bar{T}}{\partial \zeta} + \tilde{J}_\sigma = 0 \quad (4.68)
\]
Where,

\[ \tilde{A} = \frac{\partial \bar{P}}{\partial T} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\xi_z}{\varepsilon} & -\frac{\xi_y}{\varepsilon} \\ 0 & 0 & 0 & -\frac{\xi_z}{\varepsilon} & 0 & \frac{\xi_x}{\varepsilon} \\ 0 & 0 & 0 & \frac{\xi_y}{\varepsilon} & -\frac{\xi_x}{\varepsilon} & 0 \\ 0 & -\frac{\xi_z}{\mu} & \frac{\xi_y}{\mu} & 0 & 0 & 0 \\ \frac{\xi_z}{\mu} & 0 & -\frac{\xi_x}{\mu} & 0 & 0 & 0 \\ -\frac{\xi_y}{\mu} & \frac{\xi_x}{\mu} & 0 & 0 & 0 & 0 \end{bmatrix} \]

\[ \tilde{B} = \frac{\partial \bar{Q}}{\partial T} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\eta_z}{\varepsilon} & -\frac{\eta_y}{\varepsilon} \\ 0 & 0 & 0 & -\frac{\eta_z}{\varepsilon} & 0 & \frac{\eta_x}{\varepsilon} \\ 0 & 0 & 0 & \frac{\eta_y}{\varepsilon} & -\frac{\eta_x}{\varepsilon} & 0 \\ 0 & -\frac{\eta_z}{\mu} & \frac{\eta_y}{\mu} & 0 & 0 & 0 \\ \frac{\eta_z}{\mu} & 0 & -\frac{\eta_x}{\mu} & 0 & 0 & 0 \\ -\frac{\eta_y}{\mu} & \frac{\eta_x}{\mu} & 0 & 0 & 0 & 0 \end{bmatrix} \]

\[ \tilde{C} = \frac{\partial \bar{R}}{\partial T} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\zeta_z}{\varepsilon} & -\frac{\zeta_y}{\varepsilon} \\ 0 & 0 & 0 & -\frac{\zeta_z}{\varepsilon} & 0 & \frac{\zeta_x}{\varepsilon} \\ 0 & 0 & 0 & \frac{\zeta_y}{\varepsilon} & -\frac{\zeta_x}{\varepsilon} & 0 \\ 0 & -\frac{\zeta_z}{\mu} & \frac{\zeta_y}{\mu} & 0 & 0 & 0 \\ \frac{\zeta_z}{\mu} & 0 & -\frac{\zeta_x}{\mu} & 0 & 0 & 0 \\ -\frac{\zeta_y}{\mu} & \frac{\zeta_x}{\mu} & 0 & 0 & 0 & 0 \end{bmatrix} \]
The eigenvalues of the Jacobian matrices $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$ are presented in equation (4.70), (4.71) and (4.72), respectively. The theoretical aspects of the eigenvalues were discussed for 2D model equations and therefore, are not repeated here.

$$\lambda_{1A} = 0$$

$$\lambda_{2A} = 0$$

$$\lambda_{3A} = -\frac{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}{\sqrt{\mu \varepsilon}} = -c \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}$$

$$\lambda_{4A} = -\frac{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}{\sqrt{\mu \varepsilon}} = -c \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}$$

(4.70)

$$\lambda_{5A} = \frac{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}{\sqrt{\mu \varepsilon}} = c \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}$$

$$\lambda_{6A} = \frac{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}}{\sqrt{\mu \varepsilon}} = c \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}$$
\[ \lambda_{1b} = 0 \]

\[ \lambda_{2b} = 0 \]

\[ \lambda_{3b} = -\frac{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}}{\sqrt{\mu\varepsilon}} = -c\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} \]

\[ \lambda_{4b} = -\frac{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}}{\sqrt{\mu\varepsilon}} = -c\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} \hspace{1cm} (4.71) \]

\[ \lambda_{5b} = \frac{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}}{\sqrt{\mu\varepsilon}} = c\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} \]

\[ \lambda_{6b} = \frac{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}}{\sqrt{\mu\varepsilon}} = c\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} \]
\[ \lambda_{1c} = 0 \]

\[ \lambda_{2c} = 0 \]

\[ \lambda_{3c} = -\frac{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}}{\sqrt{\mu \epsilon}} = -c \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]

\[ \lambda_{4c} = -\frac{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}}{\sqrt{\mu \epsilon}} = -c \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]  \hspace{1cm} (4.72)

\[ \lambda_{5c} = \frac{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}}{\sqrt{\mu \epsilon}} = c \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]

\[ \lambda_{6c} = \frac{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}}{\sqrt{\mu \epsilon}} = c \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]

Let us define,

\[ \psi = \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]

\[ \theta = \sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} \]

\[ \varsigma = \sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \]

And impedance of a material is defined as,

\[ Z = \frac{\mu}{\sqrt{\epsilon}} \]
The resultant eigenvector matrix of the Jacobian matrices \( \bar{A} \), \( \bar{B} \) and \( \bar{C} \) are

\[
\chi_A = \begin{bmatrix}
0 & \frac{\xi_x}{\xi_z} & \frac{\xi_y Z}{\psi} & -\frac{\xi_z Z}{\psi} & -\frac{\xi_y Z}{\psi} & \frac{\xi_z Z}{\psi} \\
0 & \frac{\xi_y}{\xi_z} & -\frac{(\xi_x^2 + \xi_z^2) Z}{\xi_x \psi} & -\frac{\xi_y \xi_z Z}{\xi_x \psi} & \frac{(\xi_x^2 + \xi_z^2) Z}{\xi_x \psi} & \frac{\xi_y \xi_z Z}{\xi_x \psi} \\
0 & 1 & \frac{\xi_y \xi_z Z}{\xi_x \psi} & \frac{(\xi_x^2 + \xi_y^2) Z}{\xi_x \psi} & -\frac{\xi_y \xi_z Z}{\xi_x \psi} & -\frac{(\xi_x^2 + \xi_y^2) Z}{\xi_x \psi} \\
\frac{\xi_x}{\xi_z} & 0 & -\frac{\xi_z}{\xi_x} & -\frac{\xi_y}{\xi_x} & -\frac{\xi_z}{\xi_x} & -\frac{\xi_y}{\xi_x} \\
\frac{\xi_y}{\xi_z} & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 0
\end{bmatrix}
\]

\[
\chi_B = \begin{bmatrix}
0 & \frac{\eta_x}{\eta_z} & \frac{\eta_y Z}{\vartheta} & -\frac{\eta_z Z}{\vartheta} & -\frac{\eta_y Z}{\vartheta} & \frac{\eta_z Z}{\vartheta} \\
0 & \frac{\eta_y}{\eta_z} & -\frac{(\eta_x^2 + \eta_z^2) Z}{\eta_x \vartheta} & -\frac{\eta_y \eta_z Z}{\eta_x \vartheta} & \frac{(\eta_x^2 + \eta_z^2) Z}{\eta_x \vartheta} & \frac{\eta_y \eta_z Z}{\eta_x \vartheta} \\
0 & 1 & \frac{\eta_y \eta_z Z}{\eta_x \vartheta} & \frac{(\eta_x^2 + \eta_y^2) Z}{\eta_x \vartheta} & -\frac{\eta_y \eta_z Z}{\eta_x \vartheta} & -\frac{(\eta_x^2 + \eta_y^2) Z}{\eta_x \vartheta} \\
\frac{\eta_x}{\eta_z} & 0 & -\frac{\eta_z}{\eta_x} & -\frac{\eta_y}{\eta_x} & -\frac{\eta_z}{\eta_x} & -\frac{\eta_y}{\eta_x} \\
\frac{\eta_y}{\eta_z} & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 0
\end{bmatrix}
\]
\[
\chi_c = \begin{bmatrix}
0 & \frac{\zeta_x}{\zeta_z} & \frac{\zeta_y Z}{\zeta} & -\frac{\zeta_z Z}{\zeta} & -\frac{\zeta_y Z}{\zeta} & \frac{\zeta_z Z}{\zeta} \\
0 & \frac{\zeta_y}{\zeta_z} & -\frac{(\zeta_x^2 + \zeta_y^2) Z}{\zeta_x Z} & -\frac{\zeta_y Z}{\zeta_x Z} & \frac{(\zeta_x^2 + \zeta_y^2) Z}{\zeta_x Z} & \frac{\zeta_y Z}{\zeta_x Z} \\
0 & 1 & \frac{\zeta_y Z}{\zeta_x Z} & \frac{(\zeta_x^2 + \zeta_y^2) Z}{\zeta_x Z} & -\frac{\zeta_y Z}{\zeta_x Z} & \frac{(\zeta_x^2 + \zeta_y^2) Z}{\zeta_x Z} \\
\frac{\zeta_x}{\zeta_z} & 0 & -\frac{\zeta_y}{\zeta_x} & -\frac{\zeta_x}{\zeta_x} & \frac{\zeta_y}{\zeta_x} & -\frac{\zeta_x}{\zeta_x} \\
\frac{\zeta_y}{\zeta_z} & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 0
\end{bmatrix}
\]

4.5 Numerical Model Development

In this section, the fourth-order modified Runge-Kutta formulation of the model equation in computational domain is presented.

4.5.1 Grid Scheme

As we know that the Yee’s FDTD grid [1], also known as the staggered grid, is the standard method of specifying electric and magnetic field variables on the grid points for simulating propagation of electromagnetic waves, however, we have performed initial investigations in two-dimensions using both unstaggered or collocated grid and staggered grid approach. Hence, we will present two-dimensional formulation using both approaches and three-dimensional formulation using staggered grid approach in the following sections. Before continuing with the formulation, brief theoretical aspects of the two approaches are presented in this section.
4.5.1.1 Unstaggered or Collocated Grid

In the unstaggered grid approach, the electric and magnetic field variables are specified at each grid points within the domain, as shown in Figure 4.1.(a). By using such an approach, the distance between two cells is specified by unit grid step, $\Delta x$ and $\Delta y$. This approach is used rarely for simulating electromagnetic phenomena. Liu [124] has established that the requirement of a minimum number of grid points per smallest wavelength increases when unstaggered approach is used in order to maintain the acceptable level of accuracy.

4.5.1.2 Staggered Grid

According to this approach, the electric field vector and magnetic field vectors are solved on two different grids separated by half cells, $\Delta x/2$ and $\Delta y/2$, as shown in Figure 4.1.(b) in space and hence two grids can be named as primary and secondary grid systems. As a result of this approach, each electric field variable is surrounded by four magnetic field variables and each magnetic field variable is surrounded by two electric field variables. In addition to grid staggering, time staggering or leapfrog is also employed to reduce dissipation errors. For electromagnetic applications, the staggered grid approach is known to be more accurate than any other approach in finite difference time domain techniques.
We have presented initial investigations using unstaggered grid approach and subsequently, a comparison is presented between the unstaggered grid and the staggered grid approaches to demonstrate the accuracy of the two approaches. Henceforth, the staggered grid approach will be used for all investigations.

4.5.2 Two-Dimensional Formulation in Transformed Coordinate

Before proceeding ahead with the finite difference approximation of Maxwell’s equations, a prerequisite is to rearrange terms associated with $\bar{T}_1$ on right hand side of Eq. (4.74). Rewrite equation (4.34) in the finite-difference form as

$$
\bar{T}_{1_{i,j}}^{n+1} = \bar{T}_{1_{i,j}}^{n} - \frac{\Delta \tau}{\epsilon_{i,j}} \left[ \left( \frac{\Delta \bar{P}_1}{\Delta \xi} \right)_{i,j}^{n} + \left( \frac{\Delta \bar{Q}_1}{\Delta \eta} \right)_{i,j}^{n} + K_{\sigma_{i,j}} \bar{T}_{1_{i,j}}^{n} \right]
$$

The resultant equation is

$$
\bar{T}_{1_{i,j}}^{n+1} = \left( 1 - \frac{\Delta \tau}{\epsilon_{i,j}} K_{\sigma_{i,j}} \right) \bar{T}_{1_{i,j}}^{n} - \frac{\Delta \tau}{\epsilon_{i,j}} \left[ \left( \frac{\Delta \bar{P}_1}{\Delta \xi} \right)_{i,j}^{n} + \left( \frac{\Delta \bar{Q}_1}{\Delta \eta} \right)_{i,j}^{n} \right]
$$

(4.75)

It is observed that the variable $\bar{T}_1$ is computed at time step, $n+1$ using the known vector quantities at time step, $n$. However, a standard procedure as defined in the literature is to approximate the electric field variable on the right-hand side of the governing equation by time-averaging the value over two time steps.

4.5.2.1 Unstaggered Grid Approach

The application of fourth-order Runge-Kutta approximation to the model equations (4.34) - (4.36) is presented next. Using the approach similar to equation (4.75), the MRK representation for $\bar{T}_1$ is obtained as presented in equation (4.76).
The convective terms in equation (4.76) are estimated using second-order central differencing scheme; the formulation is provided in equation (4.77).

\[
\left( \frac{\partial \bar{P}_1}{\partial \xi} \right)_{i,j}^{n} + \left( \frac{\partial \bar{Q}_1}{\partial \eta} \right)_{i,j}^{n} = \frac{\bar{p}^{n}_{i+1,j} - \bar{p}^{n}_{i-1,j}}{2\Delta \xi} + \frac{\bar{q}^{n}_{i,j+1} - \bar{q}^{n}_{i,j-1}}{2\Delta \eta}
\]
In a similar manner, MRK approximation for $T_2$, and $T_3$, is described in equation (4.78) and (4.80), respectively.

$$\bar{T}_{2,i,j}^{(1)} = \bar{T}_{2,i,j}^n$$

1st stage:

$$\bar{T}_{2,i,j}^{(2)} = \bar{T}_{2,i,j}^n - \frac{\Delta \tau}{3\mu_{i,j}} \left[ \left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^{(1)} + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^{(1)} \right]$$

2nd stage:

$$\bar{T}_{2,i,j}^{(3)} = \bar{T}_{2,i,j}^n - \frac{\Delta \tau}{2\mu_{i,j}} \left[ \left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^{(2)} + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^{(2)} \right]$$

3rd stage:

$$\bar{T}_{2,i,j}^{(4)} = \bar{T}_{2,i,j}^n - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^{(3)} + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^{(3)} \right]$$

4th stage:

$$\bar{T}_{2,i,j}^{n+1} = \bar{T}_{2,i,j}^n - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^{(4)} \right]$$

The formulation for solving convective terms in equation (4.78) by second-order approximation is given as

$$\left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^n + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^n = \frac{\bar{P}_{2,i+1,j}^n - \bar{P}_{2,i-1,j}^n}{2\Delta \xi} + \frac{\bar{Q}_{2,i,j+1}^n - \bar{Q}_{2,i,j-1}^n}{2\Delta \eta}$$

(4.79)
\[
\overline{T}_{3,ij}^{(1)} = \overline{T}_{3,ij}^n
\]

1\textsuperscript{st} stage:
\[
\overline{T}_{3,ij}^{(2)} = \overline{T}_{3,ij}^n - \frac{\Delta \tau}{4\mu_i,j} \left[ \left( \frac{\partial P_3}{\partial \xi} \right)_{i,j}^{(1)} + \left( \frac{\partial Q_3}{\partial \eta} \right)_{i,j}^{(1)} \right]
\]

2\textsuperscript{nd} stage:
\[
\overline{T}_{3,ij}^{(3)} = \overline{T}_{3,ij}^n - \frac{\Delta \tau}{3\mu_i,j} \left[ \left( \frac{\partial P_3}{\partial \xi} \right)_{i,j}^{(2)} + \left( \frac{\partial Q_3}{\partial \eta} \right)_{i,j}^{(2)} \right]
\]

3\textsuperscript{rd} stage:
\[
\overline{T}_{3,ij}^{(4)} = \overline{T}_{3,ij}^n - \frac{\Delta \tau}{2\mu_i,j} \left[ \left( \frac{\partial P_3}{\partial \xi} \right)_{i,j}^{(3)} + \left( \frac{\partial Q_3}{\partial \eta} \right)_{i,j}^{(3)} \right]
\]

4\textsuperscript{th} stage:
\[
\overline{T}_{3,ij}^{n+1} = \overline{T}_{3,ij}^n - \frac{\Delta \tau}{\mu_i,j} \left[ \left( \frac{\partial P_3}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial Q_3}{\partial \eta} \right)_{i,j}^{(4)} \right]
\]

Where,
\[
\left( \frac{\partial P_3}{\partial \xi} \right)_{i,j}^n + \left( \frac{\partial Q_3}{\partial \eta} \right)_{i,j}^n = \frac{P_{3,i+1,j}^n - P_{3,i-1,j}^n}{2\Delta \xi} + \frac{Q_{3,i+1,j}^n - Q_{3,i-1,j}^n}{2\Delta \eta}
\]  

(4.81)

Using the equations (4.76), (4.78) and (4.80), flux vector components \(\overline{T}_1\), \(\overline{T}_2\), and \(\overline{T}_3\) will be computed in the following way; First stage for solving \(\overline{T}_1\), \(\overline{T}_2\), and \(\overline{T}_3\) is computed at \(n+1\) time level at all \((i, j)\) index locations using the values from the previous time step, update \(\overline{T}_1 \rightarrow E_z\), \(\overline{T}_2 \rightarrow H_x\), \(\overline{T}_3 \rightarrow H_y\), update flux vectors \(P\) and \(Q\) from primitive variables \(E_z\), \(H_x\), and \(H_y\). Subsequently, the second, third, and fourth stages will be computed using the values from the previous stage of the same time level. The solution will advance in time until it reaches the desired time level for time dependence analysis or until the solution is converged in case of steady state analysis.
### 4.5.2.2 Staggered Grid Approach

The fourth-order MRK approximation on the staggered grid is very similar to the unstaggered grid approach, however, the difference between the two approaches is the specification of the central difference approximation of the spatial derivatives and the leapfrog approach for temporal discretization. Recall from Figure 4.1(b) that the electric field variable is specified at integer index locations \((x, x+\Delta x, x+2\Delta x,\ldots)\), \((y, y+\Delta y, y+2\Delta y,\ldots)\) and the magnetic field variables are specified at \((\Delta x/2, x+\Delta x/2, x+3\Delta x/2,\ldots)\) and \((\Delta y/2, y+\Delta y/2, y+3\Delta y/2,\ldots)\) and the distance between the cells is \(\Delta x/2\) and \(\Delta y/2\). Using the standard notation, the index locations is written as \(i+1/2\) or \(i-1/2\), however, only the integer arrays can be defined in programming the numerical approximations. Therefore, the index location of \(i+1/2\) is assumed as \(i\) on secondary grid and the index location of \(i-1/2\) is assumed as \(i-1\). Similar approach is applicable of \(j\) indices in \(y\)-coordinate.

Consider the example equation (4.82) for better understanding, where the mathematical representation of central difference approximation of a variable \(f\) on staggered grid is presented.

\[
\left(\frac{\partial f}{\partial x}\right)_{i,j} = \frac{f_{i+1/2,j} - f_{i-1/2,j}}{2(\Delta x/2)}
\]  

(4.82)

As we know that such representation is impossible to specify in a programming language, a slightly different specification given below will allow us to easily code the staggered grid approach.

\[
\left(\frac{\partial f}{\partial x}\right)_{i,j} = \frac{f_{i,j} - f_{i-1,j}}{2(\Delta x/2)}
\]  

(4.83)

Using a similar approach, the central differencing of spatial derivatives in the MRK method can be easily specified. We are presenting the approximation equations in both standard notation form as well as the form that is easily readable by the computer program to establish the clear difference between two specifications. The fourth-stage of the MRK approximation of \(T_1\), \(T_2\), and \(T_3\) is presented in standard notation is given in equations (4.84) through (4.86), respectively.

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\[ \overline{T}_{1,i,j}^{n+1} = \left(1 - \frac{\Delta \tau}{\varepsilon K_{\sigma_{ij}}} \right) \overline{T}_{1,i,j}^{n} - \frac{\Delta \tau}{\varepsilon_{i,j}} \left[ \left( \frac{\partial \overline{P}_{1}}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial \overline{Q}_{1}}{\partial \eta} \right)_{i,j}^{(4)} \right] \] (4.84)

\[ \overline{T}_{2,i,j+1/2}^{n+1} = \overline{T}_{2,i,j+1/2}^{n} - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{2}}{\partial \xi} \right)_{i,j+1/2}^{(4)} + \left( \frac{\partial \overline{Q}_{2}}{\partial \eta} \right)_{i,j+1/2}^{(4)} \right] \] (4.85)

\[ \overline{T}_{3,i+1/2,j}^{n+1} = \overline{T}_{3,i+1/2,j}^{n} - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{3}}{\partial \xi} \right)_{i+1/2,j}^{(4)} + \left( \frac{\partial \overline{Q}_{3}}{\partial \eta} \right)_{i+1/2,j}^{(4)} \right] \] (4.86)

Where,

\[ \left( \frac{\partial \overline{P}_{1}}{\partial \xi} \right)_{i,j}^{n} + \left( \frac{\partial \overline{Q}_{1}}{\partial \eta} \right)_{i,j}^{n} = \frac{\overline{P}_{1,i+1/2,j}^{n} - \overline{P}_{1,i-1/2,j}^{n}}{\Delta \xi} + \frac{\overline{Q}_{1,i,j+1/2}^{n} - \overline{Q}_{1,i,j-1/2}^{n}}{\Delta \eta} \] (4.87)

\[ \left( \frac{\partial \overline{P}_{2}}{\partial \xi} \right)_{i,j+1/2}^{n} + \left( \frac{\partial \overline{Q}_{2}}{\partial \eta} \right)_{i,j+1/2}^{n} = \frac{\overline{P}_{2,i+1/2,j+1/2}^{n} - \overline{P}_{2,i-1/2,j+1/2}^{n}}{\Delta \xi} + \frac{\overline{Q}_{2,i,j+1}^{n} - \overline{Q}_{2,i,j}^{n}}{\Delta \eta} \] (4.88)

\[ \left( \frac{\partial \overline{P}_{3}}{\partial \xi} \right)_{i+1/2,j}^{n} + \left( \frac{\partial \overline{Q}_{3}}{\partial \eta} \right)_{i+1/2,j}^{n} = \frac{\overline{P}_{3,i+1/2,j+1/2}^{n} - \overline{P}_{3,i,j+1/2}^{n}}{\Delta \xi} + \frac{\overline{Q}_{3,i,j}^{n} - \overline{Q}_{3,i,j-1/2}^{n}}{\Delta \eta} \] (4.89)

The finite difference approximation of the staggered approach specified in the computer codes is

\[ \overline{T}_{1,i,j}^{n+1} = \left(1 - \frac{\Delta \tau}{\varepsilon K_{\sigma_{ij}}} \right) \overline{T}_{1,i,j}^{n} - \frac{\Delta \tau}{\varepsilon_{i,j}} \left[ \left( \frac{\partial \overline{P}_{1}}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial \overline{Q}_{1}}{\partial \eta} \right)_{i,j}^{(4)} \right] \] (4.90)

\[ \overline{T}_{2,i,j}^{n+1} = \overline{T}_{2,i,j}^{n} - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{2}}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial \overline{Q}_{2}}{\partial \eta} \right)_{i,j}^{(4)} \right] \] (4.91)

\[ \overline{T}_{3,i,j}^{n+1} = \overline{T}_{3,i,j}^{n} - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{3}}{\partial \xi} \right)_{i,j}^{(4)} + \left( \frac{\partial \overline{Q}_{3}}{\partial \eta} \right)_{i,j}^{(4)} \right] \] (4.92)
Where,

$$
\left( \frac{\partial \bar{P}_1}{\partial \xi} \right)_{i,j}^n + \left( \frac{\partial \bar{Q}_1}{\partial \eta} \right)_{i,j}^n = \frac{\bar{P}_{1,i,j}^n - \bar{P}_{1,i-1,j}^n}{\Delta \xi} + \frac{\bar{Q}_{1,i,j}^n - \bar{Q}_{1,i,j-1}^n}{\Delta \eta}
$$

(4.93)

$$
\left( \frac{\partial \bar{P}_2}{\partial \xi} \right)_{i,j}^n + \left( \frac{\partial \bar{Q}_2}{\partial \eta} \right)_{i,j}^n = \frac{\bar{P}_{2,i+1,j}^n - \bar{P}_{2,i,j}^n}{\Delta \xi} + \frac{\bar{Q}_{2,i,j+1}^n - \bar{Q}_{2,i,j}^n}{\Delta \eta}
$$

(4.94)

$$
\left( \frac{\partial \bar{P}_3}{\partial \xi} \right)_{i,j}^n + \left( \frac{\partial \bar{Q}_3}{\partial \eta} \right)_{i,j}^n = \frac{\bar{P}_{3,i+1,j}^n - \bar{P}_{3,i,j}^n}{\Delta \xi} + \frac{\bar{Q}_{3,i,j+1}^n - \bar{Q}_{3,i,j}^n}{\Delta \eta}
$$

(4.95)

Upon comparison of the approximation equations for spatial derivatives, there is an obvious difference in the notations. This difference is due to the reason that the $\bar{T}_2$ and $\bar{T}_3$ vectors in equation (4.91) and (4.92) corresponds to magnetic field variables which are specified on secondary grid located at half integer indices. The magnetic field variables are calculated using electric field variables from the neighboring locations which is the primary grid. In equation (4.90), $\bar{T}_1$ corresponds to the electric field variable which is computed using neighboring magnetic field variables on secondary grid whose index locations $i+1/2$ and $j+1/2$ are treated as $i$ and $j$, respectively. This sums up the approach of specifying MRK approximation using staggered grid approach.

### 4.5.2.3 Leapfrog Modified Runge Kutta Approach

We have altered the MRK method by introducing the concept of leapfrogging the stages. The leapfrog time stepping is the fundamental approach in Yee-FDTD [1] method. The MRK method, as will be shown later in this report, is prone to dissipation errors. We have found that when the solution is setup to initial conditions as the source of excitation, there is no dissipation, whereas for applications such as in far field scattering, soft sources or hard sources excitation method is used. Such an approach results in the amplitude dissipation. The dissipation errors of MRK method is well recorded in the published literature, however, MRK is still a very popular numerical method because the advantages of the MRK method far outweighs the cost of dissipation error. Therefore, with the aim to reduce the dissipation and to utilize the stability benefits of MRK scheme, we investigated the results obtained by staggering the stages of MRK in time. In our knowledge, this approach has not been investigated in the past. We found that by using such
an approach the dissipation was greatly reduced which is discussed in the results chapter. The description of the leapfrog Modified Runge-Kutta scheme is presented next.

Using the equations (4.76), (4.78) and (4.80), flux vector components $\overline{T}_1$, $\overline{T}_2$, and $\overline{T}_3$ will be computed in the following way; the first stage for solving $\overline{T}_1$ is computed at $n+1$ time level at all $(i,j)$ index locations using the values of $H_x$, and $H_y$ from the previous time step and update $\overline{T}_1 \rightarrow E_z$. Subsequently, update flux vectors $P$ and $Q$ from primitive variable $E_z$. The first stage for $\overline{T}_2$, and $\overline{T}_3$ is computed at $n+1/2$ using the updated values of $E_z$ calculated in the first stage. After computing at all grid points, update, $\overline{T}_2 \rightarrow H_x$, $\overline{T}_3 \rightarrow H_y$, and flux vectors $P$ and $Q$ from primitive variables $H_x$ and $H_y$. Subsequently, the second, third, and fourth stages will be computed using the values from the interleaved stages of the same time level. The solution will advance in time until it reaches the desired time level for time dependence analysis or until the solution is converged in case of steady state analysis. The spatial derivatives are computed by the staggered grid approach presented in Section 4.5.2.2.

The results of the simulation of travelling waves in one-dimension is presented in Figure 4.2.

Figure 4.2. Numerical simulation of a sine wave traveling with frequency, $f = 3.0$ GHz, 201 grid points. The frequency of simulated sine wave is 3.0 GHz and 201 grid are selected that corresponds to a sampling rate of 20 points per wavelength. The comparison of the results obtained from the MRK scheme, MRK-
leapfrog and the FDTD method at different time steps suggests that the amplitude of waves predicted by MRK is reduced by 50% as compared with the FDTD method that is dissipation-less in one-dimension. The numerical results computed with MRK-leapfrog demonstrates an acceptable level of accuracy.

### 4.5.3 Three Dimensional Formulation in Transformed Coordinates

Using a similar approach described previously for two dimensional formulation on staggered grid, three-dimensional approximation equations on staggered grid are derived and presented in this section. The four stages of the MRK with leapfrogging of stages is utilized to advance in time. In three-dimensions, let’s recall that the flux vectors components $\vec{T}_1$, $\vec{T}_2$, and $\vec{T}_3$ corresponds to electric field variables and the vectors components $\vec{T}_4$, $\vec{T}_5$, and $\vec{T}_6$ corresponds to magnetic field variables. Since the index specification of the $\vec{T}_1$, $\vec{T}_2$, and $\vec{T}_3$ will be same, only the MRK approximation of $\vec{T}_1$ is presented in equation (4.96) and a similar formulation is obtained for $\vec{T}_2$, and $\vec{T}_3$.

$$T^{(1)}_{1,i,j,k} = T^n_{1,i,j,k}$$

1st stage:  
$$T^{(2)}_{1,i,j,k} = \left(1 - \frac{\Delta \tau}{4\varepsilon_{i,j}} K_{\sigma_{i,j}}\right) T^n_{1,i,j,k} - \frac{\Delta \tau}{4\varepsilon_{i,j}} \left[ \left(\frac{\partial P_1}{\partial \xi}\right)_{i,j,k}^{(1)} + \left(\frac{\partial Q_1}{\partial \eta}\right)_{i,j,k}^{(1)} + \left(\frac{\partial R_1}{\partial \zeta}\right)_{i,j,k}^{(1)} \right]$$

2nd stage:  
$$T^{(3)}_{1,i,j,k} = \left(1 - \frac{\Delta \tau}{3\varepsilon_{i,j}} K_{\sigma_{i,j}}\right) T^n_{1,i,j,k} - \frac{\Delta \tau}{3\varepsilon_{i,j}} \left[ \left(\frac{\partial P_1}{\partial \xi}\right)_{i,j,k}^{(2)} + \left(\frac{\partial Q_1}{\partial \eta}\right)_{i,j,k}^{(2)} + \left(\frac{\partial R_1}{\partial \zeta}\right)_{i,j,k}^{(2)} \right]$$

3rd stage:  
$$T^{(4)}_{1,i,j,k} = \left(1 - \frac{\Delta \tau}{2\varepsilon_{i,j}} K_{\sigma_{i,j}}\right) T^n_{1,i,j,k} - \frac{\Delta \tau}{2\varepsilon_{i,j}} \left[ \left(\frac{\partial P_1}{\partial \xi}\right)_{i,j,k}^{(3)} + \left(\frac{\partial Q_1}{\partial \eta}\right)_{i,j,k}^{(3)} + \left(\frac{\partial R_1}{\partial \zeta}\right)_{i,j,k}^{(3)} \right]$$

4th stage:  
$$T^{n+1}_{1,i,j,k} = \left(1 - \frac{\Delta \tau}{\varepsilon_{i,j}} K_{\sigma_{i,j}}\right) T^n_{1,i,j,k} - \frac{\Delta \tau}{\varepsilon_{i,j}} \left[ \left(\frac{\partial P_1}{\partial \xi}\right)_{i,j,k}^{(4)} + \left(\frac{\partial Q_1}{\partial \eta}\right)_{i,j,k}^{(4)} + \left(\frac{\partial R_1}{\partial \zeta}\right)_{i,j,k}^{(4)} \right]$$
Where, the convective terms are approximated by second-order central difference approximation as presented in equation (4.97).

\[
\left( \frac{\partial \overline{P}_{1}^{n}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{1}^{n}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{1}^{n}}{\partial \zeta} \right)_{i,j,k} = \frac{\overline{P}_{1,i,j,k}^{n} - \overline{P}_{1,i-1,j,k}^{n}}{\Delta \xi} + \frac{\overline{Q}_{1,i,j,k}^{n} - \overline{Q}_{1,i,j-1,k}^{n}}{\Delta \eta} + \frac{\overline{R}_{1,i,j,k}^{n} - \overline{R}_{1,i,j-1,k}^{n}}{\Delta \zeta}
\]

Similarly, the MRK approximation of only \( T_{4} \) is presented in equation (4.98) in the notations as specified in computer codes and \( \overline{T}_{5} \) and \( \overline{T}_{6} \) is formulated in a similar manner.

\[
\overline{T}_{4,i,j,k}^{(1)} = \overline{T}_{4,i,j,k}^{n}
\]

1st stage:

\[
\overline{T}_{4,i,j,k}^{(2)} = \overline{T}_{4,i,j,k}^{n} - \frac{\Delta \tau}{4 \mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{4}^{(1)}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{4}^{(1)}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{4}^{(1)}}{\partial \zeta} \right)_{i,j,k} \right]
\]

2nd stage:

\[
\overline{T}_{4,i,j,k}^{(3)} = \overline{T}_{4,i,j,k}^{n} - \frac{\Delta \tau}{3 \mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{4}^{(2)}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{4}^{(2)}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{4}^{(2)}}{\partial \zeta} \right)_{i,j,k} \right]
\]

3rd stage:

\[
\overline{T}_{4,i,j,k}^{(4)} = \overline{T}_{4,i,j,k}^{n} - \frac{\Delta \tau}{2 \mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{4}^{(3)}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{4}^{(3)}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{4}^{(3)}}{\partial \zeta} \right)_{i,j,k} \right]
\]

4th stage:

\[
\overline{T}_{4,i,j,k}^{n+1} = \overline{T}_{4,i,j,k}^{n} - \frac{\Delta \tau}{\mu_{i,j}} \left[ \left( \frac{\partial \overline{P}_{4}^{(4)}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{4}^{(4)}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{4}^{(4)}}{\partial \zeta} \right)_{i,j,k} \right]
\]

The space derivatives are approximated using second-order central difference approximation presented in equation (4.99).

\[
\left( \frac{\partial \overline{P}_{4}^{n}}{\partial \xi} \right)_{i,j,k} + \left( \frac{\partial \overline{Q}_{4}^{n}}{\partial \eta} \right)_{i,j,k} + \left( \frac{\partial \overline{R}_{4}^{n}}{\partial \zeta} \right)_{i,j,k} = \frac{\overline{P}_{4,i+1,j,k}^{n} - \overline{P}_{4,i,j,k}^{n}}{\Delta \xi} + \frac{\overline{Q}_{4,i+1,j,k}^{n} - \overline{Q}_{4,i,j,k}^{n}}{\Delta \eta} + \frac{\overline{R}_{4,i+1,j,k}^{n} - \overline{R}_{4,i,j,k}^{n}}{\Delta \zeta}
\]
4.6 Boundary and Interface Conditions

In the mathematics of partial differential equations, the set of constraints are imposed to restrict the region where the governing equations will be valid. The set of constraints are the boundary conditions which can be determined using the physics of the problem represented by the governing equations. A well-posed boundary condition ensures the accuracy of the solution. In computational simulations, the size of the computational domain is restricted by the application of boundary conditions. The dependent variable or its derivative is specified at the boundary to terminate the simulation region. The inaccurate modeling of boundary conditions leads to spurious reflections, unknown non-physical errors, introduce instability in the solution, or affect solution convergence. The modeling of boundary conditions depends on the application. For example, in computational electromagnetics, the boundary conditions in waveguide application are specified by the properties of the perfect conductor. Applications involving open region are generally modeled using Perfectly Matched Layer boundary conditions. Investigators have presented several methods to accurately incorporate boundary conditions for open-region applications. The other categories are the periodic boundary condition, impedance boundary conditions, to name a few. In this section, the useful boundary conditions for applications involving simulation of EM waves in open region are discussed.

4.6.1 Outer Boundaries

The imposition of boundary conditions at the outer edges is performed either to restrict the simulation space of the open problem or accurately specify the physics of the problem, such as in the case of waveguides. Open problems are the class of application where the modeled device is surrounded by a free space and therefore, extent of the boundaries can be infinite. The various types of boundary condition that can be imposed at the boundaries open problem are described next.

Perfect Conducting Boundary Conditions

The studies presented in the paper are the open problems and the outer boundaries are specified by the application of the ideal boundary conditions known as the perfectly conducting boundary conditions which assumes the presence of electric or magnetic conductors at the outer edges. Mathematically, such conditions for perfect electrical conductors (PEC) are represented as
It is because no tangential electric field exists at the surface of the PEC that results in the normal magnetic fields at the surface equals to zero. These boundaries conditions are straightforward to apply, however, not an accurate representation of the open problem as it will lead to artificial reflections of the waves from the boundary that will corrupt the solution. This limitation is overcome by increasing the size of the domain to a larger size than required such that important physical phenomenon can be captured before any wave reach the boundary, subsequently, stop the simulation right before the wave is about to reach the boundary to avoid non-physical reflections.

For the open problems, several classes of boundary conditions have been developed and presented by the researchers. The most notable developments are the absorbing boundary conditions and the perfectly matched layer boundary conditions. Brief discussion and historical developments pertaining to them are presented next for informational purpose. However, we have used the PEC boundary conditions in the studied cases.

*Absorbing Boundary Conditions*

The purpose of the absorbing boundary conditions is to prevent the reflection of non-physical waves back into the simulation region in such a manner that the wave appears to be propagating outwards at all boundaries as it would in a physical world. The advantage of using ABCs is that the required results can be obtained by using a much smaller simulation region, which leads to fewer grid points and faster computations. The application of absorbing boundary conditions in electromagnetic simulations was first reported by Taylor et al. [125] wherein they used a simple linear interpolation technique for specifying field variables at the boundaries of the domain. Taflove and Brodwin [12] presented an approach that would interpolate the wave using field values from adjacent interior points from the previous time step, which is exact for 1-D applications, however, approximate for 2-D and 3-D applications because of the oblique
incidence of waves on the boundaries. Subsequently, Taflove [4] presented another work on ABC by introducing conductivity within the free space region to dampen the outgoing fields as it would happen in the lossy dielectric, however, it was an inefficient method for absorption of waves. Engquist and Majda [2] developed localized boundary conditions for the scalar wave equation. Based on this approach, Mur[3] presented a superior method of boundary truncation for electromagnetic applications.

Perfectly Matched Layer Boundary Conditions

Perfectly Matched layer, as defined by Berenger[5], a class of absorbing boundary condition was introduced in 1994 for FDTD methods. The application of PML for wave structure interaction was demonstrated in Berenger[5]. PML are the upgraded version of the ABCs and the fundamental purpose to absorb the outgoing electromagnetic waves without reflection remains same. Subsequently, Katz et al. [6] extended the application of PML to the three-dimensional space. Eventually, PML method became the benchmark in electromagnetic problems. The PMLs are demonstrated to be the most efficient method of terminating the boundaries of open problem without spurious reflections and several developments based on the PML method have been reported in the literature till date.

4.6.2 Material Interfaces

The material investigations presented in this report assumes three types of materials, viz. lossless, lossy and PEC. The conditions at the boundaries of the lossless and lossy materials are represented as

\[ n \cdot (D_1 - D_2) = 0 \]
\[ n \times (E_1 - E_2) = 0 \]
\[ n \cdot (B_1 - B_2) = 0 \]
\[ n \times (H_1 - H_2) = 0 \]

(4.101)

The subscripts 1 and 2 in the interface conditions represent the regions within the domain where 1 represents the free space region and 2 represents any other material surrounded by free space region. These conditions are implicitly satisfied at the material boundaries in the finite difference approximation equations and
therefore, are not required to be explicitly stated in the codes. The material properties, however, are specified at each grid points within the domain based on the problem definition to define the presence of the material.

The PEC-free space interfaces are represented using the PEC boundary conditions in equation (4.100). No electric field and the magnetic fields exist at the grid points within the PEC material. However, on the surface of material i.e. the wall boundary condition, only the electric fields and the normal component of the magnetic fields are zero. The surface of the PEC is analogous to a no-slip wall in fluid dynamics. The existence of volume current density on the surface of metals, requires a slight modification in the boundary specification for magnetic fields.

\[ n \times (H_1 - H_2) = J \]  \hspace{1cm} (4.102)

4.7 Post-Processing

Post-processing of the time-domain data, obtained from the finite difference computations of Maxwell’s equation, by transforming the time-domain results to a more meaningful, quantifiable form is a vital step in electromagnetic investigations. The post-processing is performed to evaluate the spectral response of the scattering object at discrete frequencies of interest. The transformation of time-domain results to the frequency-domain results is carried out by using Fast Fourier Transform (FFT) method. The FFT method is very efficient to obtain the response of the device to multiple frequencies in a single simulation using impulse as a source. Another method to obtain a quantifiable data is to use sine waveform as the source. The frequency response can be obtained at a frequency of interest and subsequently the amplitude and phase can be determined. However, the drawback of this method is that the separate simulation run is required to obtain frequency response of different frequencies. Therefore, FFT method is the preferred choice for calculating frequency domain data.

The objective in this report is to present investigations using qualitative analysis, and since the frequency-domain data is used for quantitative analysis, therefore, the frequency domain results are
presented only for limited two-dimensional cases. A brief description of the FFT method given in Sullivan [118] is presented here.

The Fourier transform of time-domain electric field $E_z(t)$ at a frequency, $f$ is given by equation (4.103).

$$E_z(f) = \int_{0}^{T} E_z(t) \cdot e^{-i(2\pi ft)} dt$$  \hspace{1cm} (4.103)$$

Equation (4.104) is the finite difference form of the integral equation.

$$E_z(f) = \sum_{n=0}^{NM} E_z(n\Delta t) \cdot e^{-i(2\pi fn\Delta t)}$$  \hspace{1cm} (4.104)$$

Where $NM$ is the total number of time steps at which the solution is obtained. Using complex identity in equation (4.105), the finite difference expression in equation (4.104) is rewritten as in equation (4.106)

$$e^{-i\theta} = \cos \theta - i \sin \theta$$  \hspace{1cm} (4.105)$$

$$E_z(f) = \sum_{n=0}^{NM} E_z(n\Delta t) \cdot \{\cos(2\pi fn\Delta t) - i \sin(2\pi fn\Delta t)\}$$  \hspace{1cm} (4.106)$$

In computer program, a subroutine is added after the MRK subroutine for calculating the real and imaginary components of the electric field at all frequencies of interest, all grid point locations and at every time step until the time marching is aborted. The equations used in the computer codes are presented in equations (4.107) and (4.108). The flow of equations is in such a manner that the field values in time-domain will be computed at $n+1$ time step using the MRK formulation at all grid locations within the domain and subsequently using the electric field values at $n+1$ time step, the real and imaginary components at each frequency will be computed.

$$E_{z,real}^{n+1}_{f,i,j} = E_{z,real}^{n}_{f,i,j} + E_{z,real}^{n}_{f,i,j} \cdot \cos(2\pi fn\Delta t)$$  \hspace{1cm} (4.107)$$
\[ E_{z,\text{imag}}^{n,f,i,j} = E_{z,\text{imag}}^{n-1,f,i,j} - E_{z,i}^{n,f,i,j} \cdot \cos(2\pi fn\Delta t) \] (4.108)

After the code has looped through \( N \) time steps and the time-domain and frequency-domain results are obtained at the desired time level, the amplitude and phase at all frequencies is determined using the equations (4.109) and (4.110), respectively.

\[ \text{Amp}_{f,i,j} = \sqrt{(E_{z,\text{real}}^{NM,f,i,j})^2 + (E_{z,\text{imag}}^{NM,f,i,j})^2} \] (4.109)

\[ \text{Ph}_{f,i,j} = \tan^{-1}\left(\frac{E_{z,\text{imag}}^{NM,f,i,j}}{E_{z,\text{real}}^{NM,f,i,j}}\right) \] (4.110)

The computed amplitude and phase values are still not meaningful unless they are normalized using some reference quantity. Usually the reference quantity for normalizing output data is the frequency domain data of source field. There are several ways of using source field for normalization based on the source field specification, however, we have used the pointwise normalization of the total field using source field. The frequency domain source field data is obtained simultaneously with frequency domain total field at each locations and at all frequencies of interest. Subsequently, the total field amplitude is divided by source field amplitude at the locations of interest to determine various non-dimensional coefficients, such as transmittance and reflectance.

The flow chart presented in Figure 4.3 demonstrates the step-by-step algorithm for obtaining time-domain results as well as frequency-domain results.
Figure 4.3. Code algorithm for two-dimensional four-stage Runge-Kutta solver with post-processing.
CHAPTER 5
TOTAL FIELD-SCATTERED FIELD FORMULATION ON STAGGERED GRID

A brief fundamental idea of the total field-scattered field formulation has been discussed in Section 3.4.2.2. An assumed feature of the plane wave is that it retains its properties even after traveling large distances. Ideally, true plane waves are not possible, however, the plane waves can be assumed to exists in the localized region at a distance far away from the source. This property makes the plane wave an ideal candidate for simulation applications that involve far-field scattering. By implementing the TF-SF formulation and exciting the source field right outside the imaginary TF-SF boundary, the incoming source wave appears to have been generated at a far distance away from the scatterer and hence the requirement of increasing the computational domain to represent the physical distance can be overcome using such formulation. With temporal advance, the wave propagates through the region of interest and interact with the device located inside this region.

The TF-SF formulation for both two-dimensional and three-dimensional applications are presented in this Chapter. Generally, a plane wave is used to study far-field scattering pattern, however, the presented formulation assumes that the incoming wave is a cylindrical for two-dimensional applications and spherical for three-dimensional applications. The basic idea of TF-SF formulation method has been taken from Taflove [65], and Inan [116] and further derived in the transformed coordinate system for conducting the investigations to remain consistent with the proposed finite difference approximation method.

5.1 Methodology

The TF-SF formulation is based on the linearity of the Maxwell’s equations. Since the governing Maxwell’s equations are written in the flux vector form in transformed coordinate system, the TF-SF formulation must be derived using the same form. Therefore, linearity of Maxwell’s equation is expressed in terms of the flux vector. Due to this linearity, the scattered field, \( \vec{T}_{\text{scat}} \) and the incident field, \( \vec{T}_{\text{inc}} \) in equation (5.1) separately satisfy the governing Maxwell’s equations and therefore, the total field can be decomposed to the sum of the incident field and the scattered field as shown
Another useful assumption to make here is that the incident wave exists in the absence of any scatterer, like a wave propagating in free space. Therefore, the incident wave is calculated using the model equation (5.2) within the domain with the material properties of a free space. The two-dimensional model equation results in a cylindrical waves that will serve as an excitation source at a point on the TF-SF boundary.

\[
\frac{\partial T_{\text{inc}}}{\partial \tau} + X_0 \frac{\partial P_{\text{inc}}}{\partial \xi} + Y_0 \frac{\partial Q_{\text{inc}}}{\partial \eta} = 0
\]

(5.2)

Where the coefficients in the model equation are given as,

\[
X_0 = Y_0 = {\begin{bmatrix}
\frac{1}{\varepsilon_0} & 0 & 0 \\
0 & \frac{1}{\mu_0} & 0 \\
0 & 0 & \frac{1}{\mu_p}
\end{bmatrix}}
\]

(5.3)

As mentioned previously, the domain is divided into two regions namely, the total field region and the scattered field region, separated by the TF-SF boundary as shown in Figure 5.1 for the two-dimensional geometry. The total field region is the region of interest where the scattering device is located, and the scattered field regions surrounds the total field region. One of the method to introduce the incident wave is to define the incident waveform at a location in the scattered field region, so that it appears to have originated outside the simulation region, i.e., the total field region. The boundary separating the total field and the scattered field regions is assumed to be imaginary and it can be of any shape, preferably rectangular so that it can be accurately represented by the grid points, irrespective of the shape of the scatterer. However, with the method proposed in this research, the imaginary TF-SF boundary can be made parallel to the boundary of the scatterer. Since the staggered grid formulation is used in the MRK approximation of governing equations, the TF-SF boundary is aligned with the primary grid where the electric field variables are specified. The importance of such specification is discussed within the TF-SF formulation in the subsequent sub-sections.
5.2 Two-Dimensional Formulation

The framework for the TF-SF development for the two-dimensional applications is as follows; While computing the field variables using TF-SF formulation, it is required that the total fields must be calculated using field values only from the total field region and similarly, scattered fields must be calculated using field values from the scattered field regions to provide consistency to the formulation. Therefore, the finite difference equations on the TF-SF boundaries must be modified. Consider the finite difference equations at the boundaries of the TF-SF located at the grid points $i_a, i_b$ on the $\xi$-coordinate and at grid points $j_a, j_b$ on the $\eta$-coordinate. The central differencing of convective terms includes the field values from the scattered field region to compute variables located on the four boundaries that is in the total field region. This is explained by using the finite difference equation for approximation of $\bar{T}_1$ on the
imaginary TF-SF boundaries of the total field region. As stated previously, that the TF-SF boundaries are
aligned with the primary grid system, hence the electric field variables exist on the four boundaries.

Therefore, correction on the boundaries is performed only for $T_1$ vector.

\[ i = ia, ja < j < jb: \]
\[ T_1^{n+1}{_{ia,j}} = T_1^n{_{ia,j}} - \Delta \tau \epsilon_{ia,j} \left[ \frac{p^n{_{1ia,j}} - p^n{_{1ia-1,j}}}{\Delta \xi} + \frac{q^n{_{1ia,j}} - q^n{_{1ia,j-1}}}{\Delta \eta} \right] \]  
(5.4)

\[ i = ib, ja < j < jb: \]
\[ T_1^{n+1}{_{ib,j}} = T_1^n{_{ib,j}} - \Delta \tau \epsilon_{ib,j} \left[ \frac{p^n{_{1ib,j}} - p^n{_{1ib-1,j}}}{\Delta \xi} + \frac{q^n{_{1ib,j}} - q^n{_{1ib,j-1}}}{\Delta \eta} \right] \]  
(5.5)

\[ ia < i < ib, j = ja: \]
\[ T_1^{n+1}{_{i,ja}} = T_1^n{_{i,ja}} - \Delta \tau \epsilon_{i,ja} \left[ \frac{p^n{_{i,ja}} - p^n{_{i-1,ja}}}{\Delta \xi} + \frac{q^n{_{i,ja}} - q^n{_{i,ja-1}}}{\Delta \eta} \right] \]  
(5.6)

\[ ia < i < ib, j = jb: \]
\[ T_1^{n+1}{_{i,jb}} = T_1^n{_{i,jb}} - \Delta \tau \epsilon_{i,jb} \left[ \frac{p^n{_{i,jb}} - p^n{_{i-1,jb}}}{\Delta \xi} + \frac{q^n{_{i,jb}} - q^n{_{i,jb-1}}}{\Delta \eta} \right] \]  
(5.7)

The term $p^n{_{1ia-1,j}}$ in equation (5.4) is the scattered field value, whereas all other terms are in the
total field region. Therefore, the formulation is inconsistent. Using the linearity of Maxwell’s equations
given in equation (5.1), this equation can be made consistent by adding the incident term which can be
called as the correction term, and therefore, the term becomes a total field value, as shown in equation (5.8).

Upon rearrangement of terms, it can be shown that the equation (5.8) is equivalent to the form expressed in
equation (5.9). The first term on the right-hand side of equation (5.9) is the expression calculated from
equation (5.4) and the second term is the added correction term. Therefore, in the Runge-Kutta formulation,
the correction term is added to the variable $T_1$, at locations $i = ia, ja < j < jb$, obtained after executing the
computation of four stages within the entire domain.

\[ T_1^{n+1}{_{ia,j}} = T_1^n{_{ia,j}} - \Delta \tau \epsilon_{ia,j} \left[ \frac{p^n{_{1ia,j}} - p^n{_{1ia-1,j}} + p^n{_{1incia-1,j}}}{\Delta \xi} + \frac{q^n{_{1ia,j}} - q^n{_{1ia,j-1}}}{\Delta \eta} \right] + \Delta \tau \epsilon_{ia,j} \Delta \xi p^n{_{1incia-1,j}} \]  
(5.8)

\[ T_1^{n+1} = \left( T_1^n{_{ia,j}} + \Delta \tau \epsilon_{ia,j} p^n{_{1incia-1,j}} \right) \]  
(5.9)
Similar corrections are applied at locations $ia < i < ib, j = ja$, in the total field region;

\[
\tilde{T}^{n+1}_{1,ja} = \tilde{T}^n_{1,ja} - \frac{\Delta \tau}{\epsilon_{i,ja}} \left[ \frac{P^n_{1,ja} - P^n_{1,i-1,ja}}{\Delta \xi} + \frac{\overline{Q}^n_{1,ja} - (\overline{Q}^n_{1,ja-1} + \overline{Q}^n_{1\text{inc}_{i,ja-1}})}{\Delta \eta} \right]
\] (5.10)

\[
\tilde{T}^{n+1}_{1,ja} = \{ \tilde{T}^n_{1,ja} \} + \frac{\Delta \tau}{\epsilon_{i,ja} \Delta \eta} \overline{Q}^n_{1\text{inc}_{i,ja-1}}
\] (5.11)

However, at locations $i = ib, ja < j < jb$ and at $ia < i < ib, j = jb$, the formulation is slightly different.

\[
\tilde{T}^{n+1}_{1,ib,j} = \tilde{T}^n_{1,ib,j} - \frac{\Delta \tau}{\epsilon_{ib,j}} \left[ \frac{(P^n_{1,ib,j} + P^n_{1\text{inc}_{ib,j}}) - P^n_{1,i-1,ib,j}}{\Delta \xi} + \frac{\overline{Q}^n_{1,ib,j} - \overline{Q}^n_{1,ib-1,j}}{\Delta \eta} \right]
\] (5.12)

\[
\tilde{T}^{n+1}_{1,ib,j} = \{ \tilde{T}^n_{1,ib,j} \} - \frac{\Delta \tau}{\epsilon_{ib,j} \Delta \xi} P^n_{1\text{inc}_{ib,j}}
\] (5.13)

\[
\tilde{T}^{n+1}_{1,ib} = \tilde{T}^n_{1,ib} - \frac{\Delta \tau}{\epsilon_{i,jb}} \left[ \frac{P^n_{1,ib} - P^n_{1,i-1,jb}}{\Delta \xi} + \frac{(\overline{Q}^n_{1,ib} + \overline{Q}^n_{1\text{inc}_{i,jb}}) - \overline{Q}^n_{1,i-1,jb}}{\Delta \eta} \right]
\] (5.14)

\[
\tilde{T}^{n+1}_{1,ib} = \{ \tilde{T}^n_{1,ib} \} - \frac{\Delta \tau}{\epsilon_{i,jb} \Delta \eta} \overline{Q}^n_{1\text{inc}_{i,jb}}
\] (5.15)

Special care must be taken at the vertices $(ia, ja), (ia, jb), (ib, ja)$ and $(ib, jb)$ of the TF-SF boundary as the two correction terms will be added at these location to comply with the principle of the TF-SF formulation, otherwise, it will lead to inaccurate results.

\[
\tilde{T}^{n+1}_{1,ia,ja} = \tilde{T}^n_{1,ia,ja} - \frac{\Delta \tau}{\epsilon_{ia,ja}} \left[ \frac{P^n_{1,ia,ja} - (P^n_{1,ia-1,ja} - P^n_{1\text{inc}_{ia-1,ja}})}{\Delta \xi} + \frac{\overline{Q}^n_{1,ia,ja} - (\overline{Q}^n_{1,ia-1,ja} - \overline{Q}^n_{1\text{inc}_{ia-1,ja-1}})}{\Delta \eta} \right]
\] (5.16)

\[
\tilde{T}^{n+1}_{1,ia,ja} = \{ \tilde{T}^n_{1,ia,ja} \} + \frac{\Delta \tau}{\epsilon_{ia,ja} \Delta \xi} P^n_{1\text{inc}_{ia-1,ja}} + \frac{\Delta \tau}{\epsilon_{ia,ja} \Delta \eta} \overline{Q}^n_{1\text{inc}_{ia,ja-1}}
\] (5.17)
\[
\ddot{T}_{1i,ja}^{n+1} = \ddot{T}_{1i,ja}^{n} - \frac{\Delta \tau}{\varepsilon_{ia,ja}} \left[ \frac{P_{1i,ja}^{n} - P_{1i,ja-1}^{n} - P_{1inc,ja-1}^{n}}{\Delta \xi} + \frac{Q_{1i,ja}^{n} - Q_{1inc,ja}^{n} - Q_{1i,ja-1}^{n}}{\Delta \eta} \right] 
\]

(5.18)

\[
\ddot{T}_{1ib,ja}^{n+1} = \{\ddot{T}_{1ib,ja}^{n+1}\} + \frac{\Delta \tau}{\varepsilon_{ia,ja}} \frac{P_{1inc,ja}^{n-1} - P_{1inc,ja}^{n}}{\Delta \xi} - \frac{\Delta \tau}{\varepsilon_{ia,ja}} \frac{Q_{1inc,ja}^{n-1} - Q_{1inc,ja}^{n}}{\Delta \eta} 
\]

(5.19)

\[
\ddot{T}_{1ib,ja}^{n+1} = \ddot{T}_{1ib,ja}^{n} - \frac{\Delta \tau}{\varepsilon_{ib,ja}} \left[ \frac{P_{1ib,ja}^{n} - P_{1inc,ja}^{n} - P_{1ib-1,ja}^{n}}{\Delta \xi} + \frac{Q_{1ib,ja}^{n} - Q_{1inc,ja}^{n} - Q_{1ib-1,ja}^{n}}{\Delta \eta} \right] 
\]

(5.20)

\[
\ddot{T}_{1ib,ja}^{n+1} = \{\ddot{T}_{1ib,ja}^{n+1}\} - \frac{\Delta \tau}{\varepsilon_{ib,ja}} \frac{P_{1inc,ja}^{n} - P_{1inc,ja}^{n}}{\Delta \xi} + \frac{\Delta \tau}{\varepsilon_{ib,ja}} \frac{Q_{1inc,ja}^{n} - Q_{1inc,ja}^{n}}{\Delta \eta} 
\]

(5.21)

\[
\ddot{T}_{1ib,ja}^{n+1} = \ddot{T}_{1ib,ja}^{n} - \frac{\Delta \tau}{\varepsilon_{ib,ja}} \left[ \frac{P_{1ib,ja}^{n} - P_{1inc,ja}^{n} - P_{1ib-1,ja}^{n}}{\Delta \xi} + \frac{Q_{1ib,ja}^{n} - Q_{1inc,ja}^{n} - Q_{1ib-1,ja}^{n}}{\Delta \eta} \right] 
\]

(5.22)

\[
\ddot{T}_{1ib,ja}^{n+1} = \{\ddot{T}_{1ib,ja}^{n+1}\} - \frac{\Delta \tau}{\varepsilon_{ib,ja}} \frac{P_{1inc,ja}^{n} - P_{1inc,ja}^{n}}{\Delta \xi} + \frac{\Delta \tau}{\varepsilon_{ib,ja}} \frac{Q_{1inc,ja}^{n} - Q_{1inc,ja}^{n}}{\Delta \eta} 
\]

(5.23)

After obtaining the correction terms corresponding to \(E_z\), similar corrections are required at the grid points adjacent to the TF-SF boundary where \(H_x\) and \(H_y\) components are located. The central difference approximation of spatial derivatives at the grid points \((ia-1, ja<j<jb)\), \((ib, ja<j<jb)\), \((ia<i<ib, ja-1)\), and \((ia<i<ib, jb)\) contains term from the total field that needs to be corrected as the given grid points lie in the scattered field region. Therefore, by application of a similar procedure described above for the correction in the approximation of \(\ddot{T}_{1i,j}^{n+1}\), will yield consistent approximations for \(\ddot{T}_{2i,j}^{n+1}\) and \(\ddot{T}_{3i,j}^{n+1}\).

\[
ia < i < ib, j = ja-1: \quad \ddot{T}_{2i,ja-1}^{n+1} = \{\ddot{T}_{2i,ja-1}^{n+1}\} + \frac{\Delta \tau}{\mu_{i,ja-1}} \frac{Q_{2inc,ja}^{n}}{\Delta \eta} 
\]

(5.24)

\[
ia < i < ib, j = ja-1: \quad \ddot{T}_{3i,ja-1}^{n+1} = \{\ddot{T}_{3i,ja-1}^{n+1}\} + \frac{\Delta \tau}{\mu_{i,ja-1}} \frac{Q_{3inc,ja}^{n}}{\Delta \eta} 
\]

(5.25)
\[ ia < i < ib, j = jb: \]
\[ T^{n+1}_{2i,jb} = \{ T^{n+1}_{2i,jb} \} - \frac{\Delta \tau}{\mu_{i,jb} \Delta \eta} Q^{n}_{2inc,jb} \quad (5.26) \]

\[ ia < i < ib, j = jb: \]
\[ T^{n+1}_{3i,jb} = \{ T^{n+1}_{3i,jb} \} - \frac{\Delta \tau}{\mu_{i,jb} \Delta \eta} Q^{n}_{3inc,jb} \quad (5.27) \]

\[ i = ia-1, ja < j < jb: \]
\[ T^{n+1}_{2ia-1,j} = \{ T^{n+1}_{2ia-1,j} \} + \frac{\Delta \tau}{\mu_{ia-1,j} \Delta \xi} P^{n}_{2inc,ia,j} \quad (5.28) \]

\[ i = ia-1, ja < j < jb: \]
\[ T^{n+1}_{3ia-1,j} = \{ T^{n+1}_{3ia-1,j} \} + \frac{\Delta \tau}{\mu_{ia-1,j} \Delta \xi} P^{n}_{3inc,ia,j} \quad (5.29) \]

\[ i = ib, ja < j < jb: \]
\[ T^{n+1}_{2ib,j} = \{ T^{n+1}_{2ib,j} \} - \frac{\Delta \tau}{\mu_{ib,j} \Delta \xi} P^{n}_{2inc,ib,j} \quad (5.30) \]

\[ i = ib, ja < j < jb: \]
\[ T^{n+1}_{3ib,j} = \{ T^{n+1}_{3ib,j} \} - \frac{\Delta \tau}{\mu_{ib,j} \Delta \xi} P^{n}_{3inc,ib,j} \quad (5.31) \]

### 5.3 Three-Dimensional Formulation

The implementation of TF-SF formulation on three-dimensional grid is quite exhaustive. The correction terms for approximating \( \bar{T}_1, \bar{T}_2, \bar{T}_3 \) are added or subtracted at six faces, twelve edges and eight vertices to accurately model the TF-SF formulation, whereas \( \bar{T}_4, \bar{T}_5, \bar{T}_6 \) are approximated at the six faces adjacent to the TF-SF boundary in the scattered field region. Similar to the two-dimensional formulation, the TF-SF boundary is aligned with the primary grid and hence, electric field variables lie on the grid points on the TF-SF boundaries. The complete set of equations in the three-dimensional approximation using TF-SF formulation is presented in this section.
- At face $F1$: $ia+1 < i < ib-1$, $ja+1 < j < jb-1$, $k = ka$

\[ T_{1,i,ka}^{n+1} = \left( T_{1,i,ka}^{n+1} \right) + \frac{\Delta \tau}{\epsilon_{i,j,ka} \Delta \zeta} R_{1inc_{i,j,ka-1}}^n \]  

(5.32)

\[ T_{2,i,ka}^{n+1} = \left( T_{2,i,ka}^{n+1} \right) + \frac{\Delta \tau}{\epsilon_{i,j,ka} \Delta \zeta} R_{2inc_{i,j,ka-1}}^n \]  

(5.33)

\[ T_{3,i,ka}^{n+1} = \left( T_{3,i,ka}^{n+1} \right) + \frac{\Delta \tau}{\epsilon_{i,j,ka} \Delta \zeta} R_{3inc_{i,j,ka-1}}^n \]  

(5.34)
- At face F2; \( ia+1 < i < ib-1, ja+1 < j < jb-1, k = kb \)

\[
\begin{align*}
T_{1,i,j,kb}^{n+1} &= \{T_{1,i,j,kb}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,j,kb}} Q_{1inc_{i,j,kb}}^{n} \quad (5.35) \\
T_{2,i,j,kb}^{n+1} &= \{T_{2,i,j,kb}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,j,kb}} Q_{2inc_{i,j,kb}}^{n} \quad (5.36) \\
T_{3,i,j,kb}^{n+1} &= \{T_{3,i,j,kb}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,j,kb}} Q_{3inc_{i,j,kb}}^{n} \quad (5.37)
\end{align*}
\]

- At face F3; \( ia+1 < i < ib-1, j = ja, ka+1 < k < kb-1 \)

\[
\begin{align*}
\tilde{T}_{1,i,ja,k}^{n+1} &= \{\tilde{T}_{1,i,ja,k}^{n+1}\} + \frac{\Delta \tau}{\epsilon_{i,ja,k}} Q_{1inc_{i,ja-1,k}}^{n} \quad (5.38) \\
\tilde{T}_{2,i,ja,k}^{n+1} &= \{\tilde{T}_{2,i,ja,k}^{n+1}\} + \frac{\Delta \tau}{\epsilon_{i,ja,k}} Q_{2inc_{i,ja-1,k}}^{n} \quad (5.39) \\
\tilde{T}_{3,i,ja,k}^{n+1} &= \{\tilde{T}_{3,i,ja,k}^{n+1}\} + \frac{\Delta \tau}{\epsilon_{i,ja,k}} Q_{3inc_{i,ja-1,k}}^{n} \quad (5.40)
\end{align*}
\]

- At face F4; \( ia+1 < i < ib-1, j = jb, ka+1 < k < kb-1 \)

\[
\begin{align*}
\tilde{T}_{1,i,jb,k}^{n+1} &= \{\tilde{T}_{1,i,jb,k}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,jb,k}} Q_{1inc_{i,jb}}^{n} \quad (5.41) \\
\tilde{T}_{2,i,jb,k}^{n+1} &= \{\tilde{T}_{2,i,jb,k}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,jb,k}} Q_{2inc_{i,jb}}^{n} \quad (5.42) \\
\tilde{T}_{3,i,jb,k}^{n+1} &= \{\tilde{T}_{3,i,jb,k}^{n+1}\} - \frac{\Delta \tau}{\epsilon_{i,jb,k}} Q_{3inc_{i,jb}}^{n} \quad (5.43)
\end{align*}
\]
- At face F5; $i = i_a, j_a < j < j_b - 1, k_a, k < k_b - 1$

$$T^{n+1}_{1i_a,j,k} = \left( T^{n+1}_{1i_a,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i_a,j,k} \Delta \xi} P^{n}_{1\text{inc}_{i_a-1,j,k}}$$ (5.44)

$$T^{n+1}_{2i_a,j,k} = \left( T^{n+1}_{2i_a,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i_a,j,k} \Delta \xi} P^{n}_{2\text{inc}_{i_a-1,j,k}}$$ (5.45)

$$T^{n+1}_{3i_a,j,k} = \left( T^{n+1}_{3i_a,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i_a,j,k} \Delta \xi} P^{n}_{3\text{inc}_{i_a-1,j,k}}$$ (5.46)

- At face F6; $i = i_b, j_a < j < j_b - 1, k_a, k < k_b - 1$

$$T^{n+1}_{1i_b,j,k} = \left( T^{n+1}_{1i_b,j,k} \right) - \frac{\Delta \tau}{\epsilon_{i_b,j,k} \Delta \xi} P^{n}_{1\text{inc}_{i_b,j,k}}$$ (5.47)

$$T^{n+1}_{2i_b,j,k} = \left( T^{n+1}_{2i_b,j,k} \right) - \frac{\Delta \tau}{\epsilon_{i_b,j,k} \Delta \xi} P^{n}_{2\text{inc}_{i_b,j,k}}$$ (5.48)

$$T^{n+1}_{3i_b,j,k} = \left( T^{n+1}_{3i_b,j,k} \right) - \frac{\Delta \tau}{\epsilon_{i_b,j,k} \Delta \xi} P^{n}_{3\text{inc}_{i_b,j,k}}$$ (5.49)

- At edge E1; $i_a + 1 < i < i_b - 1, j = j_a, k = k_a$

$$T^{n+1}_{1i,j,k} = \left( T^{n+1}_{1i,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \eta} Q^{n}_{1\text{inc}_{i,j-1,k}} + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \zeta} R^{n}_{1\text{inc}_{i,j,k-1}}$$ (5.50)

$$T^{n+1}_{2i,j,k} = \left( T^{n+1}_{2i,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \eta} Q^{n}_{2\text{inc}_{i,j-1,k}} + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \zeta} R^{n}_{2\text{inc}_{i,j,k-1}}$$ (5.51)

$$T^{n+1}_{3i,j,k} = \left( T^{n+1}_{3i,j,k} \right) + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \eta} Q^{n}_{3\text{inc}_{i,j-1,k}} + \frac{\Delta \tau}{\epsilon_{i,j,k} \Delta \zeta} R^{n}_{3\text{inc}_{i,j,k-1}}$$ (5.52)
- At edge E2; \( ia+1 < i < ib-1, j = jb, k = ka \)

\[
\bar{T}_{1i,jb,ka}^{n+1} = \left\{ \bar{T}_{1i,jb,ka}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \eta} \bar{Q}_{1inc_{i,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \zeta} \bar{R}_{1inc_{i,jb,ka}}^{n} \tag{5.53}
\]

\[
\bar{T}_{2i,jb,ka}^{n+1} = \left\{ \bar{T}_{2i,jb,ka}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \eta} \bar{Q}_{2inc_{i,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \zeta} \bar{R}_{2inc_{i,jb,ka}}^{n} \tag{5.54}
\]

\[
\bar{T}_{3i,jb,ka}^{n+1} = \left\{ \bar{T}_{3i,jb,ka}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \eta} \bar{Q}_{3inc_{i,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{i,jb,ka} \Delta \zeta} \bar{R}_{3inc_{i,jb,ka}}^{n} \tag{5.55}
\]

- At edge E3; \( ia+1 < i < ib-1, j = ja, k = kb \)

\[
\bar{T}_{1i,ja,kb}^{n+1} = \left\{ \bar{T}_{1i,ja,kb}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \eta} \bar{Q}_{1inc_{i,ja-1,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \zeta} \bar{R}_{1inc_{i,ja,kb}}^{n} \tag{5.56}
\]

\[
\bar{T}_{2i,ja,kb}^{n+1} = \left\{ \bar{T}_{2i,ja,kb}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \eta} \bar{Q}_{2inc_{i,ja-1,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \zeta} \bar{R}_{2inc_{i,ja,kb}}^{n} \tag{5.57}
\]

\[
\bar{T}_{3i,ja,kb}^{n+1} = \left\{ \bar{T}_{3i,ja,kb}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \eta} \bar{Q}_{3inc_{i,ja-1,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,ja,kb} \Delta \zeta} \bar{R}_{3inc_{i,ja,kb}}^{n} \tag{5.58}
\]

- At edge E4; \( ia+1 < i < ib-1, j = jb, k = kb \)

\[
\bar{T}_{1i,jb,kb}^{n+1} = \left\{ \bar{T}_{1i,jb,kb}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \eta} \bar{Q}_{1inc_{i,jb,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \zeta} \bar{R}_{1inc_{i,jb,kb}}^{n} \tag{5.59}
\]

\[
\bar{T}_{2i,jb,kb}^{n+1} = \left\{ \bar{T}_{2i,jb,kb}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \eta} \bar{Q}_{2inc_{i,jb,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \zeta} \bar{R}_{2inc_{i,jb,kb}}^{n} \tag{5.60}
\]

\[
\bar{T}_{3i,jb,kb}^{n+1} = \left\{ \bar{T}_{3i,jb,kb}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \eta} \bar{Q}_{3inc_{i,jb,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{i,jb,kb} \Delta \zeta} \bar{R}_{3inc_{i,jb,kb}}^{n} \tag{5.61}
\]
- At edge $E5$: $i = ia, ja+1 < j < jb-1, k = ka$

$$
\begin{align*}
\overline{T}_{1_{ia,ka}}^{n+1} &= \left\{ \overline{T}_{1_{ia,ka}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{p}_{1inc_{ia-1,ka}}^n + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{R}_{1inc_{ia,ka-1}}^n \\
\overline{T}_{2_{ia,ka}}^{n+1} &= \left\{ \overline{T}_{2_{ia,ka}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{p}_{2inc_{ia-1,ka}}^n + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{R}_{2inc_{ia,ka-1}}^n \\
\overline{T}_{3_{ia,ka}}^{n+1} &= \left\{ \overline{T}_{3_{ia,ka}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{p}_{3inc_{ia-1,ka}}^n + \frac{\Delta \tau}{\epsilon_{ia,j,ka}} \overline{R}_{3inc_{ia,ka-1}}^n
\end{align*}
$$  \tag{5.62}

- At edge $E6$: $i = ib, ja+1 < j < jb-1, k = ka$

$$
\begin{align*}
\overline{T}_{1_{ib,ka}}^{n+1} &= \left\{ \overline{T}_{1_{ib,ka}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{p}_{1inc_{ib,j,ka}}^n + \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{R}_{1inc_{ib,ka-1}}^n \\
\overline{T}_{2_{ib,ka}}^{n+1} &= \left\{ \overline{T}_{2_{ib,ka}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{p}_{2inc_{ib,j,ka}}^n + \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{R}_{2inc_{ib,ka-1}}^n \\
\overline{T}_{3_{ib,ka}}^{n+1} &= \left\{ \overline{T}_{3_{ib,ka}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{p}_{3inc_{ib,j,ka}}^n + \frac{\Delta \tau}{\epsilon_{ib,j,ka}} \overline{R}_{3inc_{ib,ka-1}}^n
\end{align*}
$$  \tag{5.65}

- At edge $E7$: $i = ia, ja+1 < j < jb-1, k = kb$

$$
\begin{align*}
\overline{T}_{1_{ia,kb}}^{n+1} &= \left\{ \overline{T}_{1_{ia,kb}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{p}_{1inc_{ia-1,kb}}^n - \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{R}_{1inc_{ia,kb}}^n \\
\overline{T}_{2_{ia,kb}}^{n+1} &= \left\{ \overline{T}_{2_{ia,kb}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{p}_{2inc_{ia-1,kb}}^n - \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{R}_{2inc_{ia,kb}}^n \\
\overline{T}_{3_{ia,kb}}^{n+1} &= \left\{ \overline{T}_{3_{ia,kb}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{p}_{3inc_{ia-1,kb}}^n - \frac{\Delta \tau}{\epsilon_{ia,j,kb}} \overline{R}_{3inc_{ia,kb}}^n
\end{align*}
$$  \tag{5.68}

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- At edge E8; \( i = ib, ja+1 < j < jb-1, k = kb \)

\[
\begin{align*}
\bar{T}_{1_{ib,j,kb}}^{n+1} &= \left\{ \bar{T}_{1_{ib,j,kb}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{P}_{1\text{inc}_{ib,j,kb}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{Q}_{1\text{inc}_{ib,j,kb}}^{n} \\
\bar{T}_{2_{ib,j,kb}}^{n+1} &= \left\{ \bar{T}_{2_{ib,j,kb}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{P}_{2\text{inc}_{ib,j,kb}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{Q}_{2\text{inc}_{ib,j,kb}}^{n} \\
\bar{T}_{3_{ib,j,kb}}^{n+1} &= \left\{ \bar{T}_{3_{ib,j,kb}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{P}_{3\text{inc}_{ib,j,kb}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,kb} \Delta \xi} \bar{Q}_{3\text{inc}_{ib,j,kb}}^{n}
\end{align*}
\] (5.71) (5.72) (5.73)

- At edge E9; \( i = ia, j = ja, ka+1 < k < kb-1 \)

\[
\begin{align*}
\bar{T}_{1_{ia,j,a,k}}^{n+1} &= \left\{ \bar{T}_{1_{ia,j,a,k}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{P}_{1\text{inc}_{ia,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{Q}_{1\text{inc}_{ia,j,a-1,k}}^{n} \\
\bar{T}_{2_{ia,j,a,k}}^{n+1} &= \left\{ \bar{T}_{2_{ia,j,a,k}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{P}_{2\text{inc}_{ia,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{Q}_{2\text{inc}_{ia,j,a-1,k}}^{n} \\
\bar{T}_{3_{ia,j,a,k}}^{n+1} &= \left\{ \bar{T}_{3_{ia,j,a,k}}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{P}_{3\text{inc}_{ia,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ia,j,a,k} \Delta \xi} \bar{Q}_{3\text{inc}_{ia,j,a-1,k}}^{n}
\end{align*}
\] (5.74) (5.75) (5.76)

- At edge E10; \( i = ib, j = ja, ka+1 < k < kb-1 \)

\[
\begin{align*}
\bar{T}_{1_{ib,j,a,k}}^{n+1} &= \left\{ \bar{T}_{1_{ib,j,a,k}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{P}_{1\text{inc}_{ib,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{Q}_{1\text{inc}_{ib,j,a-1,k}}^{n} \\
\bar{T}_{2_{ib,j,a,k}}^{n+1} &= \left\{ \bar{T}_{2_{ib,j,a,k}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{P}_{2\text{inc}_{ib,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{Q}_{2\text{inc}_{ib,j,a-1,k}}^{n} \\
\bar{T}_{3_{ib,j,a,k}}^{n+1} &= \left\{ \bar{T}_{3_{ib,j,a,k}}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{P}_{3\text{inc}_{ib,j,a,k}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,j,a,k} \Delta \xi} \bar{Q}_{3\text{inc}_{ib,j,a-1,k}}^{n}
\end{align*}
\] (5.77) (5.78) (5.79)
- At edge $E11; i = ia, j = jb, ka+1 < k < kb-1$
\[
\overline{R}^{n+1}_{1ia,jb,k} = \{\overline{R}^{n+1}_{1ia,jb,k}\} + \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \xi} \overline{P}^{n}_{1inc_{ia-1,jb,k}} - \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \eta} \overline{Q}^{n}_{1inc_{ia,ja,ka}}
\]

(5.80)

\[
\overline{R}^{n+1}_{2ia,jb,k} = \{\overline{R}^{n+1}_{2ia,jb,k}\} + \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \xi} \overline{P}^{n}_{2inc_{ia-1,jb,k}} - \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \eta} \overline{Q}^{n}_{2inc_{ia,ja,ka}}
\]

(5.81)

\[
\overline{R}^{n+1}_{3ia,jb,k} = \{\overline{R}^{n+1}_{3ia,jb,k}\} + \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \xi} \overline{P}^{n}_{3inc_{ia-1,jb,k}} - \frac{\Delta \tau}{\epsilon_{ia,jb,k} \Delta \eta} \overline{Q}^{n}_{3inc_{ia,ja,ka}}
\]

(5.82)

- At edge $E12; i = ib, j = ja, ka+1 < k < kb-1$
\[
\overline{R}^{n+1}_{1ib,ja,k} = \{\overline{R}^{n+1}_{1ib,ja,k}\} - \frac{\Delta \tau}{\epsilon_{ib,ja,k} \Delta \xi} \overline{P}^{n}_{1inc_{ib,ja,k}} - \frac{\Delta \tau}{\epsilon_{ib,ja,k} \Delta \eta} \overline{Q}^{n}_{1inc_{ia,ja,ka}}
\]

(5.83)

(5.84)

(5.85)

- At vertex $V1; i = ia, j = ja, k = ka$
\[
\overline{R}^{n+1}_{1ia,ja,ka} = \{\overline{R}^{n+1}_{1ia,ja,ka}\} + \frac{\Delta \tau}{\epsilon_{ia,ja,ka} \Delta \xi} \overline{P}^{n}_{1inc_{ia-1,ja,ka}} + \frac{\Delta \tau}{\epsilon_{ia,ja,ka} \Delta \eta} \overline{Q}^{n}_{1inc_{ia,ja-1,ka}}
\]

(5.86)

\[
\overline{R}^{n+1}_{2ia,ja,ka} = \{\overline{R}^{n+1}_{2ia,ja,ka}\} + \frac{\Delta \tau}{\epsilon_{ia,ja,ka} \Delta \xi} \overline{P}^{n}_{2inc_{ia-1,ja,ka}} + \frac{\Delta \tau}{\epsilon_{ia,ja,ka} \Delta \eta} \overline{Q}^{n}_{2inc_{ia,ja-1,ka}}
\]

(5.87)
\[ T_3^{n+1} = (T_3^{n+1})_{ia,ja,ka} \] + \frac{\Delta \tau}{\epsilon_{ia,ja,ka}} \vec{P}_{3inc_{ia-1,ja,ka}}^{n} \] + \frac{\Delta \tau}{\epsilon_{ia,ja,ka}} \vec{R}_{3inc_{ia,ja,ka-1}}^{n} 

(5.88)

At vertex V2: i = ia, j = jb, k = ka

\[ T_1^{n+1} = (T_1^{n+1})_{ia,jb,ka} \] + \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{P}_{1inc_{ia-1,jb,ka}}^{n} \] - \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{Q}_{1inc_{ia,jb,ka}}^{n} 

(5.89)

\[ T_2^{n+1} = (T_2^{n+1})_{ia,jb,ka} \] + \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{P}_{2inc_{ia-1,jb,ka}}^{n} \] - \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{Q}_{2inc_{ia,jb,ka}}^{n} 

(5.90)

\[ T_3^{n+1} = (T_3^{n+1})_{ia,jb,ka} \] + \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{P}_{3inc_{ia-1,jb,ka}}^{n} \] - \frac{\Delta \tau}{\epsilon_{ia,jb,ka}} \vec{Q}_{3inc_{ia,jb,ka}}^{n} 

(5.91)

- At vertex V3: i = ib, j = ja, k = ka

\[ T_1^{n+1} = (T_1^{n+1})_{ib,ja,ka} \] - \frac{\Delta \tau}{\epsilon_{ib,ja,ka}} \vec{P}_{1inc_{ib,ja,ka}}^{n} \] + \frac{\Delta \tau}{\epsilon_{ib,ja,ka}} \vec{Q}_{1inc_{ib,ja-1,ka}}^{n} 

(5.92)

\[ T_2^{n+1} = (T_2^{n+1})_{ib,ja,ka} \] - \frac{\Delta \tau}{\epsilon_{ib,ja,ka}} \vec{P}_{2inc_{ib,ja,ka}}^{n} \] + \frac{\Delta \tau}{\epsilon_{ib,ja,ka}} \vec{Q}_{2inc_{ib,ja-1,ka}}^{n} 

(5.93)
\[
\hat{T}_{3,ib,ja,ka}^{n+1} = \left( \hat{T}_{3,ib,ja,ka}^{n+1} \right) = \frac{\Delta \tau}{\epsilon_{ib,ja,ka} \Delta \xi} P_{3inc_{ib,ja,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,ja,ka} \Delta \eta} Q_{3inc_{ib,ja-1,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,ja,ka} \Delta \zeta} R_{3inc_{ib,ja,ka-1}}^{n} 
\]

(5.94)

- At vertex V4: \( i = ib, j = jb, k = ka \)

\[
\hat{T}_{1,ib,jb,ka}^{n+1} = \left( \hat{T}_{1,ib,jb,ka}^{n+1} \right) - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \xi} P_{1inc_{ib,jb,ka}}^{n} - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \eta} Q_{1inc_{ib,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \zeta} R_{1inc_{ib,jb,ka-1}}^{n} 
\]

(5.95)

\[
\hat{T}_{2,ib,jb,ka}^{n+1} = \left( \hat{T}_{2,ib,jb,ka}^{n+1} \right) - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \xi} P_{2inc_{ib,jb,ka}}^{n} - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \eta} Q_{2inc_{ib,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \zeta} R_{2inc_{ib,jb,ka-1}}^{n} 
\]

(5.96)

\[
\hat{T}_{3,ib,jb,ka}^{n+1} = \left( \hat{T}_{3,ib,jb,ka}^{n+1} \right) - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \xi} P_{3inc_{ib,jb,ka}}^{n} - \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \eta} Q_{3inc_{ib,jb,ka}}^{n} + \frac{\Delta \tau}{\epsilon_{ib,jb,ka} \Delta \zeta} R_{3inc_{ib,jb,ka-1}}^{n} 
\]

(5.97)

- At vertex V5: \( i = ia, j = ja, k = kb \)

\[
\hat{T}_{1,ia,ja,kb}^{n+1} = \left( \hat{T}_{1,ia,ja,kb}^{n+1} \right) + \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \xi} P_{1inc_{ia,ja-1,kb}}^{n} + \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \eta} Q_{1inc_{ia,ja-1,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \zeta} R_{1inc_{ia,ja,kb}}^{n} 
\]

(5.98)

\[
\hat{T}_{2,ia,ja,kb}^{n+1} = \left( \hat{T}_{2,ia,ja,kb}^{n+1} \right) + \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \xi} P_{2inc_{ia,ja-1,kb}}^{n} + \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \eta} Q_{2inc_{ia,ja-1,kb}}^{n} - \frac{\Delta \tau}{\epsilon_{ia,ja,kb} \Delta \zeta} R_{2inc_{ia,ja,kb}}^{n} 
\]

(5.99)
\[ T_{3i_1a,j_1k_1}^{n+1} = \left\{ T_{3i_1a,j_1k_1}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} P_{3inc_{i_1a,j_1k_1}}^{n} + \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \eta} Q_{3inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} R_{3inc_{i_1a,j_1k_1}}^{n} \]  

(5.100)

- At vertex \( V_6 \); \( i = i_a, j = j_b, k = k_b \)

\[ T_{1i_1a,j_1k_1}^{n+1} = \left\{ T_{1i_1a,j_1k_1}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} P_{1inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \eta} Q_{1inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} R_{1inc_{i_1a,j_1k_1}}^{n} \]  

(5.101)

\[ T_{2i_1a,j_1k_1}^{n+1} = \left\{ T_{2i_1a,j_1k_1}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} P_{2inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \eta} Q_{2inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} R_{2inc_{i_1a,j_1k_1}}^{n} \]  

(5.102)

\[ T_{3i_1a,j_1k_1}^{n+1} = \left\{ T_{3i_1a,j_1k_1}^{n+1} \right\} + \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} P_{3inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \eta} Q_{3inc_{i_1a,j_1k_1}}^{n} - \frac{\Delta \tau}{\epsilon_{i_1a,j_1k_1} \Delta \zeta} R_{3inc_{i_1a,j_1k_1}}^{n} \]  

(5.103)

- At vertex \( V_7 \); \( i = i_b, j = j_a, k = k_b \)

\[ T_{1i_2a,j_2k_2}^{n+1} = \left\{ T_{1i_2a,j_2k_2}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \zeta} P_{1inc_{i_2a,j_2k_2}}^{n} + \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \eta} Q_{1inc_{i_2a,j_2k_2}}^{n} - \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \zeta} R_{1inc_{i_2a,j_2k_2}}^{n} \]  

(5.104)

\[ T_{2i_2a,j_2k_2}^{n+1} = \left\{ T_{2i_2a,j_2k_2}^{n+1} \right\} - \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \zeta} P_{2inc_{i_2a,j_2k_2}}^{n} + \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \eta} Q_{2inc_{i_2a,j_2k_2}}^{n} - \frac{\Delta \tau}{\epsilon_{i_2a,j_2k_2} \Delta \zeta} R_{2inc_{i_2a,j_2k_2}}^{n} \]  

(5.105)
\[
\begin{align*}
\bar{T}_{3ib,ja,kb}^{n+1} &= \{\bar{T}_{3ib,ja,kb}^n\} - \frac{\Delta \tau}{\epsilon_{ib,ja,kb} \Delta \xi} \bar{P}_{3inc_{ib,ja,kb}}^n + \frac{\Delta \tau}{\epsilon_{ib,ja,kb} \Delta \eta} \bar{Q}_{3inc_{ib,ja-1,kb}}^n \\
&\quad - \frac{\Delta \tau}{\epsilon_{ib,ja,kb} \Delta \zeta} \bar{R}_{3inc_{ib,ja,kb}}^n
\end{align*}
\] (5.106)

- At vertex V8; \( i = ib, j = jb, k = kb \)

\[
\begin{align*}
\bar{T}_{1ib,jb,kb}^{n+1} &= \{\bar{T}_{1ib,jb,kb}^n\} - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \xi} \bar{P}_{1inc_{ib,jb,kb}}^n - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \eta} \bar{Q}_{1inc_{ib,jb,kb}}^n \\
&\quad - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \zeta} \bar{R}_{1inc_{ib,jb,kb}}^n
\end{align*}
\] (5.107)

\[
\begin{align*}
\bar{T}_{2ib,jb,kb}^{n+1} &= \{\bar{T}_{2ib,jb,kb}^n\} - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \xi} \bar{P}_{2inc_{ib,jb,kb}}^n - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \eta} \bar{Q}_{2inc_{ib,jb,kb}}^n \\
&\quad - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \zeta} \bar{R}_{2inc_{ib,jb,kb}}^n
\end{align*}
\] (5.108)

\[
\begin{align*}
\bar{T}_{3ib,jb,kb}^{n+1} &= \{\bar{T}_{3ib,jb,kb}^n\} - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \xi} \bar{P}_{3inc_{ib,jb,kb}}^n - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \eta} \bar{Q}_{3inc_{ib,jb,kb}}^n \\
&\quad - \frac{\Delta \tau}{\epsilon_{ib,jb,kb} \Delta \zeta} \bar{R}_{3inc_{ib,jb,kb}}^n
\end{align*}
\] (5.109)

Since the grid points adjacent to the TF-SF boundary falls on the secondary grid, where magnetic field variables are specified, therefore, the finite difference approximation terms for \( \bar{T}_4, \bar{T}_5, \bar{T}_6 \) at these grid points must be corrected by adding or subtracting the total field value using the linearity of the model equation. The formulation is presented next for the six faces that are adjacent to TF-SF boundary in the scattered zone. No separate correction is required at the edges or vertices as they are included in the formulation.
- At face adjacent to face F1; $ia < i < ib, ja < j < jb, k = ka-1$

$$T_{4i,ka-1}^{n+1} = \left\{ T_{4i,ka-1}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ka-1} \Delta \zeta} R_{4inci,ja}^n$$  \hspace{1cm} (5.110)$$

$$T_{5i,ka-1}^{n+1} = \left\{ T_{5i,ka-1}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ka-1} \Delta \zeta} R_{5inci,ja}^n$$  \hspace{1cm} (5.111)$$

$$T_{6i,ka-1}^{n+1} = \left\{ T_{6i,ka-1}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ka-1} \Delta \zeta} R_{6inci,ja}^n$$  \hspace{1cm} (5.112)$$

- At plane adjacent to face F2; $ia < i < ib, ja < j < jb, k = kb$

$$T_{4i,kb}^{n+1} = \left\{ T_{4i,kb}^n \right\} - \frac{\Delta \tau}{\mu_{i,j,kb} \Delta \zeta} R_{4inci,kb}^n$$  \hspace{1cm} (5.113)$$

$$T_{5i,kb}^{n+1} = \left\{ T_{5i,kb}^n \right\} - \frac{\Delta \tau}{\mu_{i,j,kb} \Delta \zeta} R_{5inci,kb}^n$$  \hspace{1cm} (5.114)$$

$$T_{6i,kb}^{n+1} = \left\{ T_{6i,kb}^n \right\} - \frac{\Delta \tau}{\mu_{i,j,kb} \Delta \zeta} R_{6inci,kb}^n$$  \hspace{1cm} (5.115)$$

- At plane adjacent to face F3; $ia < i < ib, ja = ja-1, ka < k < kb$

$$T_{4i,ja-1,k}^{n+1} = \left\{ T_{4i,ja-1,k}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ja-1,k} \Delta \eta} Q_{4inci,ja,k}^n$$  \hspace{1cm} (5.116)$$

$$T_{5i,ja-1,k}^{n+1} = \left\{ T_{5i,ja-1,k}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ja-1,k} \Delta \eta} Q_{5inci,ja,k}^n$$  \hspace{1cm} (5.117)$$

$$T_{6i,ja-1,k}^{n+1} = \left\{ T_{6i,ja-1,k}^n \right\} + \frac{\Delta \tau}{\mu_{i,j,ja-1,k} \Delta \eta} Q_{6inci,ja,k}^n$$  \hspace{1cm} (5.118)$$

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- At plane adjacent to face $F_4$; $ia < i < ib, ja < j < jb, ka < k < kb$

\[
\bar{T}^{n+1}_{4i,jb,k} = \{T^{n+1}_{4i,jb,k}\} - \frac{\Delta \tau}{\mu_{i,jb,k}} Q^n_{4inc_{i,jb,k}}
\] (5.119)

\[
\bar{T}^{n+1}_{5i,jb,k} = \{T^{n+1}_{5i,jb,k}\} - \frac{\Delta \tau}{\mu_{i,jb,k}} Q^n_{5inc_{i,jb,k}}
\] (5.120)

\[
\bar{T}^{n+1}_{6i,jb,k} = \{T^{n+1}_{6i,jb,k}\} - \frac{\Delta \tau}{\mu_{i,jb,k}} Q^n_{6inc_{i,jb,k}}
\] (5.121)

- At plane adjacent to face $F_5$; $i = ia-1, ja < j < jb, ka < k < kb$

\[
\bar{T}^{n+1}_{4ia-1,j,k} = \{T^{n+1}_{4ia-1,j,k}\} + \frac{\Delta \tau}{\mu_{ia-1,j,k}} P^n_{4inc_{ia,j,k}}
\] (5.122)

\[
\bar{T}^{n+1}_{5ia-1,j,k} = \{T^{n+1}_{5ia-1,j,k}\} + \frac{\Delta \tau}{\mu_{ia-1,j,k}} P^n_{5inc_{ia,j,k}}
\] (5.123)

\[
\bar{T}^{n+1}_{6ia-1,j,k} = \{T^{n+1}_{6ia-1,j,k}\} + \frac{\Delta \tau}{\mu_{ia-1,j,k}} P^n_{6inc_{ia,j,k}}
\] (5.124)

- At plane adjacent to face $F_6$; $i = ib, ja < j < jb, ka < k < kb$

\[
\bar{T}^{n+1}_{4ib,j,k} = \{T^{n+1}_{4ib,j,k}\} - \frac{\Delta \tau}{\mu_{ib,j,k}} P^n_{4inc_{ib,j,k}}
\] (5.125)

\[
\bar{T}^{n+1}_{5ib,j,k} = \{T^{n+1}_{5ib,j,k}\} - \frac{\Delta \tau}{\mu_{ib,j,k}} P^n_{5inc_{ib,j,k}}
\] (5.126)

\[
\bar{T}^{n+1}_{6ib,j,k} = \{T^{n+1}_{6ib,j,k}\} - \frac{\Delta \tau}{\mu_{ib,j,k}} P^n_{6inc_{ib,j,k}}
\] (5.127)
5.4 Approximation of Incident Wave

It is to be noted that the incident field values are required to be known only at the boundaries and at the grid points adjacent to the boundaries for making the finite difference equations consistent. The question now arises how to obtain the source terms for addition or subtraction at the imaginary TF-SF boundaries? An approach to approximate incident field has been presented in this section that is used in the computation of numerical results for TF-SF applications. There are several efficient approaches available in the literature, however, for detailed investigations on accuracy of the numerical scheme for the total field as well as the incident field computations and to monitor the propagation of incident wave within the entire domain, the fourth-order Modified Runge-Kutta approximations on transformed coordinates is used to advance the incident field in time and space within the entire domain. The MRK method on the transformed coordinates is used for incident field propagation to remain consistent with the total field computations. For two-dimensional applications, the incident fields are defined on an auxiliary two-dimensional domain which is assumed to be of same size as of total-field propagation domain in the proposed formulations. The difference between the two domains is that the auxiliary domain is a free space domain without the presence of any scatterer. The $z$-component of electric field is hard-coded at a location $(sx, sy)$ by using the gaussian pulse or a sinusoidal waveform to excite the incident field. The description of the gaussian and sine waveform is presented in Section 3.4.1. The location of $(sx, sy)$ corresponds to a location within the scattered field region on the grid that computes total-field.

\[
\begin{align*}
T_{1inc_{i,j}}^{n+1} &= T_{1inc_{i,j}}^n - \frac{\Delta \tau}{4\epsilon_0} \left[ \frac{\bar{P}_{1inc_{i+1/2,j}}^n - \bar{P}_{1inc_{i-1/2,j}}^n}{\Delta \xi} + \frac{\bar{Q}_{1inc_{i+1/2,j}}^n - \bar{Q}_{1inc_{i-1/2,j}}^n}{\Delta \eta} \right] \\
T_{1inc_{i,j}}^{n+1} &= T_{1inc_{i,j}}^n - \frac{\Delta \tau}{3\epsilon_0} \left[ \frac{\bar{P}_{1inc_{i+1/2,j}}^n - \bar{P}_{1inc_{i-1/2,j}}^n}{\Delta \xi} + \frac{\bar{Q}_{1inc_{i+1/2,j}}^n - \bar{Q}_{1inc_{i-1/2,j}}^n}{\Delta \eta} \right] \\
T_{1inc_{i,j}}^{n+1} &= T_{1inc_{i,j}}^n - \frac{\Delta \tau}{2\epsilon_0} \left[ \frac{\bar{P}_{1inc_{i+1/2,j}}^n - \bar{P}_{1inc_{i-1/2,j}}^n}{\Delta \xi} + \frac{\bar{Q}_{1inc_{i+1/2,j}}^n - \bar{Q}_{1inc_{i-1/2,j}}^n}{\Delta \eta} \right]
\end{align*}
\]
\[
\tilde{T}_{1inc_{i,j}}^{n+1} = \frac{\Delta \tau}{\varepsilon_0} \left[ \frac{P_{1inc_{i+1/2,j}}^n - P_{1inc_{i-1/2,j}}^n}{\Delta \xi} + \frac{Q_{1inc_{i+1/2,j}}^n - Q_{1inc_{i-1/2,j}}^n}{\Delta \eta} \right]
\] (5.131)

After the four-stage MRK approximation, the source is introduced as the hard source at a location within the scattered field zone as specified in equation (5.132). By using such specification, any previously computed value at \((sx, sy)\) will be overwritten by the value of gaussian pulse at that time level.

\[
\tilde{T}_{1inc_{sx, sy}}^{n+1} = \text{pulse}
\] (5.132)

Hence, the incident field will advance in space and time and as it strikes the nearest TF-SF boundary, the wavefront will be visible in the total-field region due to the correction applied on the TF-SF boundary using the incident term. The incident wave will continue to propagate on the auxiliary grid as if it is propagating in free space whereas the total-field will propagate on the actual grid where it will interact with the scatterer. In the examples presented in this research, the scattered field region has been made large compared to the total field region to avoid artificial reflections from the boundary as no PML is incorporated at the boundaries.
CHAPTER 6
RESULTS AND DISCUSSION

The numerical algorithms discussed previously in this report have been used to develop several two and three-dimensional computer codes based on the application. In this chapter, results are presented for different applications and geometries. Subsequently, the computer codes are validated by comparing the numerical results with the analytical solution, for the benchmark problems, wherever applicable.

The initial step in the validation of numerical algorithms consist of simulating the electromagnetic waves in a simple two-dimensional homogeneous rectangular geometry with the closed form solution. The initial and the boundary conditions are obtained from the exact solution, hence, no additional efforts were required to avoid artificial reflections from the boundaries. Subsequently, a non-homogeneous rectangular geometry with the available analytical solution is considered by placing a dielectric medium in the free space. Similar to the previous problem, the initial and the boundary conditions were derived from exact solution. These two classes of problems have been adopted in several published literature for initial verification and analysis of the numerical methods.

Next, the computer codes were modified for the TF-SF implementation and numerical simulation of the wave propagation within several different media configurations of rectangular geometries were obtained. The post-processing stage for transformation of time-domain fields to frequency-domain data has also been implemented in the computer algorithm, however, since the objective of the research is to perform qualitative analysis; only the time-domain investigations are presented. Subsequently, the scattering from a circular cylindrical geometry with the properties of a lossless dielectric and the scattering from an airfoil configuration with the properties of the perfect conductor were considered to demonstrate the application of the numerical model to simulate complex geometries.
Finally, the three dimensional electromagnetic solver is developed. The scattering of waves from a lossless dielectric cube is simulated on the clustered grid system. Such configurations are considered as electrically large systems and requires enormous amount of computational resources to obtain a solution with an acceptable level of accuracy.

6.1 Standing-Wave Simulation in a Homogeneous Medium

The domain considered for simulation of a standing-wave within a homogeneous medium is a two-dimensional domain with a rectangular cross-section. The material is assumed to be filled with a medium with properties of a free space medium. The material properties are specified as input at each grid point within the domain before the time stepping of the solution. The material parameters and the domain dimensions are specified in Table 6.1. and the reference values for non-dimensionalization of variables are mentioned in Table 6.2.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of medium $\epsilon_1$</td>
<td>$8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium $\mu_1$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical conductivity $\sigma$</td>
<td>0.0 S/m</td>
</tr>
<tr>
<td>Domain length $A$</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Domain height $B$</td>
<td>1.0 m</td>
</tr>
</tbody>
</table>
TABLE 6.2
REFERENCE VALUES FOR NON-DIMENSIONALIZATION OF VARIABLES IN THE GOVERNING EQUATION

<table>
<thead>
<tr>
<th>Reference Variables</th>
<th>Reference Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference electrical permittivity</td>
<td>$\varepsilon_0 =$</td>
</tr>
<tr>
<td></td>
<td>$8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Reference magnetic permeability</td>
<td>$\mu_0 =$</td>
</tr>
<tr>
<td></td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Speed of light in vacuum</td>
<td>$c_0 =$</td>
</tr>
<tr>
<td></td>
<td>$3.0 \times 10^8$ m/s</td>
</tr>
<tr>
<td>Reference length</td>
<td>$L =$</td>
</tr>
<tr>
<td></td>
<td>$1.0$ m</td>
</tr>
<tr>
<td>Reference electric field</td>
<td>$E_0 =$</td>
</tr>
<tr>
<td></td>
<td>$1.0$ V/m</td>
</tr>
</tbody>
</table>

The analytical solution for this example obtained from Ref. [16] is given as

$$E_z(x, y, t) = \sin(3\pi x - 5\pi t) \sin(4\pi y) \quad \text{in V/m}$$

The simulation was started using initial conditions as the source condition. The initial conditions for the electric and magnetic field variables at time level, $t = 0$ seconds is obtained from the exact solution. Similarly, boundary conditions for the field components in TM mode are derived from exact solution. The derived initial and the boundary conditions are presented next.

Initial Conditions:

$$E_z(x, y, 0) = \sin(3\pi x) \sin(4\pi y) \quad \text{in V/m}$$

$$H_x(x, y, 0) = -\frac{4}{5} \cos(3\pi x) \sin(4\pi y) \quad \text{in A/m}$$

$$H_y(x, y, 0) = -\frac{3}{5} \sin(3\pi x) \sin(4\pi y) \quad \text{in A/m}$$
Boundary Conditions:

\[
E_z(0, y, t) = -\sin(5\pi t) \sin(4\pi y) \quad \text{in } V/m
\]

\[
E_z(1, y, t) = \sin(3\pi - 5\pi t) \sin(4\pi y) \quad \text{in } V/m
\]

\[
E_z(x, 0, t) = 0.0 \quad \text{in } V/m
\]

\[
E_z(x, 1, t) = 0.0 \quad \text{in } V/m
\]

The accuracy of the numerical solution is calculated by obtaining analytical solution at all grid points and subsequently, computing the error distribution within the entire domain using the expression:

\[
ERROR\% = \left(\frac{E_{z\text{numerical}} - E_{z\text{analytical}}}{E_{z\text{analytical}}}\right) \times 100
\]

The simulated results from the developed codes with the above mentioned specifications is presented next. Presently, an unstaggered grid has been used to perform time-dependent simulations. A description of the unstaggered grid approach is presented in Section 4.5.2.1. Following investigations have been considered for the initial analysis:

- Comparison of solutions obtained using various configuration of numerical formulation on uniform and clustered grid; and

- Grid independence study.

6.1.1 Solutions Using Different Numerical Approach

The initial validation was performed by comparing results using various configurations of the numerical algorithm. The numerical algorithms considered are presented as follows:

- MRK scheme in transformed coordinates with non-dimensional variables;

- MRK scheme in transformed coordinates with dimensional variables;

- MRK scheme in physical domain with dimensional variables;

For the sake of simplicity in referencing, let us define the given algorithms in an abbreviated form as MRK1, MRK2, and MRK3, respectively. The numerical solutions and the error analysis on a uniform
grid are presented in Figure 6.1 – Figure 6.10 in Section 6.1.1.1 and on a clustered grid are presented in Figures 6.12 – Figure 6.15 in Section 6.1.1.2. The electric field and the magnetic field data within the domain are recorded as the output at each grid points, however, only the electric field variables are presented in the results as a function of x and at y-locations as described in the figure captions.

6.1.1.1 Uniform Mesh

The mesh with 501×501, 201x201, 101x101 and 51x51 grid points were selected and the corresponding grid step values of ∆x and ∆y on a uniform grid is presented in Table 6.3. Based on the grid spacing, the time step, ∆t was computed such that the Courant stability condition is satisfied.

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Grid Size, ∆x = ∆y</th>
</tr>
</thead>
<tbody>
<tr>
<td>51 × 51</td>
<td>0.02 m</td>
</tr>
<tr>
<td>101 × 101</td>
<td>0.01 m</td>
</tr>
<tr>
<td>201 × 201</td>
<td>0.005 m</td>
</tr>
<tr>
<td>501 × 501</td>
<td>0.002 m</td>
</tr>
</tbody>
</table>

It is demonstrated in the electric field and the errors distribution plots that the numerical solutions obtained by MRK1, MRK2, and MRK3 algorithms are in good agreement with the analytical solution where the observed error distribution is $ERROR \% \ll 0.005$ which is an acceptable level of accuracy. The sinusoidal behavior of the standing wave has been accurately predicted by the developed computer codes. The study presented here is the simplest problem in electromagnetics where there are no material interfaces that would results in the penetration or reflection of the waves. However, based on the analysis presented, it can be concluded that the fourth-order MRK scheme can be used to accurately simulate the complex electromagnetic phenomena.
Figure 6.1. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2$ m and grid system = 501x501 on a uniform grid.

Figure 6.2. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2$ m and grid system = 501x501 on a uniform grid.
Figure 6.3. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.6$ m and grid system = 501x501 on a uniform grid.

Figure 6.4. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.6$ m and grid system = 501x501 on a uniform grid.
Figure 6.5. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at \(y = 0.6\) m and grid system = 201x201 on a uniform grid.

Figure 6.6. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at \(y = 0.6\) m and grid system = 201x201 on a uniform grid.
Figure 6.7. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2$ m and grid system = 101x101 on a uniform grid.

Figure 6.8. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2$ m and grid system = 101x101 on a uniform grid.
Figure 6.9. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2m$ and grid system = 51x51 on a uniform grid.

Figure 6.10. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), MRK scheme in computational domain (dimensional variables) and MRK scheme in physical domain (dimensional variables) at $y = 0.2m$ and grid system = 51x51 on a uniform grid.
6.1.1.2 Clustered Mesh

To further demonstrate the applicability of the numerical model to a non-uniform mesh, the domain is clustered along the length of the domain as illustrated in Figure 6.11. The density of the grid points is high near the outer boundary, whereas the grid point distribution is sparse at the center of the domain. The purpose of clustering of grid points here is to validate the accuracy and stability of the solution on the non-uniform mesh, thus the location of clustering can be selected anywhere within the grid in this case primarily due to the underlying physics of this problem.

![Illustration of a clustered mesh with 101x101 grid points.](image)

Figure 6.11. Illustration of a clustered mesh with 101x101 grid points.

The grid density parameter, $\beta$ is used in the grid generation module to specify the density of the grids at the desired location within the domain. The value of $\beta$ ranges from 1 to $\infty$ where the grid density increases as the value approaches 1.0. The grid presented here is generated with $\beta = 1.005$. The solution obtained on a 101x101 grid and 51x51 grid shows an excellent agreement with the exact solution in Figure 6.12 and Figure 6.14 and the error distribution in Figure 6.13 and Figure 6.15 is less than the order of $10^{-3}$. A similar order of accuracy is obtained on the uniform grid as well. Therefore, it can be concluded that a stable and an accurate solution of wave propagation can be obtained on a clustered grid using the Runge-Kutta method on transformed coordinates.
Figure 6.12. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables), at $y = 0.2$ m and grid system = $101 \times 101$ with grid clustering along $x$-axis.

Figure 6.13. Error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables) at $y = 0.2$ m and grid system = $101 \times 101$ with grid clustering along $x$-axis.
Figure 6.14. Comparison of numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables) at $y = 0.2$ m and grid system = 51x51 with grid clustering along $x$-axis.

Figure 6.15. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables) at $y = 0.2$m and grid system = 51x51 with grid clustering along $x$-axis.
6.1.2 Grid Independence Study

In this section, grid independence investigations are presented. The objective of the grid independence investigation is to understand the effect of the spatial step size on the accuracy of the simulated results. The simulated results were obtained by the MRK1, MRK2, and MRK3 algorithms that have been discussed previously. The investigations were performed on four different grid sizes presented in Table 3. The error distributions are plotted at locations \( y = 0.2 \text{ m} \) and \( y = 0.6 \text{ m} \).

To obtain a stable solution, the time step was selected to satisfy the Courant stability condition for all grid configurations. It is demonstrated in Figure 6.16 through Figure 6.21 that the numerical solution is not affected by the choice of the grid size and the error for each numerical configuration \( \text{ERROR \%} \ll 0.01 \). Since the domain consisted of homogeneous material having same properties at all locations, the standing sinusoidal wave was oscillating at the same velocity within the entire domain. Therefore, it was expected that the simulated results are independent of spatial step size for the given grid sizes. However, the requirement of the minimum number of grid points to resolve the maximum wavelength for the selected frequency must be satisfied to obtain meaningful results from the simulations. The explanation of such requirement is presented later in this report in Section 6.3.1.1. Similarly, the grid independence investigations using the MRK1 algorithm on the clustered grid are presented in Figure 6.22 and Figure 6.23 where a similar level of accuracy is observed.

![Figure 6.16](image)

Figure 6.16. Effect of \( \Delta x \) and \( \Delta t \) on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at \( y = 0.2 \text{ m} \) on a uniform grid.
Figure 6.17. Effect of Δ𝑥 and Δ𝑡 on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at y = 0.6 m on a uniform grid.

Figure 6.18. Effect of Δ𝑥 and Δ𝑡 on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (dimensional variables) at y = 0.2 m on a uniform grid.

Figure 6.19. Effect of Δ𝑥 and Δ𝑡 on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (dimensional variables) at y = 0.6 m on a uniform grid.
Figure 6.20. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in physical domain (dimensional variables) at $y = 0.2$ m on a uniform grid.

Figure 6.21. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in physical domain (dimensional variables) at $y = 0.6$ m on a uniform grid.

Figure 6.22. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.2$ m with grid clustering along x-axis.
Figure 6.23. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.6$ m with grid clustering along $x$-axis.

The electric field distribution plot within the entire domain is presented as surface plots in Figure 6.24 (b) and the corresponding analytical solution is presented in Figure 6.24 (a).

6.2 Standing-Wave Simulation in a Non-Homogeneous Medium

The region of interest considered for this application is a two-dimensional domain with rectangular cross-section. The non-homogenous medium is assumed to consist of a free space and a lossless dielectric medium wherein the dielectric medium is surrounded by the free space on either side as illustrated in Figure
6.25. The dielectric medium is represented by the shaded region in the schematic, whereas the unshaded regions correspond to free space.

Figure 6.25. Geometry and nomenclature of the domain for standing wave in an inhomogeneous medium. Assuming that the free space is designated as medium 1 and the dielectric medium is designated as medium 2, the material parameters and the domain dimensions are specified in Table 6.4 where subscripts denotes the related medium. The non-dimensionalization of the variables was performed by using the reference values given in Table 6.2.

**TABLE 6.4**

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of medium 1</td>
<td>$\epsilon_1 = 8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 1</td>
<td>$\mu_1 = 1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical permittivity of medium 2</td>
<td>$\epsilon_2 = 2 \times 8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 2</td>
<td>$\mu_2 = 1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 1 and 2</td>
<td>$\sigma = 0.0$ S/m</td>
</tr>
<tr>
<td>Domain length</td>
<td>$A = 2.0$ m</td>
</tr>
<tr>
<td>Domain height</td>
<td>$B = 1.0$ m</td>
</tr>
</tbody>
</table>
The non-homogenous property of the domain is included in the computer codes by assigning the material properties as the constant initial values at each grid point for the corresponding medium. For example, the grid point \(i = 1, j = 1\) lies in medium 1, and hence, the material properties of free space are specified at this grid point.

**A note of caution:** Technically, free space is also a lossless dielectric medium with relative permittivity, \(\varepsilon^* = 1.0\), and therefore, to mention that the simulation domain consist of free space and a dielectric medium is misleading. However, to distinguish between the two lossless media, where one medium is having the dielectric properties of unity and the other medium has the dielectric properties other than unity, we have chosen to define that the domain consists of free space medium and a dielectric medium, wherever required.

Due to the lossless property of both media, the electrical conductivity is zero and hence no source of losses within the domain. Relative permittivity of a material is obtained in a similar manner as the non-dimensional electric permittivity and is defined by the expression:

\[
\varepsilon_r = \varepsilon^* = \frac{\varepsilon}{\varepsilon_0}
\]

The equations representing the exact solution for the given application are obtained from [16].

\[
E_z = \begin{cases} 
2 \cos\left(\frac{2\pi x}{3}\right) \cos(\omega t) \sin(K_y y) & \text{for } |x| \leq 0.5, 0 \leq y \leq 1.0 \\
\exp\left(\frac{\pi \sqrt{3}}{3}\right) \exp\left(-\frac{2\pi \sqrt{3}|x|}{3}\right) \cos(\omega t) \sin(K_y y) & \text{for } |x| \geq 0.5, 0 \leq y \leq 1.0
\end{cases}
\]

\[
H_x = \begin{cases} 
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \cos\left(\frac{2\pi x}{3}\right) \sin(\omega t) \cos(K_y y) & \text{for } |x| \leq 0.5, 0 \leq y \leq 1.0 \\
-\frac{\sqrt{\varepsilon_1 - 3\varepsilon_2}}{2} \exp\left(\frac{\pi \sqrt{3}}{3}\right) \exp\left(-\frac{2\pi \sqrt{3}|x|}{3}\right) \sin(\omega t) \cos(K_y y) & \text{for } |x| \geq 0.5, 0 \leq y \leq 1.0
\end{cases}
\]
\[ H_y = \begin{cases} -\sqrt{\epsilon_2 - \epsilon_1} \sin \left( \frac{2\pi x}{3} \right) \sin(\omega t) \sin(K_y y) & \text{for } |x| \leq 0.5, 0 \leq y \leq 1.0 \\ -\frac{\sqrt{3(\epsilon_2 - \epsilon_1)}}{2} \exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( -\frac{2\pi \sqrt{3} x}{3} \right) \sin(\omega t) \sin(K_y y) & \text{for } x \geq 0.5, 0 \leq y \leq 1.0 \\ \frac{\sqrt{3(\epsilon_2 - \epsilon_1)}}{2} \exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( \frac{2\pi \sqrt{3} x}{3} \right) \sin(\omega t) \sin(K_y y) & \text{for } x \leq -0.5, 0 \leq y \leq 1.0 \end{cases} \]

Where \( K_y \) and \( \omega \) are given as

\[ K_y = \frac{2\pi}{3} \sqrt{\epsilon_1 + 3\epsilon_2} \]
\[ \omega = \frac{4\pi}{3\sqrt{\epsilon_2 - \epsilon_1}} \]

Subsequently, the initial and the boundary conditions are obtained from the given exact solution. The initial conditions act as a source for excitation of standing waves within the domain. The boundary conditions are specified to restrict the size of the domain and to avoid any non-physical reflections from the boundary.

Initial Conditions \( E_z, H_x, \) and \( H_y \):

\[ E_z(x, y, 0) = \begin{cases} 2 \cos \left( \frac{2\pi x}{3} \right) \sin(K_y y) & \text{for } |x| \leq 0.5, 0 \leq y \leq 1.0 \\ \exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( -\frac{2\pi \sqrt{3} |x|}{3} \right) \sin(K_y y) & \text{for } |x| \geq 0.5, 0 \leq y \leq 1.0 \end{cases} \]

\[ H_x(x, y, 0) = 0 \]

\[ H_y(x, y, 0) = 0 \]
Boundary Conditions for $E_z$, $H_x$, and $H_y$:

$$E_z(-1, y, t) = \exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( -\frac{2\pi \sqrt{3}}{3} \right) \cos(\omega t) \sin(K_y y)$$

$$E_z(1, y, t) = \exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( -\frac{2\pi \sqrt{3}}{3} \right) \cos(\omega t) \sin(K_y y)$$

$$E_z(x, 0, t) = 0$$

$$E_z(x, 1, t) = \begin{cases} 
2 \cos \left( \frac{2\pi x}{3} \right) \cos(\omega t) \sin(K_y) & \text{for } |x| \leq 0.5 \\
\exp \left( \frac{\pi \sqrt{3}}{3} \right) \exp \left( -\frac{2\pi \sqrt{3}|x|}{3} \right) \cos(\omega t) \sin(K_y) & \text{for } |x| \geq 0.5 
\end{cases}$$

$$H_x(-1, y, t) = \begin{cases} 
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \cos \left( -\frac{2\pi}{3} \right) \sin(\omega t) \cos(K_y y) \\
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \frac{\pi \sqrt{3}}{3} \exp \left( -\frac{2\pi \sqrt{3}|x|}{3} \right) \sin(\omega t) \cos(K_y y) 
\end{cases}$$

$$H_x(1, y, t) = \begin{cases} 
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \cos \left( \frac{2\pi x}{3} \right) \sin(\omega t) \cos(K_y y) \\
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \frac{\pi \sqrt{3}}{3} \exp \left( -\frac{2\pi \sqrt{3}|x|}{3} \right) \sin(\omega t) \cos(K_y y) 
\end{cases}$$

$$H_x(x, 0, t) = \begin{cases} 
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \cos \left( \frac{2\pi x}{3} \right) \sin(\omega t) & \text{for } |x| \leq 0.5 \\
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \frac{\pi \sqrt{3}}{3} \exp \left( -\frac{2\pi \sqrt{3}|x|}{3} \right) \sin(\omega t) \cos(K_y y) & \text{for } |x| \geq 0.5 
\end{cases}$$

$$H_x(x, 1, t) = \begin{cases} 
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \cos \left( \frac{2\pi x}{3} \right) \sin(\omega t) \cos(K_y y) & \text{for } |x| \leq 0.5 \\
-\sqrt{\varepsilon_1 - 3\varepsilon_2} \frac{\pi \sqrt{3}}{3} \exp \left( -\frac{2\pi \sqrt{3}|x|}{3} \right) \sin(\omega t) \cos(K_y y) & \text{for } |x| \geq 0.5 
\end{cases}$$
The objective of simulating a non-homogenous domain is to investigate the accuracy of the numerical algorithm in the presence of material discontinuities. The following investigations are considered in the study of inhomogeneous medium and the relevant results are presented next.

1. Investigate the accuracy of the computer algorithm and grid independence in a non-homogenous medium;

2. Investigate the effect of electric permittivity of the lossless dielectric medium on the electric field distribution within the domain; and

3. Investigate the time dependence of the solution
6.2.1 Lossless Dielectric with Electric Permittivity, $\varepsilon_2^* = 2.0$

The numerical solution was obtained by the MRK1 algorithm on four different grid systems specified in Table 6.5.

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Grid Step, $\Delta x$</th>
<th>Grid Step, $\Delta y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$51 \times 51$</td>
<td>0.04 m</td>
<td>0.02 m</td>
</tr>
<tr>
<td>$101 \times 101$</td>
<td>0.02 m</td>
<td>0.01 m</td>
</tr>
<tr>
<td>$201 \times 201$</td>
<td>0.01 m</td>
<td>0.005 m</td>
</tr>
<tr>
<td>$501 \times 501$</td>
<td>0.004 m</td>
<td>0.002 m</td>
</tr>
</tbody>
</table>

The time step for the simulations was selected such that it satisfies the Courant stability condition for all grid size configuration. The numerical solution of computed electric field after 500 time steps as a function of $x$ at $y = 0.2$ m and $y = 0.6$ m is presented in the plots in Figure 6.26 – Figure 6.29. It is observed that the simulated results are in excellent agreement with the analytical solution. This is further demonstrated by the error distribution plots where $ERROR \% \ll 0.1$, which demonstrate an acceptable level of accuracy. The error plot shows that the MRK1 algorithm can be used to simulate electromagnetic fields within the complex media accurately. Figure 6.30 illustrates the electric field distribution of the analytically computed and numerically simulated waves within the entire domain.
Figure 6.26. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.2$ m on a uniform grid.

Figure 6.27. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables at $y = 0.2$ m for various grid system on a uniform grid.
Figure 6.28. Effect of $\Delta x$ and $\Delta t$ on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.6$ m on a uniform grid.

Figure 6.29. Comparison of error distribution for the numerical solutions of Maxwell’s equations obtained by MRK scheme in computational domain (non-dimensional variables) at $y = 0.6$ m for various grid systems on a uniform grid.
6.2.2 Effect of Electric Permittivity in the Lossless Dielectric Material on the Electric Field in the Domain

In this section, the effect of electric permittivity on the propagation of wave is presented. The plots of the numerical solution are presented as a function of $x$ at $y = 0.2$ m and $y = 0.6$ m. The grid size used for computations is $51 \times 51$ and the corresponding $\Delta x$ and $\Delta y$ is given in Table 6.5. Three different dielectric permittivity values have been considered, viz. $\varepsilon_2^* = 2.0$, $\varepsilon_2^* = 4.0$ and $\varepsilon_2^* = 8.0$ and the results are plotted for comparison to demonstrate the effect of electric permittivity on the electric field.

It is observed in Figure 6.31 and Figure 6.32 that the amplitude of the electric field varies with respect to $\varepsilon_2^*$. At $y = 0.2$ m, the electric field values are higher when $\varepsilon_2^* = 2.0$ and least for $\varepsilon_2^* = 8.0$. Since the standing wave is an oscillatory sine wave, the amplitude of the standing wave is a representation of the velocity. The amplitude of the wave is reduced with the increase in the dielectric permittivity because of the reduction in the velocity. The speed of the electromagnetic wave in the dielectric medium in obtained using the expression $c_2 = 1/\sqrt{\mu_2 \varepsilon_2}$, where wave velocity is inversely proportional to dielectric permittivity for a constant permeability parameter.
Figure 6.31. Effect of electric permittivity on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.2$ m on a uniform grid.

Figure 6.32. Effect of electric permittivity on the solution of Maxwell’s equations by Modified Runge-Kutta method in computational domain (non-dimensional variables) at $y = 0.6$ m on a uniform grid.
### 6.2.3 Time Dependence Study

To investigate the time dependence nature of the problem, the numerical solutions obtained at time level $t^* > 0.1$ are presented, unlike in the previous solutions where the time level was considerably small (i.e., $t^* = 0.0005$). The results demonstrate the effect of time level on the computed electric field and verifies the stability and accuracy of the scheme.

![Graph showing electric field over domain length (x) at different time levels $t^*$](image)

**Figure 6.33.** MRK1 solution obtained at $y = 0.2$ m on uniform grid at low time levels ($t^* \ll 0.1$).

![Graph showing electric field over domain length (x) at different time levels $t^*$](image)

**Figure 6.34.** MRK1 solution obtained at $y = 0.2$ m on uniform grid at time levels, $t^* > 0.1$. 

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From Figure 6.33, it is evident that at time levels $t^* = 0.0001$, 0.0002, and 0.0005, the solutions remain constant which suggest that the waves are stationary. This is because the time levels are small and do not produce any change in the solution. However, when the solution is obtained at a higher time level of $t^* > 0.1$, the dependency of the electric field on time can be seen. The oscillatory behavior of the standing wave is demonstrated from the simulated results at higher time levels. The numerical solutions obtained at time level, $t^* = 0.1$, 0.2, 0.5, and 0.8 are plotted in Figure 6.34. All solutions are obtained on a grid size of $201 \times 51$, by using the MRK1 algorithm.

Upon close inspection while performing the investigations on time dependency, it was discovered that at higher time levels, there are oscillations in the solution, which become prominent at these higher time levels. For example, referring to the plots in Figure 6.35 and Figure 6.36, oscillations are visible at $t^* = 0.5$ and at $t^* = 0.8$, and the oscillations can be seen as early as $t^* = 0.2$. Next, the root cause of the error and its mitigation is presented in Section 6.2.4.

![Figure 6.35. Numerical solution obtained at $y = 0.2$ m, $t^* = 0.5$ on unstaggered, uniform grid system.](image-url)
6.2.4 Staggered Grid Approach vs Unstaggered Grid Approach

As discussed in the previous section while investigating the effects of time marching on the electric field values, oscillations in the solution were noticed at higher time levels. The observations suggest that the oscillations were originated near the interface boundaries and propagated on either directions of the boundaries. While investigating the source of the oscillations, it was discovered that they are the result of unstaggered gridding. To illustrate these findings, the staggered, fourth-order Modified-Runge Kutta method on transformed coordinates system with non-dimensional variables have been used to obtain the numerical solution. On a staggered grid, as presented previously, the electric and magnetic field variables are computed on primary and secondary grid systems, respectively, while all other parameters remain the same. Let us define this algorithm as MRK-S, which is a modification of MRK1, wherein unstaggered field components were considered. Additionally, the temporal advancement of fields was performed by leapfrog approach coupled with four-stages of Runge-Kutta method in the MRK-S algorithm.

As demonstrated in Figure 6.37 and Figure 6.38, there are no oscillations in the solution at the given time levels. Therefore, investigations demonstrate that the occurrence of the non-physical oscillations can be attributed to the unstaggered gridding approach, hence solely a numerical error. The central-differencing approximation on unstaggered or collocated grid leads to the divergence instability of the solution due to
odd-even decoupling [126]. Such errors are prominent in the presence of material discontinuity. However, these errors can be mitigated by the application of staggered grid systems. Similar phenomena have been reported as the classical checkerboard pattern for pressure calculation in the CFD related literature. Thus, the staggering scheme is more accurate when using centered space approximations. Henceforth, based on the conclusions, the MRK-S algorithm has been used for all subsequent investigations to achieve the objectives of this research.

Figure 6.37. Numerical solution obtained at $y = 0.2$ m, $t^* = 0.5$ on staggered, uniform grid system.

Figure 6.38. Numerical solution obtained at $y = 0.2$ m, $t^* = 0.8$ on staggered, uniform grid system.
6.3 Reflection and Penetration Simulation of Waves Using TF-SF Formulation

In this section of the investigation, the total field-scattered field formulation is incorporated in the MRK-S algorithm to simulate the far-field reflection and penetration patterns of different scatterer shapes having different material properties. Let us abbreviate the modified algorithm as MRK-STFSF and the computer codes were developed based on this algorithm. The objective of TF-SF implementation is discussed in Chapter 5. This section starts with the discussion on some fundamental concepts that one must know for setting up simulations. The relevant simulated results are presented to understand such fundamentals. Subsequently, the simulation of traveling wave in inhomogeneous media is considered. Various investigations that may affect the quality of the predicted results are presented. The investigations are carried out for the following scenarios:

- Interaction of waves with a lossless and a lossy dielectric square cylinder;
- Interaction of waves with a lossless dielectric circular cylinder;
- Interaction of waves with a perfectly conducting airfoil; and
- Interaction of waves with a lossless dielectric cube.

These investigations are representative of far-field applications. In Chapter 7, near-field investigations are presented by simulating the interaction of electromagnetic waves with the biological tissues. The study is to demonstrate that the numerical algorithm can be used for solving practical algorithms. The computer algorithm is modified to incorporate the dispersive properties of the biological tissues which is presented in Chapter 7.

A note of caution: Most practical electromagnetic phenomena may include a scattering object that is inhomogeneous in itself. Such scattering objects consists of various layers, each having their own unique material properties and each layer acts as a separate complex-shaped scatterer. However, for the investigations presented in this Chapter, we have used the term inhomogeneous media to describe that the simulation domain consists of different materials, however, the scattering object is considered to be homogenous. For example, a dielectric square cylinder is a homogeneous material surrounded by free space medium.
6.3.1 Some Preliminary Investigations

In this section, we will present some preliminary investigation results to gain understanding of various fundamental principles in computational electromagnetics. Such fundamental knowledge can be used as the foundation for the subsequent in-depth investigations. The results presented in this section provides an initial validation of the numerical algorithm.

6.3.1.1 Sampling Rate

While selecting a grid size for meshing of the domain, it is important to ensure that selected grid size is sufficient to resolve a wavelength for a highest frequency within the domain to avoid inaccuracies in simulation. The sampling rate is defined as the number of points to resolve the minimum wavelength accurately. Past studies have demonstrated that the sampling rate of 10 points per wavelength produces an acceptable level of accuracy, however, a wave resolved with 20 points or more produces the desirable level of accuracy. Grid points less than 10 points per wavelength lead to the dispersion errors and phase errors. The sampling rate calculation is explained with an example here. Assuming that the wave propagating with the frequency of 1 GHz in a free space is to be simulated using the finite difference method, the minimum wavelength of the electromagnetic wave is calculated as

$$\lambda = \frac{c_0}{f_{\text{max}} * n_{\text{max}}} = \frac{3 \times 10^8 \text{ m/s}}{(1 \times 10^9) \text{ Hz} \times 1} = 0.3 \text{ m}$$

Where, $f_{\text{max}}$ and $n_{\text{max}}$ are maximum wave frequency and maximum refractive index within the domain, respectively. Subsequently, if we choose to resolve this wavelength with number of grid points per wavelength, $N_\lambda = 20$ points, the spatial step size is computed as shown.

$$\Delta x = \frac{\lambda}{N_\lambda} = 0.015 \text{ m}$$
6.3.1.2 Transverse Magnetic Field Propagation of a Continuous Sinusoid and an Impulse Function

A discussion on various types of sources was presented in Section 3.4. To illustrate the difference in the propagation of fields upon excitation by a continuous sinusoid and an impulse function, we will use the two commonly used sources, a sine wave function and a gaussian pulse. The sources are specified as the hard sources, and the simulation region is homogenous with free space material properties. The wave is allowed to propagate until it reaches the outer boundaries. The outer boundaries have to be defined by appropriate boundary conditions to restrict the computational region. As demonstrated in Figure 6.39, the simulated values of the electric field are stable, and no extremes are observed within the domain.

Figure 6.39. Wave propagation illustration of (a) gaussian impulse and (b) sinusoidal wave computed on a 201x201 uniform grid.

The difference between the wave propagation of the two fields are obvious. The gaussian function is a short impulse that propagates within the domain and contain wideband frequency spectrum. The sinusoidal waveform, to the contrary, is a continuous waveform, that emits the waves continuously from the source point. The simulation of electromagnetic waves must be terminated at certain point based on the nature of investigations. When using a gaussian pulse, a steady state is generally observed when all the propagating fields have died out within the observed region and frequency response is obtained at that time, whereas, the steady state for the sine waveform is observed when the changes in the domain are negligible with
respect to time. The magnitude of the two waves in Figure 6.39(a) and Figure 6.39(b) are of different orders because of difference in their attenuation factor.

6.3.1.3 Verification of Total Field-Scattered Field Implementation

A simple check to validate the correct implementation of the TF-SF formulation in the MRK-STFSF algorithm can be performed by comparing the numerical results with the theoretical principle of TF-SF formulation. According to the TF-SF formulation, the wave is introduced within the region of interest, known as the total field region by the addition or subtraction of incident waves at the TF-SF boundaries. The waves will continue to propagate within this region and upon impingement on the scatterer, the scattered fields can be recorded in the scattered field region for reflection analysis. In the absence of any scattering object within the total field region, the wave will continue to propagate as if it is propagating in a vacuum and exit from the other side of the total-field boundary and consequently, no fields will be observed in the scattered field region. As shown in Figure 6.40(a) and Figure 6.40(b), when there is no scattering device in the total-field region, the wave will enter the total-field region at one corner and disappear from the other corner, without being scattered; hence, no field values and leakage are recorded in the scattered-field region. The imaginary TF-SF boundaries are depicted by red lines in Figure 6.40.

Figure 6.40. Illustration of wave propagation in free space using TF-SF source.
The effect on wave propagation in the presence of the lossless ($\sigma = 0 \text{ S/m}$) scattering device can be observed in Figure 6.41(a) and Figure 6.41(b). When the traveling wavefront impinges on the scattering device, reflections can be noticed in the scattered-field region, as shown in Figure 6.41(b). The boundaries of the scattering material are depicted by the cyan colored lines in Figure 6.41.

![Figure 6.41. Illustration of wave propagation in the presence of a scatterer using TF-SF source.](image)

Before the wavefront reaches the device, scattered regions will not detect any reflections, and the wave will keep propagating within the domain without any distortion of the wavefront. Eventually the wave will exit the space from the far corner of the total-field region. Thus, the presented results demonstrate the correct implementation of the TF-SF formulation in the computer codes and henceforth, the computer codes based on the MRK-STFSF algorithm are used to perform the simulations that involve far-field scattering investigations.

Ideally, there should not be any leakage or back-scattering from the TF-SF boundary, however, there is always some leakage of fields into scattered field region. The cause and an alternative approach to reduce such errors have been reported in literature discussed in Section 2.2.
6.3.1.4 Plane Waves and Cylindrical Waves

The plots presented in Figure 6.42 compares the propagation of a plane wave and a cylindrical wave in the total-field region. Numerically, the plane waves are generated addition or subtraction of source field values on the 2-D or 3-D TF-SF boundaries.

![Wave propagation in free space excited by a gaussian pulse](image)

(a) using 1-D source  
(b) using 2-D source

Figure 6.42. Wave propagation in free space excited by a gaussian pulse (a) plane wave source, (b) cylindrical wave source.

The correction terms are obtained by the propagation of source fields on a one-dimensional propagation axis and thus, requires computation of only two field components. The model equation is obtained by reducing equation (5.2) to a one-dimensional form.

As observed, a TF-SF boundary acts as source of excitation for introduction of plane waves into the total field region, whereas, a point on the TF-SF boundary acts as a source of a cylindrical or a spherical wave. Physically, the incoming waves are assumed as the plane waves for scattering investigations and therefore, the simulation of EM wave scattering is performed by using plane wave. However, there are limitations of plane waves that poses accuracy concerns due to which we have used both cylindrical and plane wave source depending on the investigations performed. Nevertheless, the studies presented are limited to the development and validation analysis of the algorithm, which can be conducted using either of the source.
The selection of the source must not compromise the numerical quality of the solution and therefore, we have based our decision to select a particular method of source based on the known numerical advantages and disadvantages listed here.

➢ The physical plane waves, ideally, does not lose its properties after travelling large distance. On the other hand, the cylindrical or spherical waves attenuates at the rate of $1/r^2$, where $r$ is the propagation radius of the cylindrical wavefront.

➢ The plane waves are obtained by solving only two-field components of one-dimensional arrays each, whereas cylindrical source propagation requires three variables in a TM mode specified as two-dimensional arrays. Hence, cylindrical (or spherical in 3-D) waves are computationally expensive. A more efficient method has been presented by Taflove [65] to introduce oblique plane waves into the total field region.

➢ Simulation on a clustered grid using plane waves results in artificial leakage in the scattered field region due to the phase errors and dispersion errors. Cylindrical waves produced better results on clustered grid because the Jacobian and metrics of the transformation varies along both $x$ and $y$ coordinates and to match the phase of the source field and total field at all TF-SF boundaries, two dimensional source fields are computed on the same clustered grid.

### 6.3.1.5 Simulation of Scattering and Penetration of Waves by Rectangular Interfaces

The simulation of the wave propagation, reflection and penetration phenomenon is considered in this section. The domain specification and the simulation set-up to obtain the results presented in this section are given in Table 6.6 and Table 6.7, respectively. The reference values for non-dimensionalization are obtained from Table 6.2. of wave interaction with the object. The traveling wave is specified by sine wave propagating along $x$-axis and introduced in the total field region using the TF-SF formulation.
### TABLE 6.6
OPERATING CONDITIONS FOR WAVE SCATTERING BY A LOSSLESS DIELECTRIC

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of medium 1 $\epsilon_1$</td>
<td>$8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 1 $\mu_1$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical permittivity of medium 2 $\epsilon_2$</td>
<td>$5 \times 8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 2 $\mu_2$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 1 and 2 $\sigma$</td>
<td>0.0 S/m</td>
</tr>
<tr>
<td>Domain length $A$</td>
<td>0.6 m</td>
</tr>
<tr>
<td>Domain height $B$</td>
<td>0.6 m</td>
</tr>
</tbody>
</table>

### TABLE 6.7
SIMULATION SET-UP FOR WAVE SCATTERING BY A LOSSLESS DIELECTRIC

<table>
<thead>
<tr>
<th>Simulation set-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
</tr>
<tr>
<td>Frequency of interest $f_0$</td>
</tr>
<tr>
<td>Source field</td>
</tr>
<tr>
<td>Grid points</td>
</tr>
<tr>
<td>Spatial step size $\Delta x = \Delta y$</td>
</tr>
<tr>
<td>Time Step $\Delta t$</td>
</tr>
<tr>
<td>CFL</td>
</tr>
<tr>
<td>Grid feature</td>
</tr>
</tbody>
</table>
Figure 6.43 illustrates the snapshots of the simulation at four different time levels. The scattering object is defined such that the material boundaries are aligned with the grid axes and thus, it is termed as a square cylinder. A lossless dielectric square cylinder is considered in the simulation.

Figure 6.43. Sinusoidal plane wave propagation and scattering.
The impingement of waves on the dielectric material causes a fraction of waves to penetrate into the material and the remaining fraction of the waves are reflected and scattered. Consequently, the reflected fields are observed within the scattered field region. Ideally, the simulation should be carried until a steady state is achieved. However, since the outer boundary conditions are specified by conductors, the continuation of the wave propagation will lead to artificial reflection from the boundaries back into the simulation region and will corrupt the solution. Thus, the simulation was stopped before the fields reach the boundary. A similar analysis was carried out using the gaussian pulse as the source fields. The pulse was modeled using the parameter presented in Table 6.8 and the other properties in the simulation set-up remains same as in Table 6.7.

<table>
<thead>
<tr>
<th>TABLE 6.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAUSSIAN PULSE PARAMETERS</td>
</tr>
<tr>
<td>Gaussian pulse parameters</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

The peak frequency value is dependent on the spread of the gaussian wave and is determined from equation (3.33). The expressions for the gaussian pulse and the sinusoidal wave are presented in Section 3.4. The snapshots of simulation at four time levels are presented in Figure 6.44.
6.3.2 Effect of Courant Number

In this section, the numerical results are obtained for wave propagation in the presence of a lossless dielectric square cylinder having electric permittivity, $\varepsilon_r^2$ surrounded by free space and the effect of courant number on the quality of solution is studied. The results are obtained on various grid step sizes and time step sizes. The TM mode for source propagation is considered and the cylindrical source wave is excited...
by the gaussian pulse and introduced to the simulation domain using the TF-SF formulation on transformed coordinates.

The values of grid step, time step, the corresponding Courant number, and the time level to conduct numerical experiments to investigate the effect of Courant number are tabulated in Table 6.9. The simulation set-up is presented in Table 6.10 and the domain features are presented previously in Table 6.6.

### TABLE 6.9

**GRID STEP, TIME STEP AND CORRESPONDING COURANT NUMBER VALUES**

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Grid Step, $\Delta x = \Delta y$</th>
<th>Time Step, $\Delta t^*$</th>
<th>Courant Number, CFL</th>
<th>Time level</th>
</tr>
</thead>
<tbody>
<tr>
<td>201 x 201</td>
<td>0.003 m</td>
<td>0.0003</td>
<td>0.1</td>
<td>$n = 500, t^* = 0.15$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0006</td>
<td>0.2</td>
<td>$n = 250, t^* = 0.15$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0012</td>
<td>0.4</td>
<td>$n = 125, t^* = 0.15$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0015</td>
<td>0.5</td>
<td>$n = 100, t^* = 0.15$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0021</td>
<td>0.7</td>
<td>$n = 72, t^* = 0.1512$</td>
</tr>
<tr>
<td>626 x 626</td>
<td>0.00096 m</td>
<td>0.000096</td>
<td>0.1</td>
<td>$n = 1575, t^* = 0.1512$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.00048</td>
<td>0.5</td>
<td>$n = 315, t^* = 0.1512$</td>
</tr>
</tbody>
</table>

### TABLE 6.10

**SIMULATION SET-UP FOR CYLINDRICAL WAVE SCATTERING**

<table>
<thead>
<tr>
<th>Simulation Set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Gaussian pulse</td>
</tr>
<tr>
<td>Spread $\tau_w$</td>
<td>6.0</td>
</tr>
<tr>
<td>Delay period $n_0$</td>
<td>20.0</td>
</tr>
<tr>
<td>Source field</td>
<td>Cylindrical waves</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Uniformly spaced</td>
</tr>
</tbody>
</table>
In Figure 6.45, the surface plots of the results obtained on a grid size of 201x201 points that corresponds to $\Delta x = \Delta y = 0.003$ m and at time $t^* = 0.15$ are presented. Firstly, a comparison of total electric fields obtained numerically at Courant number of 0.2 and 0.4 is made; the corresponding time steps are $\Delta t^* = 0.0006$ and $\Delta t^* = 0.0012$, respectively. It is observed upon comparison that the solution at CFL = 0.2 produces dispersion and dissipation errors in the wake region of the wavefront.

![Figure 6.45](image)

Figure 6.45. Numerical results at $t^* = 0.15$ on a uniform grid, $\Delta x = \Delta y = 0.003$ m, (a) CFL = 0.2, and (b) CFL = 0.4.

This errors are demonstrated by plotting the computed electric field values along $x$-axis at $y = 0.354$ m as shown in Figure 6.46. The lower courant number is leading to both dispersion and dissipation errors and therefore, the time domain results at CFL = 0.2 is inaccurate.

![Figure 6.46](image)

Figure 6.46. Time domain solution on a uniform grid obtained at $t^* = 0.15$ along domain length at $y = 0.354$ m with grid step size $\Delta x = \Delta y = 0.003$ m.
The oscillatory behavior is further demonstrated in Figure 6.47 and Figure 6.48, where the results are obtained on 626\times 626 grid points i.e. $\Delta x = \Delta y = 9.6 \times 10^{-4}$ m at CFL = 0.1 and at CFL = 0.5. We are presenting results on 626\times 626 in support of the argument because from our investigations it was found that the solution does not vary drastically for $\Delta x \leq 0.0012$ m and therefore, this solution can be treated as the benchmark for comparison purposes. This grid independence of the solution is explained in Section 6.3.3.

It is again observed that the solution is oscillatory when CFL = 0.1. In Figure 6.48, the zoom image of results in Figure 6.47 is presented to illustrate the oscillations in the wake region of the wavefront when courant number is 0.1.

Figure 6.47. Normalized numerical data at $t^* \sim 0.15$ on a uniform grid, $\Delta x = \Delta y = 0.00096$ m, (a) CFL = 0.1, and (b) CFL = 0.5.

Figure 6.48. Close-up images of the numerical results presented in Figure 6.47.
The normalized total fields along the length of the domain at \( y = 0.354 \) m is presented in Figure 6.49 where the oscillations are clearly visible at CFL = 0.1. These are non-physical oscillations within the solution. However, the solution at CFL = 0.5 is smooth, free of oscillations and demonstrates the interaction of waves within the dielectric device. The results obtained from the FDTD method at CFL = 0.5 on the same mesh is included in the plots to validate the accuracy of the MRK method. It is observed that the MRK solution at CFL = 0.5 produced better scattering results than the FDTD method.

![Figure 6.49: Time domain solution on a uniform grid obtained at \( t^* \sim 0.15 \) along domain length at \( y = 0.354 \) m with grid step size \( \Delta x = \Delta y = 0.00096 \) m.](image)

Upon obtaining the solution at a later time-step \( t^* = 0.288 \) with CFL = 0.5, presented in Figure 6.50, the simulation shows that the wave has propagated further, and the scattered waves are observed within the scattered field region. At this time level, \( t^* = 0.288 \), the solution is terminated because the incident wave is about to reach the boundary, as shown in Figure 6.50 (b). Since the metal boundary conditions are employed, the non-physical waves will reflect into the domain and will corrupt the solution beyond this time level. It is to be noted the total fields in Figure 6.47, Figure 6.49 and Figure 6.50 are normalized with respect to the maximum value of the electric field in their respective solution.
Figure 6.50. Normalized numerical data at $t^* = 0.288$ on a uniform grid, $\Delta x = \Delta y = 0.00096$ m.

Similar pattern of results is observed in the numerical simulation of waves in free space. The numerical simulation in free space is carried out using plane wave source and the numerical results presented in Figure 6.5 are obtained at time level, $t^* = 0.108$. It is confirmed from the results that the numerical artifacts are introduced in the solution when CFL number is reduced. Such numerical errors are independent of the material media and the type of wave.

Figure 6.51. Numerical results at $t^* = 0.108$ on a uniform grid, $\Delta x = \Delta y = 0.00096$ m, (a) CFL = 0.1, and (b) CFL = 0.5, plane wave source in free space.

The result obtained in a free space using plane wave source is plotted along $y = 0.354$ m as a function of $x$ in Figure 6.52. The dispersion and dissipation errors are clearly visible when a lower Courant number is used.
Figure 6.52. Time domain solution on uniform grid obtained at $t^* = 0.108$ along domain length at $y = 0.354$ m with grid step size $\Delta x = \Delta y = 0.00096$ m.

In Figure 6.53 – Figure 6.54, results for the various CFL number are presented to further demonstrate the effect of Courant numbers.

Figure 6.53. Numerical results at $t^* \sim 0.15$ on a uniform grid, $\Delta x = \Delta y = 0.003$ m, at CFL = (a) 0.2, (b) 0.4, (c) 0.5, and (d) 0.7.
Based on the time-domain results presented in the investigations, the concluding observations are as follows:

- The artificial oscillations present in the solution at lower Courant numbers are caused by dispersion errors. Additionally, dissipation errors are also observed at lower CFL numbers. The inaccuracies at lower Courant numbers are verified at two different sampling. The oscillations, however, are not causing any instability in the solution.

- The application of a larger Courant number for a given grid size is preferable as it ensures that the accurate solution can be obtained.

- Higher Courant number is always desirable in the simulation set-up to reduce the computational time to obtain a transient or a steady-state solution.
6.3.3 Effect of Grid Size

The investigations pertaining to the effect of the grid size on the quality of the solution is considered here. The numerical results obtained on different grid sizes are compared. In Table 6.11, the tabulated values include the grid step, time step and courant number utilized here.

**TABLE 6.11**

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Grid Step, $\Delta x = \Delta y$</th>
<th>Time Step, $\Delta t^*$</th>
<th>Courant Number, CFL</th>
<th>Time level</th>
</tr>
</thead>
<tbody>
<tr>
<td>101 × 101</td>
<td>0.006 m</td>
<td>0.00048 0.003</td>
<td>0.08 0.5</td>
<td>$n = 315, t^* = 0.1512$ $n = 50, t^* = 0.15$</td>
</tr>
<tr>
<td>201 × 201</td>
<td>0.003 m</td>
<td>0.00048 0.0015</td>
<td>0.16 0.5</td>
<td>$n = 315, t^* = 0.1512$ $n = 100, t^* = 0.15$</td>
</tr>
<tr>
<td>501 × 501</td>
<td>0.0012 m</td>
<td>0.00048 0.0006</td>
<td>0.4 0.5</td>
<td>$n = 315, t^* = 0.1512$ $n = 252, t^* = 0.1512$</td>
</tr>
<tr>
<td>626 × 626</td>
<td>0.00096 m</td>
<td>0.00048</td>
<td>0.5</td>
<td>$n = 315, t^* = 0.1512$</td>
</tr>
<tr>
<td>1001 × 1001</td>
<td>0.0006 m</td>
<td>0.00042 0.00036 0.0003</td>
<td>0.7 0.6 0.5</td>
<td>$n = 360, t^* = 0.1512$ $n = 420, t^* = 0.1512$ $n = 504, t^* = 0.1512$</td>
</tr>
</tbody>
</table>

The numerical experiments were conducted using the set-up presented in Table 6.10. Two types of comparisons and observations relevant to the effect of grid size are presented here. Firstly, a comparison is presented in Figure 6.55 and Figure 6.56 where the numerical solutions are obtained on the different grid sizes while keeping the time step constant, and therefore the Courant number is variable. Subsequently, in Figure 6.57 – Figure 6.59, the solutions are obtained on different grid sizes, at CFL = 0.5 and therefore, the time step is variable.
From the theory of finite difference approximation methods, the solution is said to be converged when the solution approaches the exact value of the governing equation as the step size approaches zero. In practice, the finite difference equations never converge to the exact solution of the governing equations due to the discretization errors, however after considerably smaller step size, the solution becomes independent of the grid step size and the solution will not change irrespective of the grid size which suggest that the discretization errors are no longer the dominant sources of errors. This is known as grid convergence or grid independence. From the previous section, we have already established that the higher quality solution is obtained at CFL closer to 0.5. The is again observed in Figure 6.55 and Figure 6.56 that at very low CFL numbers and larger grid steps size, the solution is highly oscillatory.
This can be attributed to the discretization errors. However, as the CFL approaches 0.5, no oscillations are present in the solution. Additionally, at $\Delta x < 0.0012$, the grid independence is achieved as there is no large changes within the solution as observed in Figure 6.55 (c), (d) and Figure 6.56. The solution obtained by FDTD [1] method is also plotted. The inaccuracies in the FDTD solution is clearly demonstrated in the plot.

In Figure 6.57 and Figure 6.58, the results obtained at CFL = 0.5 on different grid sizes are plotted. Compare the solutions plotted in Figure 6.58 with the solutions in Figure 6.56. There is a large difference in the peak amplitude when solution is obtained at larger time steps, when a constant courant number is used. This difference is attributed to the modeling properties of the gaussian pulse. As we know that the gaussian pulse contains wide bandwidth of frequency depending on the modeling and the relation between the time step, $\Delta t$ and the peak frequency is given in equation (3.33). From this equation, it can be concluded that the peak frequency is inversely proportional to the time step. Considering this relation, at large time steps, the peak frequency of the gaussian is reduced and hence, the wavelength becomes comparatively large which cannot be resolved accurately at larger grid sizes.
Figure 6.57. Numerical results at $t^* \sim 0.15$ on a uniform grid, CFL = 0.5 and grid step $\Delta x = \begin{align*} & (a) \, 6.0 \times 10^{-3} \text{ m}, \\ & (b) \, 3.0 \times 10^{-3} \text{ m}, \\ & (c) \, 1.2 \times 10^{-3} \text{ m} \text{ and} \\ & (d) \, 9.6 \times 10^{-4} \text{ m}. \end{align*}$

As observed in Figure 6.57 (a) and (b), the large wavelengths are not resolved properly using the given grid sizes which has resulted in numerical errors in the solution. This phenomenon is independent of the courant number and depends mainly on the time step and the grid step. At lower time levels, however, the peak amplitudes and the wavelength are in agreement with the FDTD results as shown in Figure 6.57 and Figure 6.58. As the grid step is further reduced below 0.0012 m, the grid independence is observed, as expected. To further verify the grid independence, the solution was obtained on 1001x1001 grid points which corresponds to $\Delta x = 0.0006 \text{ m}$ at CFL 0.5 and CFL = 0.7 and is presented in Figure 6.59. No changes are observed in the solution at this grid size. Additionally, the solution is free of oscillations.
Figure 6.58. Time domain solution on a uniform grid obtained at $t^* = 0.15$ along domain length at $y = 0.354$ m for various grid sizes.

From the results presented in this section it is concluded that for the given impulse function, an accurate solution is obtained by proper modeling of the gaussian impulse based on the frequency of interest and subsequently, the grid size and the time step is selected such that the wavelength is accurately resolved. A good rule of thumb to verify a numerical formulation is to investigate the grid independence of the numerical solution.

Figure 6.59. Numerical results at $t^* \approx 0.15$ on a uniform grid size $\Delta x = 0.0006$ m, at (a) CFL = 0.5 and (b) CFL = 0.7.
6.3.4 Wave Propagation in the Presence of Lossy Dielectric Device

The simulation setup for wave interaction with a lossy dielectric medium is considered in this section. The operating conditions are given in Table 6.12 and the simulation set-up is given in Table 6.13.

**TABLE 6.12**

OPERATING CONDITIONS FOR WAVE SCATTERING BY A LOSSY DIELECTRIC

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of medium 1 $\epsilon_1$</td>
<td>$8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 1 $\mu_1$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical permittivity of medium 2 $\epsilon_2$</td>
<td>$5 \times 8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 2 $\mu_2$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 1 $\sigma_1$</td>
<td>0.0 S/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 2 $\sigma_2$</td>
<td>0.3 S/m</td>
</tr>
<tr>
<td>Domain length $A$</td>
<td>0.6 m</td>
</tr>
<tr>
<td>Domain height $B$</td>
<td>0.6 m</td>
</tr>
</tbody>
</table>

**TABLE 6.13**

SIMULATION SET-UP FOR WAVE SCATTERING BY A LOSSY DIELECTRIC

<table>
<thead>
<tr>
<th>Simulation set-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
</tr>
<tr>
<td>Spread $\tau_w$</td>
</tr>
<tr>
<td>Delay period $n_0$</td>
</tr>
<tr>
<td>Source field</td>
</tr>
<tr>
<td>Grid points</td>
</tr>
<tr>
<td>Spatial step size $\Delta x = \Delta y$</td>
</tr>
<tr>
<td>Time Step $\Delta t$</td>
</tr>
<tr>
<td>CFL</td>
</tr>
<tr>
<td>Grid feature</td>
</tr>
</tbody>
</table>
The numerical results obtained for scattering from a lossy dielectric square shaped cylinder having finite electrical conductivity, $\sigma = 0.3$ S/m is presented in Figure 6.60. The computed results are compared with the scattering results from a lossless dielectric to investigate the effects of electric conductivity on the wave propagation.

![Figure 6.60](image.png)

Figure 6.60. Numerical results at $t^* \sim 0.15$ on a uniform grid, CFL = 0.5 and grid step, $\Delta x = 9.6e-4$, in the presence of (a) a lossless scatterer, and (b) a lossy scatterer.

Theoretically, in a lossless dielectric, the EM wave power losses are negligible during its propagation and hence the attenuation is zero, however, lossy dielectric is a weak conductor and the power is lost with travel distance during its propagation. The amplitude of the wave reduces exponentially with travel distance in a lossy medium and eventually all the waves get absorbed if the lossy medium is large. The plots in Figure 6.60 and Figure 6.61 demonstrate the obvious difference between the amplitudes of total electric field within a lossless medium and a lossy medium. The attenuation of the electric field in the lossy medium is higher as compared to the lossless medium and when one calculates power using the simulated results, it is observed that the loss of power will be higher in lossy medium than in lossless medium. The image in the insert in Figure 6.61, displays the oscillations in the solution obtained by the FDTD method. Overall, the numerical results are in good agreement with the FDTD results and demonstrates the stable solution.
6.3.5 Simulation of Wave Propagation Using a Clustered Grid System

The operating conditions given in Table 6.6 is used and the simulation set-up is presented in Table 6.14.

**TABLE 6.14**

SIMULATION SET-UP FOR WAVE SCATTERING STUDY ON A CLUSTERED GRID

<table>
<thead>
<tr>
<th>Simulation set-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
</tr>
<tr>
<td>Spread</td>
</tr>
<tr>
<td>Delay period</td>
</tr>
<tr>
<td>Source field</td>
</tr>
<tr>
<td>Grid points</td>
</tr>
<tr>
<td>Time Step</td>
</tr>
<tr>
<td>CFL</td>
</tr>
<tr>
<td>Grid feature</td>
</tr>
<tr>
<td>Clustering Parameter</td>
</tr>
</tbody>
</table>
A clustered grid system employed in the simulation of electromagnetic waves in the presence of a lossless dielectric medium is presented in Figure 6.62. As illustrated, the grid points are densely distributed in the \( x \)-direction and \( y \)-direction along the boundaries of the material.

Figure 6.62. Illustration of a clustered grid system with 626x626 grid points, dashed box is TF-SF boundary and solid box is lossless medium.

Clustering of grid points is performed in the regions where large gradients are assumed to exist. The transformation of grid points from physical domain to a uniform rectangular domain helps in the straightforward implementation of the clustered grid points. The clustering density is specified by a parameter, \( \beta \) along the specified coordinate axis. Due to the clustering of grid points, the resulting metrics and the Jacobian of the transformation are not unity as in the case of a uniform grid system and hence, the evaluation of metrics distribution is required before proceeding ahead with the simulation. A smooth grid metrics distribution is desired within the domain as sharp discontinuities result in the failure of the solution or slow convergence. Due to the variable grid steps, the courant number is affected and as a result, the restrictions to the time step also becomes stringent. Additionally, since the grid step is variable, the central
differencing of the spatial derivatives is no longer second-order accurate. The error estimates and the convergence rate on the non-uniform grids are presented in previous studies [127,128]. Transformation of clustered grid in a physical domain to a uniform grid in computational domain, restores the second-order accuracy.

The grid points, as shown in Figure 6.62, are smoothly distributed within the domain without any sharp discontinuities. Verification of grid quality before running simulation ensure better accuracy, avoids extremes within the solution that may lead to the failure of the solver and helps in faster convergence of the solution. The solution obtained on 626x626 grid points are presented and compared with the solution on a uniform grid in Figure 6.63. It is observed that the quality of the solution on a clustered grid is higher than the solution obtained on uniform grid. The resolution of the absorbed waves is finely captured on the clustered grid and therefore, the discretization errors are further minimized. This phenomenon can be attributed to the fact that the CFL is dependent on the speed of the wave and since the speed of the wave is reduced within the medium as compared to the free space propagation, it results in the reduction of CFL number observed by the numerical wave within the medium. It has been demonstrated previously that the quality of the results is much better when the CFL number is close to the maximum permissible CFL by a numerical method. Consequently, clustering of grid points within the dielectric medium results in the improvement in accuracy. Furthermore, densely placing the grid points in the region of interest and sparse grid points in the region away from the scattering bodies will result in the fewer number of overall grid points, due to which a converged solution can be obtained much faster. Overall, the solution obtained is stable without any spurious oscillations and, it can be concluded that the implementation of the clustering technique can be successfully performed by the grid transformation technique.
Figure 6.63. Numerical results at $t^* \sim 0.15$ on 626x626 grid system (a) Clustered grid, (b) Uniform grid.

Next, the simulation of the plane wave propagation on a clustered grid system is presented in Figure 6.64 (a). The time-dependent solution is obtained at a time level before the wavefront has reached the dielectric scattering medium. At this time level, the scattered field must be zero as the waves have not encountered the interface boundaries yet. However, the numerical values are observed in the scattered field region. This is the leakage of the fields from the TF-SF boundary into the scattered field region due to dispersion errors and phase errors. The reason for these errors is the phase mismatch of the plane wave on the clustered grid points. This is a disadvantage of using grid clustering with plane waves and therefore, we have performed numerical experiments in section 6.3.2 – section 6.3.4 using cylindrical waves. As we know that the grid is clustered along both $x$ and $y$ coordinates, however, the computations of the plane wave is performed on an auxiliary one-dimensional axis aligned with the $x$-axis on the clustered grid. The addition or subtraction of the source plane wave at $i = ia$ location takes care of itself as the $x$-coordinates are aligned, whereas, along $j = ja$ and $j = jb$, the grids are not uniformly spaced and due to one-dimensional propagation of source wave, the metrics data along $y$-direction is not taken into consideration which results in the phase mismatch between source waves and total fields.
In order to reduce such dispersion and phase errors, one method is to use analytical fields for plane wave source specification at the interface boundaries. The drawback of analytical source is that the values must be computed in advance for each time level and stored for later use. This requires additional computation memory. Another method was proposed by Christ et al [129]. They derived a correction term from the dispersion analysis on clustered grid. Determination of a correction term for our approach based on the method described in [129] can be good prospective project.

### 6.3.6 Simulation of Scattering and Penetration by Curved Boundaries

To this point, the presented case studies consisted of the domain that involved rectangular boundaries and the comparison with either analytical solution or the benchmark FDTD method was performed to validate the numerical algorithm and the computer codes. In this section, the scattering phenomenon of the electromagnetic waves from impingement upon the non-rectangular boundaries will be analyzed. For this purpose, we have considered to utilize two curved geometries, namely, dielectric circular cylinder and a perfect conducting airfoil. These curved geometries are selected to demonstrate the benefits of using the transformation technique. Furthermore, the loss of accuracy due to the staircase approximation
of the curved boundaries can be avoided, and hence, a significant gain in the efficiency can be achieved over the FDTD method.

For each case, we will present the mesh of the domain, the associated boundary conditions, and the analysis of the results. The generated mesh for both geometries includes clustering of grid points in the region where large field gradients are expected to occur. It is demonstrated in the mesh that the clustered grid points are smoothly distributed within the domain to maintain the quality of the mesh and avoid divergence of the solution or inaccurate results.

### 6.3.6.1 Lossless Dielectric Circular Cylinder

The mesh of the domain with a lossless ($\sigma = 0$ S/m) dielectric circular cylinder is illustrated in Figure 6.65. The non-uniform grid configuration has been used.

![Illustration of clustered discretization of domain consisting of dielectric circular cylinder.](image)

Figure 6.65. Illustration of clustered discretization of domain consisting of dielectric circular cylinder.
The dielectric properties for the entire domain are obtained from Table 6.6 and the simulation set-up is specified in Table 6.15. The mesh with $321 \times 321$ grid points was generated using the algebraic method and the grid points conform to the boundary of the scatterer. The domain dimensions are $1.2 \times 1.2$ m and the radius of the scattering device is 0.096 m with origin located at (0.6 m, 0.6 m). The TF-SF source is implemented, and the total field region is enclosed within $(0.4 \leq x \leq 0.8 \text{ m, } 0.4 \leq y \leq 0.8 \text{ m})$.

**TABLE 6.15**

**SIMULATION SET-UP FOR WAVE SCATTERING BY A LOSSLESS CIRCULAR CYLINDER**

<table>
<thead>
<tr>
<th>Simulation set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Gaussian</td>
</tr>
<tr>
<td>Spread</td>
<td>$\tau = 6.0$</td>
</tr>
<tr>
<td>Delay period</td>
<td>$n_0 = 20.0$</td>
</tr>
<tr>
<td>Source field</td>
<td>Cylindrical waves</td>
</tr>
<tr>
<td>Grid points</td>
<td>$321 \times 321$</td>
</tr>
<tr>
<td>Time Step</td>
<td>$\Delta t = 6.25 \times 10^{-12}$ sec</td>
</tr>
<tr>
<td>CFL</td>
<td>0.5</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Clustered grid</td>
</tr>
</tbody>
</table>

The results were obtained at different time level and the surface plots of the wave travel after 200 and 300 time steps are presented in Figure 6.66. The waves propagate at speed of light, $c_0$, within the total-field region and after impingement on the dielectric boundary, the deformation of the wavefront occurs after approximately 200 time steps and the propagation speed is reduced. The reflections from the dielectric object is observed in the scattered field region which can be recorded by placing data monitors at appropriate locations. The waves will continue to propagate within the object at a reduced speed, $c_0/\sqrt{5}$. The simulation is stopped before the waves reach the boundary to prevent reflections. Generally, the simulation is continued until the waves have died out and a steady state has been reached. If the reflection and transmission coefficients were to be obtained after 300 time steps, the Fourier transformed frequency
domain results will be inaccurate as the energy is still absorbed within the object and the complete transmission has not occurred. The bumps around the TF-SF boundaries in Figure 6.66 are observed. It accurately represents the TF-SF boundaries because the TF-SF boundaries were specified along the lines of constant $i$, and $j$ and not along a constant $x$ and $y$ location. The imaginary TF-SF boundaries can be of any shape; however, it should be specified such that the scattering object is completely immersed within the total field region.

![Figure 6.66. Snapshots of numerical simulation in the presence of cylinder at (a) $n = 200$, (b) $n = 300$.](image)

### 6.3.6.2 Perfect Electric Conductor Airfoil

A symmetric airfoil is considered in this application and a C-grid is generated to observe scattering of electromagnetic waves from an airfoil shaped scatterer. This geometry is an example of the doubly connected domain and the branch cut procedure is used to generate the mesh. The mesh of the solution domain having $675 \times 675$ grid points is presented in Figure 6.67.
Figure 6.6. Illustration of clustered discretization of domain consisting of conducting symmetric airfoil.
The operation conditions and the simulation set-up for the study of wave scattering by a conduction symmetric airfoil is given in Table 6.16 and Table 6.17, respectively.

**TABLE 6.16**

**OPERATING CONDITIONS FOR WAVE SCATTERING BY A LOSSY DIELECTRIC**

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of medium 1 $\epsilon_1$</td>
<td>$8.854 \times 10^{-12}$ F/m</td>
</tr>
<tr>
<td>Magnetic permeability of medium 1 $\mu_1$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical permittivity of medium 2 $\epsilon_2$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Magnetic permeability of medium 2 $\mu_2$</td>
<td>$1.257 \times 10^{-6}$ H/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 1 $\sigma_1$</td>
<td>0.0 S/m</td>
</tr>
<tr>
<td>Electrical conductivity of medium 2 $\sigma_2$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Domain length $A$</td>
<td>3.0 m</td>
</tr>
<tr>
<td>Domain height $B$</td>
<td>3.0 m</td>
</tr>
<tr>
<td>Chord length $L$</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Thickness $t_c$</td>
<td>0.2 m</td>
</tr>
</tbody>
</table>

**TABLE 6.17**

**SIMULATION SET-UP FOR WAVE SCATTERING BY A CONDUCTING SYMMETRIC AIRFOIL**

<table>
<thead>
<tr>
<th>Simulation set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Gaussian</td>
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<tr>
<td>Spread $\tau_w$</td>
<td>6.0</td>
</tr>
<tr>
<td>Delay period $n_0$</td>
<td>20.0</td>
</tr>
<tr>
<td>Source field</td>
<td>Cylindrical waves</td>
</tr>
<tr>
<td>Grid points $675 \times 675$</td>
<td></td>
</tr>
<tr>
<td>Time Step $\Delta t$</td>
<td>$6.25 \times 10^{-12}$ sec</td>
</tr>
<tr>
<td>CFL</td>
<td>0.5</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Clustered grid</td>
</tr>
<tr>
<td>Clustering Parameter $\beta$</td>
<td>1.5</td>
</tr>
</tbody>
</table>
The grid points are clustered along constant \( i \) and \( j \) grid lines and it is illustrated as the insert in Figure 6.67. Since the scatterer is a perfect conductor, the electrical conductivity is very large and infinite within the object, and thus, it is assumed in the simulation that no fields exists within the conductor. Consequently, no field values exist on the surface of the conductor. Since, the efforts are directed towards the demonstration of scattering from a conductor, it is safe to assume surface currents as zero. However, if one is designing an antenna where knowing surface current distribution is of interest and thus, it cannot be ignored. The TF-SF formulation is not implemented in this investigation and therefore, it is treated as an example of near-field application where the source is located near the scatterer. This approach is implemented to illustrate the wave reflection phenomenon by the conducting surface at late time analysis. The results, normalized with respect to the maximum, obtained at four different time steps are presented in Figure 6.68. It is observed in the electric field distribution plots that the numerical scheme is stable at all time steps and there are no non-physical oscillations present within the domain. The simulation is stopped after 1600 time steps before the waves impinge on the outer boundary of the domain, illustrated in Figure 6.68 (d). The scattering behavior, as demonstrated, yields the expected pattern of the wavefront. At 400 time steps, the fields are propagating with the leading circular wavefront within the domain without any obstructions. In the absence of any reflecting boundaries, the fields will continue to propagate forward in all directions and the radius of the leading wavefront will continue to grow larger representing the wave travel distance. However, in the presented case, the waves encounter the airfoil-shaped boundary and consequently, a reflected wavefront is introduced within the domain due to reflection by the leading edge of the airfoil. The original wavefront is deflected over the conducting surface of the airfoil and will continue to propagate further. There are several wavefronts observed in the simulated results in addition to the leading wavefront. These are the reflected wavefronts introduced upon interaction of the propagating wave with the conducting boundary. Additionally, the introduction of waves using a hard source at source location also acts as conducting point. The reflected wavefront is further reflected by such hard sources which results in multiple reflected wavefronts as observed in Figure 6.68. This is known as the constructive and destructive interference pattern in the EM wave theory. The simulated wave phenomenon resembles the pattern similar
to equipotential lines emanating from a source. Theoretically, the conducting surface exhibits the similarities with an equipotential surface which is clearly observed in the simulated results. Hence, the simulated results are a good measure of the accuracy of the numerical method as the wave propagation pattern in the presence of the conductor is accurately displayed by the obtained results.

Figure 6.68. Snapshots of numerical solution in the presence of conducting airfoil at (a) $n = 400$, (b) $n = 800$, (c) $n = 1200$, (d) $n = 1600$. 
6.3.7 Simulation of Scattering and Penetration by a Three-Dimensional Object

The extension of the numerical method to three-dimensional formulation was discussed in the previous chapters. The study of the numerical solution of the wave reflection and penetration by the three-dimensional numerical model is considered in this section. The scattering object is modeled as a lossless dielectric cube and a clustered mesh is used. The operating conditions are used from Table 6.6 and the simulation set-up is presented in Table 6.18.

TABLE 6.18
SIMULATION SET-UP FOR WAVE SCATTERING FROM A LOSSLESS DIELECTRIC CUBE

<table>
<thead>
<tr>
<th>Simulation set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Sinusoidal</td>
</tr>
<tr>
<td>Source field</td>
<td>Spherical waves</td>
</tr>
<tr>
<td>Grid points</td>
<td>$101 \times 101 \times 101$</td>
</tr>
<tr>
<td>Time Step $\Delta t$</td>
<td>$8 \times 10^{-12}$ sec</td>
</tr>
<tr>
<td>CFL</td>
<td>0.4</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Clustered grid</td>
</tr>
<tr>
<td>Clustering Parameter $\beta$</td>
<td>1.5</td>
</tr>
</tbody>
</table>

The objective here is to demonstrate the applicability of the numerical method for simulating wave propagation on a three-dimensional non-uniform grid. Thereby, a mesh which is densely clustered in the vicinity of the object interface boundaries is generated, similar to the one shown in Figure 6.62 but in three-dimension. This approach of clustering is desirable because of two reasons; firstly, to capture the interaction of the rapidly attenuating waves with the dielectric medium and its boundaries, a high grid resolution in this region is required, and secondly, as we know that the wave travels at a reduced speed within a medium other than free space, selection of closely spaced grid points helps in speeding up the wave which results
in the better accuracy. A smooth mesh of good quality is generated, and it is ensured that a stable solution is obtained. The CFL number is limited by clustering of grid points, however, with the mesh considered in this section, we were able to obtain a stable solution at CFL = 0.4.

Next consideration in mesh selection is the requirement of computational resources for three dimensional simulations. The three-dimensional wave propagation requires computations of six field variables with respect to three spatial coordinates. A grid system of 101x101x101 grid points requires computation to performed on approximately 1 million grid points and on 8 million grid points for 201x201x201 grid system. This results in an enormous amount of computations to be performed and therefore, massive computational resources are required. However, due to the robustness of the Modified Runge Kutta method, the numerical solutions were carried out within a reasonable time frame. Since, a clustered mesh has been used in the simulations, source was specified by a spherical wave to avoid leakage from the TF-SF boundaries. The disadvantage of a physical spherical wave is its attenuation rate which is proportional to \(1/r^3\), where \(r\) is the radius of propagation of a spherical wave. A similar observation is made in the numerical propagation of waves, where the fields dissipate quickly. To overcome this, a dipole with two arms is typically used as a source modeling. However, at this time, we are not using the dipole source approach. The source is excited by using hard source assigned at a location on an auxiliary axis and the values of the source fields are added or subtracted at the TF-SF boundaries.

The interaction of the time domain electric fields with the dielectric device is observed by plotting numerical results at various \(z\)-planes. As expected, there is no deflection of waves at \(z = 0.31\) m and \(z = 0.32\) m in Figure 6.69 (a) and Figure 6.69 (b), respectively, as there are no material boundaries. The results plotted at plane \(z = 0.336\) m and \(z = 342\) m in Figure 6.69 (c) and Figure 6.70 (d), respectively, demonstrate the penetration and reflection of waves. The plotted numerical solution is normalized with respect to the maximum values of the fields at time steps, \(n = 60\), time level, \(t = 48\) ps. Another observation from the solution is the attenuation of waves on a three dimensional grid due to which the absolute values of the computed fields are very small. Implementation of grid clustering helps in reducing such numerical errors by selecting fine meshing in the region of interest and a coarse mesh as we move away towards the outer
boundaries. Overall, the numerical solution on a clustered three-dimensional grid is stable and no artificial leakage from the total field-scattered field boundaries suggest the correct TF-SF implementation in the algorithm.

Figure 6.69. Numerical simulation on a three-dimensional clustered grid at $n = 60$ steps, $\Delta t^* = 2.4e-3$, (a) $z = 0.31$ m, (b) $z = 0.32$ m, (c) $z = 0.336$ m, (d) $z = 0.342$ m.
CHAPTER 7
APPLICATION TO BIOELECTROMAGNETICS

We have described earlier in this report that given the nature of hyperthermia and dosimetry applications where the field interactions are largely concentrated within the small regions of biological tissues, and the order of EM absorption is in millimeters, the utilization of coordinate transformation technique may prove extremely beneficial for accurately representing the curved boundaries and for employing grid clustering without a tedious approach. Furthermore, the utilization of Runge-Kutta method for temporal discretization provides higher-order of formal accuracy and better stability to obtain faster convergence. Such benefits have already been demonstrated in the results presented in chapter six.

To utilize such benefits of the algorithm to obtain accurate absorption and reflection data in the presence of dispersive material, the numerical model based on the Runge-Kutta method on transformed coordinates is extended to include dispersive media modeling by utilizing existing techniques. In this chapter, a brief description about the inclusion of recursive convolution method in the MRK-S algorithm is presented, followed by the validation of the algorithm by considering one-dimensional studies.

7.1 Governing Equations for Biological Tissues

The frequency dependence of the material is incorporated in the governing equation by casting the Maxwell’s equations to the form presented in equations (7.1) - (7.3). Various methods to solve the constitutive relation that relates the electric flux density to electric field intensity in equation (7.2) have been presented in the literature. In the equations, permeability is assumed to be independent of frequency. As discussed previously, the finite difference approximation of the E-fields and the H-fields are not sufficient to simulate the frequency dependence of the human tissues. One drawback associated with the FDTD method to simulate dispersive material is that the permittivity and conductivity parameter obtained at specific frequency are only accurate for narrow frequency ranges in a broadband simulation.
\[
\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H}
\] (7.1)

\[
\mathbf{D}(\omega) = \varepsilon(\omega) \cdot \mathbf{E}(\omega)
\] (7.2)

\[
\mu \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}
\] (7.3)

Moreover, even if one uses an approach to simulate the absorption in biological tissues using a single frequency source using the properties of the tissues at that particular frequency, the procedure has to be repeated at every frequency of interest which makes it a tedious process. Such limitations can be overcome by utilizing an appropriate model that efficiently manages the dispersive property of any medium.

Consider the governing equations (7.1) – (7.3) with three unknowns. The equations (7.1) and (7.3) are in the time-domain form, however, the constitutive equation (7.2) is in frequency-domain. A method is required to transform equation (7.2) in the time-domain form. Here, a recursive convolutional approach is presented that is used in obtaining \( \mathbf{E} \) fields from known \( \mathbf{D} \) fields at the same time level in equation (7.2). The convolution approach is a widely accepted method in the simulation of absorption by dispersive media. An advantage of the convolution method is that it requires less memory space as compared to other existing methods. It will be observed in the equations that it stores the past history of the solution in a single variable. Additionally, it does not require the discretization of the additional equation to obtained \( \mathbf{E} \)-fields from \( \mathbf{D} \)-fields as in the case of Auxiliary Differential Equations. In ADE approach, a second-order or higher-order differential equation is obtained which is subsequently discretized and the numerical approach then involves solution of additionally discretized equations which is time-consuming. The other methods are not presented here as they are out of scope for this text.

Recall the relations in equation (4.1) for performing non-dimensionalization of the governing equations (7.1) – (7.3). The resulting non-dimensionalized equations are
\[ \frac{\partial \mathbf{D}^*}{\partial \tau^*} = \nabla^* \times \mathbf{H}^* \]  
\quad (7.4)

\[ \mathbf{D}^*(\omega) = \varepsilon^*(\omega) \cdot \mathbf{E}^*(\omega) \]  
\quad (7.5)

\[ \mu^* \frac{\partial \mathbf{H}^*}{\partial \tau^*} = -\nabla^* \times \mathbf{E}^* \]  
\quad (7.6)

The discretization of the finite difference equations is carried out in a similar manner and the resulting equations in the curvilinear coordinate is same as the non-dispersive governing equations. The three dimensional model equation in the flux-vector form for the governing equations (7.4) and (7.6) is

\[ \frac{\partial \bar{T}}{\partial \tau} + \bar{X} \frac{\partial \bar{P}}{\partial \xi} + \bar{Y} \frac{\partial \bar{Q}}{\partial \eta} + \bar{Z} \frac{\partial \bar{R}}{\partial \zeta} = 0 \]  
\quad (7.7)

Where, the flux vectors \( \bar{T}, \bar{P}, \bar{Q}, \text{ and } \bar{R} \) in transformed coordinates are related to the flux vectors in physical coordinates as shown

\[ \bar{T} = \frac{T}{f} \]

\[ \bar{P} = \frac{1}{f} (\xi_x P + \xi_y Q + \xi_z R) \]  
\quad (7.8)

\[ \bar{Q} = \frac{1}{f} (\eta_x P + \eta_y Q + \eta_z R) \]

\[ \bar{R} = \frac{1}{f} (\zeta_x P + \zeta_y Q + \zeta_z R) \]
The flux vectors containing the primitive variables are given in equation (7.9).

\[
T = \begin{bmatrix} D_x \\ D_y \\ D_z \\ H_x \\ H_y \\ H_z \end{bmatrix}
\]

\[
P = \begin{bmatrix} 0 \\ H_z \\ -H_y \\ 0 \\ -E_z \\ E_y \end{bmatrix}
\]

\[
Q = \begin{bmatrix} -H_z \\ 0 \\ H_x \\ E_z \\ 0 \\ -E_x \end{bmatrix}
\]

\[
R = \begin{bmatrix} H_y \\ -H_x \\ 0 \\ -E_y \\ E_x \\ 0 \end{bmatrix}
\]
The coefficient matrices are given as

\[
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/\mu & 0 & 0 \\
0 & 0 & 0 & 0 & 1/\mu & 0 \\
0 & 0 & 0 & 0 & 0 & 1/\mu
\end{bmatrix}
\]  

(7.10)

It is observed that the formulation of the governing equations in the transformed coordinates presented here are different than the formulation presented in chapter four. The noted observations are:

- The term \( J_\sigma \) that defines the lossy nature of the medium does not appear in the model equation (7.7). It is because the material conductivity is included in the Debye formulation.
- The flux vector \( T \) in equation (7.9) is dependent on D field variables instead of E field variables.
- The coefficient matrices in equation (7.10) contains only permeability parameter where separation formulation is required to describe the dispersive properties of the biological media.

7.2 **Dispersive Nature of Biological Tissues**

Several models to accurately define the dispersive properties of the material have been extensively studied and verified in the past studies, however, it is well-known that the Debye equation with two relaxation constants can be used to adequately describe the frequency-dependent electrical permittivity of the biological tissues. The second-order Debye equation produces accurate results for wideband simulations; however, some inaccuracies are observed in the solution at the higher and the lower end of the frequency ranges. Such inaccuracies can be removed by the implementation of higher order Debye relations, but the higher-order model lead to complexities in the numerical implementation and adds to the computational memory requirement for the simulation.
A general form of the $p$-th order Debye relation with a conductive loss term is given as [95]

$$
\varepsilon^*(\omega) = \varepsilon_\infty + \sum_{p=1}^{P} \frac{\Delta \varepsilon_p}{1 + j\omega \tau_p} + \frac{\sigma_s}{j\omega \varepsilon_0} \tag{7.11}
$$

Where, $\varepsilon_\infty$ is the permittivity of the material at infinite frequency,

$\Delta \varepsilon_p = \varepsilon_s - \varepsilon_\infty$, is the difference between the static permittivity, $\varepsilon_s$ of $p$-th order pole and permittivity at infinite frequency,

$\varepsilon_0$ is the permittivity of free space,

$\tau_p$ is the relaxation time constant of the $p^{th}$-order pole,

$p$ denotes the pole order ($p = 1, 2, 3, \ldots, P$)

Substitute the permittivity relation in equation (7.5). All equations are in the non-dimensional form and the asterisk ‘*’ from the superscript has been dropped for convenience.

$$
D(\omega) = \left( \varepsilon_\infty + \sum_{p=1}^{P} \frac{\Delta \varepsilon_p}{1 + j\omega \tau_p} + \frac{\sigma_s}{j\omega \varepsilon_0} \right) E(\omega) \tag{7.12}
$$

Since this equation is in the frequency domain form, a convolutional approach using the Fourier theorem is used as in [118,130] to transform the frequency-domain relation to the time-domain relation. According to this approach, the $1/j\omega$ term in the frequency domain is equal to the integral formulation in the time domain. Therefore, the application of inverse Fourier transform, and subsequent convolution of the terms will result in equation (7.13)

$$
D(t) = \varepsilon_\infty E(t) + \sum_{p=1}^{P} \frac{\Delta \varepsilon_p}{\tau_p} \int_{0}^{t} e^{-\frac{(t-\tau)}{\tau_p}} E(\tau) \, d\tau + \frac{\sigma_s}{\varepsilon_0} \int_{0}^{t} E(\tau) \, d\tau \tag{7.13}
$$

In the sampled time domain, the integrals in the equation is replaced by the summation as shown.

$$
D^n = \varepsilon_\infty E^n + \sum_{p=1}^{P} \frac{\Delta \varepsilon_p}{\tau_p} \Delta t \sum_{h=0}^{n} e^{-\frac{\Delta t(n-h)}{\tau_p}} E^h + \frac{\sigma_s}{\varepsilon_0} \Delta t \sum_{h=0}^{n} E^h \tag{7.14}
$$

As we will be using the $2^{nd}$ order Debye equation with two relaxation constants, the summation in equation (7.14) is expanded as shown
\[ \mathbf{D}^n = \varepsilon_\infty \mathbf{E}^n + \frac{\Delta \varepsilon_1}{\tau_1} \Delta t \sum_{h=0}^{n} e^{-\frac{\Delta t(n-h)}{\tau_1}} \mathbf{E}^h + \frac{\Delta \varepsilon_2}{\tau_2} \Delta t \sum_{h=0}^{n} e^{-\frac{\Delta t(n-h)}{\tau_2}} \mathbf{E}^h + \frac{\sigma_s}{\varepsilon_0} \Delta t \sum_{h=0}^{n} \mathbf{E}^h \] (7.15)

Let us decompose the equation (7.15) into three parts for further simplification as given in equations (7.16) – (7.18)

\[ S^n_1 = \frac{\Delta \varepsilon_1}{\tau_1} \Delta t \sum_{h=0}^{n} e^{-\frac{\Delta t(n-h)}{\tau_1}} \mathbf{E}^h \] (7.16)

\[ S^n_2 = \frac{\Delta \varepsilon_2}{\tau_2} \Delta t \sum_{h=0}^{n} e^{-\frac{\Delta t(n-h)}{\tau_2}} \mathbf{E}^h \] (7.17)

\[ S^n_2 = \frac{\sigma_s}{\varepsilon_0} \Delta t \sum_{h=0}^{n} \mathbf{E}^h \] (7.18)

Since the purpose of the formulation is to obtain the field values of \( \mathbf{E}^n \) from \( \mathbf{D}^n \), manipulation of equation (7.15) is required to obtain an equation for the computation of \( \mathbf{E} \)-fields. To derive such form, let us consider any arbitrary summation function,

\[ f = \sum_{n=0}^{m} g^n \]

Using the summation algebra, the equation can be written in the form as shown.

\[ f = g^m + \sum_{n=0}^{m-1} g^n \]

Application of the similar approach to equations (7.16) – (7.18) will results in equations (7.19) – (7.21)

\[ S^n_1 = \frac{\Delta \varepsilon_1}{\tau_1} \Delta t \left[ \mathbf{E}^n + \sum_{h=0}^{n-1} e^{-\frac{\Delta t(n-h)}{\tau_1}} \mathbf{E}^h \right] \] (7.19)

\[ S^n_2 = \frac{\Delta \varepsilon_2}{\tau_2} \Delta t \left[ \mathbf{E}^n + \sum_{h=0}^{n-1} e^{-\frac{\Delta t(n-h)}{\tau_2}} \mathbf{E}^h \right] \] (7.20)
\[
S_3^n = \frac{\sigma_s}{\epsilon_0} \Delta t \left[ E^n + \sum_{h=0}^{n-1} E^h \right]
\]  

(7.21)

In the equations (7.19), (7.20), and (7.21) the terms \( S_1^{n-1} \), \( S_2^{n-1} \) and \( S_3^{n-1} \) are introduced such that

\[
S_1^{n-1} = \frac{\Delta \varepsilon_1}{\tau_1} \Delta t e^{-\frac{\Delta t}{\tau_1} \sum_{h=0}^{n-1} e^{-\frac{\Delta t(n-h)}{\tau_1}} E^h}
\]

(7.22)

\[
S_2^{n-1} = \frac{\Delta \varepsilon_2}{\tau_2} \Delta t e^{-\frac{\Delta t}{\tau_2} \sum_{h=0}^{n-1} e^{-\frac{\Delta t(n-h)}{\tau_2}} E^h}
\]

(7.23)

\[
S_3^{n-1} = \frac{\sigma_s}{\epsilon_0} \Delta t \sum_{h=0}^{n-1} E^h
\]

(7.24)

Subsequently, using relations in equation (7.19) – (7.24), the equation (7.15) is written as

\[
D^n = \epsilon_\infty E^n + \frac{\Delta \varepsilon_1}{\tau_1} \Delta t E^n + e^{-\frac{\Delta t}{\tau_1} S_1^{n-1}} + \frac{\Delta \varepsilon_2}{\tau_2} \Delta t E^n + e^{-\frac{\Delta t}{\tau_2} S_2^{n-1}} + \frac{\sigma_s}{\epsilon_0} \Delta t E^n + S_3^{n-1}
\]

(7.25)

Rearranging terms in equation (7.25) to obtain an equation for computation of \( E \) fields at time level \( n \) and \( i,j \) locations within the grid.

\[
E_{i,j}^n = D_{i,j}^n - e^{-\frac{\Delta t}{\tau_1} S_{1i,j}^{n-1}} - e^{-\frac{\Delta t}{\tau_2} S_{2i,j}^{n-1}} - S_{3i,j}^{n-1}
\]

\[
\epsilon_\infty + \frac{\Delta \varepsilon_1}{\tau_1} \Delta t + \frac{\Delta \varepsilon_2}{\tau_2} \Delta t + \frac{\sigma_s}{\epsilon_0} \Delta t
\]

(7.26)

It is worthwhile to note that the \( E \)-fields are simply equal to \( D \)-field in the free space region. Thereafter, according to the new mathematical algorithm for the dispersive medium, flux vectors \( \overline{T}_1, \overline{T}_2, \) and \( \overline{T}_3 \) are computed in the first stage of \( n+1 \) time level at all \( (i,j) \) index locations using the values of \( H_x, H_y \) and \( H_z \) from the previous time step and update \( \overline{T} \rightarrow D \), followed by the computation of electric field intensity, \( E \), at time level, \( n+1 \) using known values of electric flux, \( D \) at the same time level, \( n+1 \) and the stored summation according to equation (7.22) – (7.24). Subsequently, update flux vectors \( P, Q, \) and \( R \) from
primitive variables $E_x, E_y,$ and $E_z$. The first stage for $\overline{T}_4, \overline{T}_5,$ and $\overline{T}_6$ is computed at $n+1/2$ time level using the updated values of E fields calculated in the first stage. After computing at all grid points, update, $\overline{T}_4 \rightarrow H_x$, $\overline{T}_5 \rightarrow H_y$, and $\overline{T}_6 \rightarrow H_z$ and flux vectors $P, Q$ and $R$ from primitive variables $H_x, H_y$ and $H_z$. Subsequently, the second, third, and fourth stages will be computed using the values from the interleaved stages of the same time level. Thus, the solution will loop over the required number of time steps according to the defined algorithm until it reaches the desired time level for time dependence analysis or until the solution is converged in case of steady state analysis. The spatial derivatives are computed by the staggered grid approach presented in Section 4.5.2.2. The known material properties of the dispersive materials are specified at each location within the domain at the start of the simulation.

Several investigators have performed rigorous experimental studies to quantify the frequency dependence of the biological tissues and once such study is presented by Gabriel et al. [97]. The values of various Debye parameters in the complex permittivity equation are obtained from the published literature. Generally, the authors in the past numerical studies have used the least square fitting method to derive the Debye constants that matches with the existing experimental data. In the presented results, we will be using the Debye constants from the cited reference papers, as their derivation is out of scope of the objective of the research at this time.

7.3 Numerical Investigations

Two one-dimensional studies are considered here to suffice the objectives of this research. The propagation of the electromagnetic waves in an air-water medium and an air-muscle medium is presented in this section. The air-water medium is considered in the investigations because of the high water content in some human tissues that affects the reflection and absorption quantities[110]. Additionally, the frequency-dependence of the water can be specified by only single Debye relaxation constant and thus, it is the simplest case to validate a numerical approach. The two investigations utilize the operating conditions and the grid size as described in Gandhi et al.[89]. Moreover, the Debye constants are assumed similar to [87,89].
The derivation of the model equation in the one-dimensional domain from the presented numerical model is straightforward by assuming the infinite domain in y and z directions and thus, no change occurs in these direction, and consequently, computation of only two primitive quantities, \( E_z \) and \( H_y \) are required. The benefit of the frequency-dependent method lies in the fact that the single simulation using an impulse function can yield frequency response of the biological tissues for a wideband spectrum. The continuous waveform like sine wave source is a single frequency source, and thus, the response at each frequency will require a separate simulation and therefore, not an efficient method for wideband simulations. To simulate at a single frequency with sine waveform, it is efficient to use frequency independent formulation instead of complex permittivity relation and specify the dielectric properties at that frequency everywhere within the domain. For wideband investigation, however, the frequency dependent method is preferred.

### 7.3.1 Wave Travel in an Air-Water Medium

The operating conditions for the simulation of wave propagation in water are presented in Table 7.1.

**TABLE 7.1**

OPERATING CONDITIONS FOR WAVE INTERACTION WITH A DISPERSIVE MEDIUM – WATER

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of AIR ( \epsilon_1 )</td>
<td>( 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Magnetic permeability of AIR ( \mu_1 )</td>
<td>( 1.257 \times 10^{-6} ) H/m</td>
</tr>
<tr>
<td>Permittivity of WATER, at infinite frequency ( \epsilon_\infty )</td>
<td>( 1.8 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Static permittivity of WATER, pole 1 ( \epsilon_{s1} )</td>
<td>( 81 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Static permittivity of WATER, pole 2 ( \epsilon_{s2} )</td>
<td>( 1.8 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Relaxation constant 1 ( \tau_1 )</td>
<td>( 9.4 \times 10^{-12} ) s</td>
</tr>
<tr>
<td>Relaxation constant 2 ( \tau_2 )</td>
<td>( 1.0 ) s</td>
</tr>
<tr>
<td>Magnetic permeability of WATER ( \mu_2 )</td>
<td>( 1.257 \times 10^{-6} ) H/m</td>
</tr>
<tr>
<td>Electrical conductivity of AIR and WATER ( \sigma )</td>
<td>( 0.0 ) S/m</td>
</tr>
<tr>
<td>Domain length ( A )</td>
<td>( 0.0374625 ) m</td>
</tr>
</tbody>
</table>
According to [87,89], the dispersive properties of the water can be accurately specified by a Debye equation with single-relaxation constant. Thus, the static permittivity of the water in the 2nd term of the Debye equation is selected equal to the permittivity of water at infinite frequency such that difference between them is zero in order to reduce the Debye equation to single order. Accordingly, the 2nd relaxation constant is not required, however, due to computational requirements, any finite value can be assigned to avoid floating point division error. The magnetic permeability is assumed non-dispersive. The source modeling parameters and other quantities in the simulation set-up are presented in Table 7.2. The frequency response of the dispersive medium is computed for the frequency range 0 to 60 GHz using the Fourier transformation method described previously in Section 4.7.

TABLE 7.2
SIMULATION SET-UP FOR WAVE INTERACTION WITH A DISPERSIVE MEDIUM – WATER

<table>
<thead>
<tr>
<th>Simulation set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Gaussian</td>
</tr>
<tr>
<td>Spread</td>
<td>( \tau_w = 152.0 )</td>
</tr>
<tr>
<td>Delay period</td>
<td>( n_0 = 400.0 )</td>
</tr>
<tr>
<td>Amplitude</td>
<td>( E_0 = 1000 ) V/m</td>
</tr>
<tr>
<td>Grid points</td>
<td>( \text{IMAX} = 1000 )</td>
</tr>
<tr>
<td>Spatial step size</td>
<td>( \Delta x = 3.75 \times 10^{-5} ) m</td>
</tr>
<tr>
<td>Time Step</td>
<td>( \Delta t = 6.25 \times 10^{-14} ) sec</td>
</tr>
<tr>
<td>CFL</td>
<td>0.5</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Uniformly spaced</td>
</tr>
</tbody>
</table>

The time-domain results are obtained at various time levels using the dispersive modeling algorithm described in this chapter as well as using the frequency-independent MRK-S method described in chapter four. Since, in a frequency-independent MRK method, the dielectric and conductive properties of a medium is specified at a constant frequency, the MRK frequency independent simulation is performed by specifying relative electric permittivity of water as 34.864 (at 20 GHz) and the conductivity as 43.43 S/m (at 20 GHz).
The results presented in Figure 7.1 to Figure 7.3 at time steps, \( n = 850 \), \( n = 1300 \) and \( n = 2000 \), respectively compares the predicted wave propagation by MRK-dispersive (MRK-D in plots) and MRK- frequency independent (MRK in plots) in domain consisting of air and water. The reflection by the air-water interface, absorption in water and subsequent attenuation is clearly observed in the presented plots.

![Figure 7.1](image1.png)

Figure 7.1. Time-domain numerical output predicted by the MRK-dispersive method and MRK-frequency independent method at \( n = 850 \) steps for an air-water interface.

![Figure 7.2](image2.png)

Figure 7.2. Time-domain numerical output predicted by the MRK-dispersive method and MRK-frequency independent method at \( n = 1300 \) steps for an air-water interface.
Figure 7.3. Time-domain numerical output predicted by the MRK-dispersive method and MRK-frequency independent method at \( n = 2000 \) steps for an air-water interface.

There is an obvious difference between the simulated results obtained from two different methods. It is demonstrated that upon interaction with the dispersive media at time levels \( n = 1300 \) and \( n = 2000 \), the frequency-dependent algorithm is incapable of accurately predicting the absorption and reflection of the EM waves by a dispersive medium. At time level, \( n = 850 \), however, when the wave is in free space, the predicted results are same as expected. The human body is made up of several tissues, and each tissue is specified by their own frequency-dependent dielectric properties and therefore, it is required to predict the absorption and reflection of waves accurately. This study is, therefore, important from validation point of view in the development of a dispersive method.

Next, the validation of accuracy is performed by obtaining the reflectance as a function of frequency and the data is compared with the analytically calculated reflection coefficient data at several frequencies. The numerical reflection is obtained using the expression in equation (7.27).

\[
\Gamma = \frac{E_z(f)|_{\text{ref}}}{E_z(f)|_{\text{inc}}} \tag{7.27}
\]
The frequency domain electric field data is obtained at the desired locations for a wideband frequency range. The reflected electric fields are obtained by placing the sensor at 10 cells away from the air-water interface to record the frequency dependent results using the Fourier transform. Similarly, the frequency domain incident electric field data are obtained by placing the sensor to record values at the interface. The total field-scattered formulation developed earlier serves as a useful tool in obtaining the reflected and incident fields as the results are obtained using a single simulation as against two separate simulation set-up used in Luebbers et al. [87]. The analytical reflection coefficient is computed using equation (7.28)

$$\Gamma_{\text{exact}} = \left| \frac{\sqrt{\varepsilon_0} - \sqrt{\varepsilon^*(\omega)}}{\sqrt{\varepsilon_0} + \sqrt{\varepsilon^*(\omega)}} \right|$$

(7.28)

Figure illustrates the comparison of numerically computed reflection coefficient at various frequencies with the exact reflection coefficients. An excellent agreement between the results is observed which validates the approach of the algorithm. The reflection data computed using the MRK frequency-independent method with properties of water at frequency of 20 GHz is also included in the figure and the inaccuracies in the results computed by the frequency-independent method is clearly visible.

Figure 7.4. Comparison of numerically computed reflection coefficient for air-water interface using the MRK-dispersive algorithm with the exact reflection coefficient data and the frequency independent MRK algorithm for the frequency range 0-60 GHz.
7.3.2 Wave Travel in an Air-Muscle Medium

According to Gandhi et al. [89], the human body can be represented by the average permittivity equivalent to 2/3 of the properties of the muscle and hence used in the studied example. Similarly, we are considering the 2/3 muscle properties obtained from [89]. The dispersive properties of the muscle tissue can be adequately specified by a second-order Debye-equation. The relative permittivity and conductivity obtained from the given Debye constants are in good agreement with the experimental data [89] and thus, can produce results with a decent accuracy within the given frequency range. The Debye constants and other operating conditions used in the simulation for the simulation of wave propagation in muscle are presented in Table 7.3. The magnetic permeability is assumed to be non-dispersive.

TABLE 7.3
OPERATING CONDITIONS FOR WAVE INTERACTION WITH A DISPERSIVE MEDIUM – 2/3 MUSCLE

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical permittivity of AIR</td>
<td>( \varepsilon_1 = 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Magnetic permeability of AIR</td>
<td>( \mu_1 = 1.257 \times 10^{-6} ) H/m</td>
</tr>
<tr>
<td>Permittivity of MUSCLE, at infinite frequency</td>
<td>( \varepsilon_\infty = 19 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Static permittivity of MUSCLE, pole 1</td>
<td>( \varepsilon_{s1} = 10019 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Static permittivity of MUSCLE, pole 2</td>
<td>( \varepsilon_{s2} = 61 \times 8.854 \times 10^{-12} ) F/m</td>
</tr>
<tr>
<td>Relaxation constant 1</td>
<td>( \tau_1 = 1.13 \times 10^{-7} ) s</td>
</tr>
<tr>
<td>Relaxation constant 2</td>
<td>( \tau_2 = 1.194 \times 10^{-11} ) s</td>
</tr>
<tr>
<td>Magnetic permeability of MUSCLE</td>
<td>( \mu_2 = 1.257 \times 10^{-6} ) H/m</td>
</tr>
<tr>
<td>Electrical conductivity of AIR and MUSCLE</td>
<td>( \sigma = 0.0 ) S/m</td>
</tr>
<tr>
<td>Domain length</td>
<td>( A = 0.126873 ) m</td>
</tr>
</tbody>
</table>
The source modeling parameters and other quantities in the simulation set-up are presented in Table 7.4.

### TABLE 7.4

**SIMULATION SET-UP FOR WAVE INTERACTION WITH A DISPERSIVE MEDIUM – 2/3 MUSCLE**

<table>
<thead>
<tr>
<th>Simulation set-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Source waveform</td>
<td>Gaussian</td>
</tr>
<tr>
<td>Spread</td>
<td>( \tau_w = 71.0 )</td>
</tr>
<tr>
<td>Delay period</td>
<td>( n_0 = 213.0 )</td>
</tr>
<tr>
<td>Grid points</td>
<td>IMAX = 1000</td>
</tr>
<tr>
<td>Spatial step size</td>
<td>( \Delta x = 1.27 \times 10^{-4} ) m</td>
</tr>
<tr>
<td>Time Step</td>
<td>( \Delta t = 2.12 \times 10^{-13} ) sec</td>
</tr>
<tr>
<td>CFL</td>
<td>0.5</td>
</tr>
<tr>
<td>Grid feature</td>
<td>Uniformly spaced</td>
</tr>
</tbody>
</table>

The time-domain propagation of the electric field component obtained at time steps, \( n = 400 \), \( n = 750 \), and \( n = 1600 \) are presented in Figure 7.5 – Figure 7.7, respectively to illustrate the wave propagation upon interaction with 2/3 muscle.

![Figure 7.5](image-url)

**Figure 7.5.** Time-domain numerical output predicted by the MRK-dispersive method at \( n = 400 \) steps for an air-2/3 muscle interface.
Figure 7.6. Time-domain numerical output predicted by the MRK-dispersive method at $n = 750$ steps for an air-2/3 muscle interface.

Figure 7.7. Time-domain numerical output predicted by the MRK-dispersive method at $n = 1600$ steps for an air-2/3 muscle interface.

The predicted results illustrate the reflection from a dispersive medium boundary and the attenuation of the absorbed waves within the dispersive medium. The results are as expected, and there are no instabilities within the solution. The accuracy of the predicted results is further demonstrated by comparing the
numerical reflection data with the analytically computed reflection at various frequencies. The comparison is presented in Figure 7.8. The analytical reflection is computed using equation (7.28).

![Figure 7.8](image)

Figure 7.8. Comparison of numerically computed reflection coefficient for air-2/3 muscle interface using the MRK-dispersive algorithm with the exact reflection coefficient data in the frequency range 0-30 GHz.

It is clearly visible that the results from MRK-dispersive algorithm are in good agreement with the analytical data. However, in Figure 7.8, some inaccuracies in the reflection coefficient at the two extremes in the frequency range are observed. Such inaccuracies are due to the specification of dispersive properties by the second-order Debye equation. The inaccuracies can be avoided by using the higher-order Debye equations that consists of more than two relaxation constants. However, the computational costs will increase by using higher order Debye formulations. Therefore, it can be concluded that the second order Debye equation can produce results with an acceptable level of accuracy.
CHAPTER 8

CONCLUSION

This research focused on the utilization of fourth-order Modified Runge-Kutta method on curvilinear coordinates to simulate non-rectangular electromagnetic applications. The two-dimensional and three-dimensional computer programs were developed, and the validity of the algorithm was validated by studying the numerical output for several cases. The standing wave problem within a homogeneous domain and an inhomogeneous domain were considered in the first stages of the research. Maxwell’s equations were solved using a fourth-order Modified Runge-Kutta scheme in both the physical domain and computational domain using a dimensionalization approach as well as non-dimensionalization approach to simulate the propagation of waves for the first two cases. The results were compared with the known analytical solution for the given case. For Case I, the accuracy of the Modified Runge-Kutta scheme on transformed coordinates and grid independence were investigated, and it was established that a stable and accurate solution was obtained, and the order of error distribution was found to be less than $10^{-5}$.

For Case II, investigations were performed for grid independence and the effect of electric permittivity on the electric field at time step $t^* = 0.0005$. The solutions obtained were found to be in excellent agreement with the analytical solution for various values of dielectric permittivity. However, in the time-dependence study, the time step $t^* = 0.0005$ was too small to show possible changes in electric field values. Hence, numerical solutions were obtained at a higher time level, $t^* > 0.2$, wherein oscillations were observed. These oscillations were due to solving field variables on an unstaggered grid system. The central differencing approximation leads to odd-even decoupling errors that causes non-physical solutions, primarily in the region where material discontinuities are encountered. The oscillations propagate into the domain from the location of such discontinuities. One method to remove such artifacts is to use grid staggering of electric and magnetic field components that does not reduces the second order accuracy of central difference approximations. This investigation on time dependency has led to the conclusion that the staggered grid approach is favorable over the unstaggered grid approach for solving Maxwell’s equation.
Next, far-field applications of the travelling waves were considered. During the preliminary investigations, we noticed large dissipation of amplitude with MRK method. To reduce the dissipation, we improvised the MRK approach by specifying the four-stages in a leapfrog order and compared the numerical results of sine wave propagation with the general MRK approach and FDTD approach in one-dimensional. The dissipation was greatly reduced by the application of leapfrog in fourth-order MRK. Subsequently, the total field-scattered field formulation was included in the numerical algorithm to investigate far-field scattering and penetration by linear, homogeneous, and non-dispersive materials. The TF-SF formulation is used to introduce incident fields that have been originated at a distant location into the region of interest known as the total field region. In this region, the waves continue to propagate in space and upon encountering a material boundary, the wave undergoes penetration and reflection based on the material property. The reflected values appear in the scattered field region and the total field region is a mix of incident and scattered fields. In the absence of any material, the wave exits from the other end of the TF-SF boundary without any deflection. This phenomenon was studied using lossless material, lossy material and conducting material and useful results were presented. The outer domain boundaries were specified using the conducting wall boundary conditions and hence, a large domain was required in order to prevent artificial reflections from the outer boundaries. The computed results were found to be stable at large CFL values and in accordance with the principles of TF-SF approach. The results were in good agreement with the benchmark FDTD method and at some locations, the results were even better than the FDTD method.

The grid independence study and the CFL dependence study resulted in useful conclusions. At low CFL numbers, the solution was highly dispersive and therefore, it was concluded that the maximum allowable CFL number for a given numerical method must be used in order to obtain the best quality simulation results. A higher CFL number also results in the faster convergence of the solution and hence, desirable. An advantage of the MRK method is its relaxed stability that allows the use of a CFL number larger than the benchmark FDTD method which makes the MRK method more appealing to researchers. We performed our tests on various grid sizes, ranging from fewer grid points to a large number of grid points.
points and it was concluded that the gain in the simulation time is roughly 20%, i.e. the FDTD method with one simulation per time step took roughly 20% more CPU time than Runge-Kutta with four stages per time step to reach the same time level.

The effect of the lossy medium on the wave propagation was studied using the developed algorithm. It was observed that the wave attenuates faster in a lossy medium as compared to the lossless medium. This was demonstrated by comparing numerical results of wave propagation in a lossy and a lossless medium. The results were found to be in adherence with the theory of physical propagation of waves in lossy medium. The usefulness of the coordinate transformation technique lies in the robustness with which the non-rectangular surfaces and boundaries can be modelled on a finite difference grid axis. Furthermore, the straightforward implementation of the clustering of grid points in the region where required, is an advantage of coordinate transformation. To demonstrate such benefits, firstly, the scattering from a rectangular lossless medium on a clustered grid was studied and subsequently, scattering from a lossless circular cylinder and a conducting airfoil were considered. The simulation of wave propagation in a square lossless medium on a clustered grid produced better results than on a uniform grid. This is due to the reason that the velocity of waves in a medium largely depends on the dielectric properties of the medium and the grid step size. A large permittivity reduces the speed of the waves in a dielectric media which can be sped up to a free space velocity by reducing the grid step size proportionately. Thus, it was concluded that finely clustering the grid points inside the dielectric and near the material interfaces and using coarse grid points near the outer boundaries results in a better quality of solution and helps in reducing the grid requirements. This conclusion will be very helpful in simulating waves in a three-dimensional space.

The scattering results from a dielectric circular cylinder and the perfectly conducting airfoil were, subsequently, investigated to demonstrate the effectiveness of coordinate transformation technique in simulation studies that involve non-rectangular boundaries. Clustering of grid points was included in the mesh. For airfoil geometry, a C-grid was generated. The time snapshots of the solution were presented, and the various underlying phenomena were explained. In the simulation of wave scattering from a symmetric airfoil, the source was specified as the hard source in the vicinity of the material and hence TF-SF
boundaries were not incorporated. Due to such approach, the constructive and destructive interference
between the reflected wavefronts and the source location was observed, as expected. Overall, a stable
solution was obtained during the simulation of waves in the presence of non-rectangular boundaries and
also when a densely clustered grid system was used.

Upon obtaining satisfactory results from the two-dimensional studies, next, the numerical model
was extended to investigations in three-dimensions and the computer program was developed to simulate
the wave propagation in the presence of a lossless dielectric cube. Due to the nature of three-dimensional
numerical algorithm, the simulation requires enormous amount of computer resources. It was highlighted
that the three dimensional structures require the computation of six field variables on at least one million
grid points to obtain an acceptable solution. This issue is further alleviated when TF-SF is included due to
computations of the source fields propagation on a similar grid size. The clustering of grid points is a useful
approach in simulating such applications as the mix of fine and coarse discretization within the domain
results in the reduction in the requirements for a large number of grid points. Simulation results on a
clustered grid system were plotted at various z-planes to demonstrate the propagation of waves in three-
dimension. The plotting of three-dimensional propagation of waves poses a challenge as additional
resources are required to plot such massive data. The observed results were stable at a fairly higher Courant
number on a clustered grid. The results were found to be in agreement with the principles of scattering and
total field-scattered field formulation.

In the last stage of the research, we extended the algorithm to simulate EM wave propagation in
the presence of a biological material such as muscles. The frequency dependence of the biological tissues
is included in the MRK formulation by using recursive convolution method. The steps in the development
of such formulation are based on existing techniques and are specified in chapter seven. The algorithm
utilizes the second order Debye equation with a lossy conductive term. Two one-dimensional cases were
considered for numerical prediction of electromagnetic wave phenomenon in the presence of biological
materials. In the first case, the reflection and absorption were studied in the air-water medium. The
numerical results indicate excellent agreement with the analytically computed reflection data. The
simulated results for the first case was also obtained by the frequency independent MRK method using the properties of water at frequency of 20 GHz. The errors using the frequency independent method are clearly demonstrated in the presented results. In the second study, an air-2/3 muscle medium was considered. The numerical results indicate excellent agreement with the analytical solution. Some inaccuracies at the lower and higher frequency ranges were observed. There errors are caused due to the specification of dispersive properties by second order Debye equation. These inaccuracies can be avoided by implementing higher order Debye accuracy but there will be a loss in efficiency of the method due to increase in computational procession time. Overall accuracy of the numerical results was observed to be reasonably good and acceptable. It is, therefore, concluded that the MRK dispersive method can be used to simulate wave phenomenon accurately in the presence of dispersive biological tissues.

During the process of investigations, several limitations were identified which require attention. Such challenges can become a part of future studies to develop an advanced solver for computational electromagnetics. Firstly, the developed algorithm needs to be modified to include plane wave source on a clustered grid without leakages. Presently, the leakage errors were observed due to the phase mismatch between the one-dimensional plane wave source and the two-dimensional simulation domain that has resulted in the dispersion and phase errors. Secondly, the implementation of absorbing boundaries in the numerical approach is required so that the steady state investigations can be performed. Presently, the time-accurate investigations were performed, however, by using absorbing boundary conditions various quantitative data, such as the reflection and transmission coefficients, can be obtained to analyze the material performance.

The inclusion of parallel computing algorithm in the developed codes is another interesting subject that requires attention. Parallel computing is the most researched and widely adopted technique presently. The simulations in three-dimensional space is largely restricted due to the limitations of single processor computational power. The implementation of parallel codes will help in alleviating the performance characteristics of the developed computer program and simulations on electrically large structures with fine discretization can be performed efficiently.
This dissertation utilized the existing numerical technique as well as presented an alternate formulation of Modified Runge-Kutta on curvilinear coordinates to study electromagnetic wave propagation in various media and made an attempt to address and reduce the numerical difficulties associated with the non-rectangular geometries.
REFERENCES


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APPENDICES
APPENDIX A

TRANSFORMATION OF EQUATIONS FROM PHYSICAL DOMAIN TO COMPUTATIONAL DOMAIN IN THREE DIMENSIONS

Chain rule of the partial differential equations given in equations (A.1) through (A.4) are used for the transformation of Maxwell’s equations from physical domain \((x, y, z)\) to computational domain \((\xi, \eta, \zeta)\)

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} + \zeta_t \frac{\partial}{\partial \zeta} \quad (A.1)
\]

\[
\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta} \quad (A.2)
\]

\[
\frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta} \quad (A.3)
\]

\[
\frac{\partial}{\partial z} = \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta} \quad (A.4)
\]

The conservative form of the non-dimensionalized Maxwell’s equations derived previously is rewritten here in equation (A.5) for convenience.

\[
\frac{\partial T}{\partial \tau} + X \frac{\partial P}{\partial \xi} + Y \frac{\partial Q}{\partial \eta} + Z \frac{\partial R}{\partial \zeta} + J_\sigma = 0 \quad (A.5)
\]

Substitute the relations given in equations (A.1) - (A.4) in equation (A.5) to obtain equation (A.6) which is further expanded as shown in equation (A.7). Since the coefficient terms \(X, Y, \) and \(Z\) contain the material parameters and are assumed as independent constants in the equation, they can be directly added in the transformed form of the equation.
\[
\left( \frac{\partial}{\partial \tau} + \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} + \zeta_t \frac{\partial}{\partial \zeta} \right) T + \left( \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta} \right) P + \left( \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta} \right) Q \\
+ \left( \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta} \right) R + J_\sigma = 0
\]  
(A.6)

\[
\frac{\partial T}{\partial \tau} + \xi_t \frac{\partial T}{\partial \xi} + \eta_t \frac{\partial T}{\partial \eta} + \zeta_t \frac{\partial T}{\partial \zeta} + \xi_x \frac{\partial P}{\partial \xi} + \eta_x \frac{\partial P}{\partial \eta} + \zeta_x \frac{\partial P}{\partial \zeta} + \xi_y \frac{\partial Q}{\partial \xi} + \eta_y \frac{\partial Q}{\partial \eta} + \zeta_y \frac{\partial Q}{\partial \zeta} + \xi_z \frac{\partial R}{\partial \xi} \\
+ \eta_z \frac{\partial R}{\partial \eta} + \zeta_z \frac{\partial R}{\partial \zeta} + J_\sigma = 0
\]

(A.7)

To obtain the conservative form of equation (A.7), divide the equation by the Jacobian of transformation, $J$, as shown in equation (A.8) and subsequently, add the terms to the equation such that the added terms sums up to zero and the net resultant remain unchanged. This manipulation is shown here for the first four terms and the conclusion is extended to the rest of the terms.

\[
\frac{1}{J} \frac{\partial T}{\partial \tau} + \frac{\xi_t}{J} \frac{\partial T}{\partial \xi} + \frac{\eta_t}{J} \frac{\partial T}{\partial \eta} + \frac{\zeta_t}{J} \frac{\partial T}{\partial \zeta} + \left[ T \frac{\partial}{\partial \tau} \left( \frac{1}{J} \right) - T \frac{\partial}{\partial \xi} \left( \frac{\xi_t}{J} \right) \right] + \left[ T \frac{\partial}{\partial \eta} \left( \frac{\eta_t}{J} \right) - T \frac{\partial}{\partial \eta} \left( \frac{\zeta_t}{J} \right) \right] \\
+ \left[ T \frac{\partial}{\partial \eta} \left( \frac{\eta_t}{J} \right) - T \frac{\partial}{\partial \eta} \left( \frac{\zeta_t}{J} \right) \right] + \left[ T \frac{\partial}{\partial \eta} \left( \frac{\eta_t}{J} \right) - T \frac{\partial}{\partial \eta} \left( \frac{\zeta_t}{J} \right) \right]
\]  
(A.8)

Rearrange the terms in the following manner

\[
\left[ \frac{1}{J} \frac{\partial T}{\partial \tau} + T \frac{\partial}{\partial \tau} \left( \frac{1}{J} \right) \right] + \left[ \xi_t \frac{\partial T}{\partial \xi} + T \frac{\partial}{\partial \xi} \left( \frac{\xi_t}{J} \right) \right] + \left[ \eta_t \frac{\partial T}{\partial \eta} + T \frac{\partial}{\partial \eta} \left( \frac{\eta_t}{J} \right) \right] + \left[ \zeta_t \frac{\partial T}{\partial \zeta} + T \frac{\partial}{\partial \zeta} \left( \frac{\zeta_t}{J} \right) \right] \\
- \left[ T \frac{\partial}{\partial \tau} \left( \frac{1}{J} \right) + T \frac{\partial}{\partial \xi} \left( \frac{\xi_t}{J} \right) + T \frac{\partial}{\partial \eta} \left( \frac{\eta_t}{J} \right) + T \frac{\partial}{\partial \zeta} \left( \frac{\zeta_t}{J} \right) \right]
\]  
(A.9)
Using the relations given in Ref. [123], the terms in the last parenthesis can be shown equal to zero. Using the calculus fundamentals, the terms in the first four parenthesis can be written in the form as shown

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{f} \right) + \frac{\partial}{\partial \xi} \left( \xi_t \frac{T}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_t \frac{T}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_t \frac{T}{f} \right)
\]

(A.10)

In a similar manner, the remaining derivatives in equation (A.7) can be derived, which results in the complete equation.

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{f} \right) + \frac{\partial}{\partial \xi} \left( \xi_t \frac{T}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_t \frac{T}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_t \frac{T}{f} \right) + \frac{\partial}{\partial \xi} \left( \xi_x \frac{P}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_x \frac{P}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_x \frac{P}{f} \right) + \frac{\partial}{\partial \xi} \left( \xi_y \frac{Q}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_y \frac{Q}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_y \frac{Q}{f} \right) + \frac{\partial}{\partial \xi} \left( \xi_z \frac{R}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_z \frac{R}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_z \frac{R}{f} \right) + J_\sigma \frac{1}{f} = 0
\]

(A.11)

Rearrange equation (A.11) to group the terms with respect to their derivatives

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{f} \right) + \left[ \frac{\partial}{\partial \xi} \left( \xi_t \frac{T}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_t \frac{T}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_t \frac{T}{f} \right) \right] + \left[ \frac{\partial}{\partial \xi} \left( \xi_x \frac{P}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_x \frac{P}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_x \frac{P}{f} \right) \right] + \left[ \frac{\partial}{\partial \xi} \left( \xi_y \frac{Q}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_y \frac{Q}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_y \frac{Q}{f} \right) \right] + \left[ \frac{\partial}{\partial \xi} \left( \xi_z \frac{R}{f} \right) + \frac{\partial}{\partial \eta} \left( \eta_z \frac{R}{f} \right) + \frac{\partial}{\partial \zeta} \left( \zeta_z \frac{R}{f} \right) \right] + J_\sigma \frac{1}{f} = 0
\]

(A.12)

Subsequently, the terms in equation (A.12) can be expressed as

\[
\frac{\partial \overline{T}}{\partial \tau} + \overline{X} \frac{\partial \overline{P}}{\partial \xi} + \overline{Y} \frac{\partial \overline{Q}}{\partial \eta} + \overline{Z} \frac{\partial \overline{R}}{\partial \zeta} + J_\sigma = 0
\]

(A.13)
Where, $\bar{T}$, $\bar{P}$, $\bar{Q}$ and $\bar{R}$ are the flux vectors in the transformed coordinates and are defined as

$$\bar{T} = \frac{T}{J}$$  \hspace{1cm} (A.14)

$$\bar{P} = \frac{1}{J} (\xi T + \xi_P + \xi_Q + \xi_R)$$  \hspace{1cm} (A.15)

$$\bar{Q} = \frac{1}{J} (\eta T + \eta_P + \eta_Q + \eta_R)$$  \hspace{1cm} (A.16)

$$\bar{R} = \frac{1}{J} (\zeta T + \zeta_P + \zeta_Q + \zeta_R)$$  \hspace{1cm} (A.17)

$$\bar{J}_\sigma = \frac{J_\sigma}{J}$$  \hspace{1cm} (A.18)
APPENDIX B

TRANSFORMATION OF EQUATIONS FROM PHYSICAL DOMAIN TO COMPUTATIONAL DOMAIN IN TWO DIMENSIONS

The reduction of the three dimensional form of the model equation in the transformed coordinate system is straightforward. A similar procedure described in Appendix A is followed to derive the equation in the desired form and presented here to avoid ambiguities. Chain rule of the partial differential equations that relates \((x, y)\) coordinates to \((\xi, \eta)\) coordinates in two dimensional axis is given by equations (B.1) through (B.3).

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} \tag{B.1}
\]

\[
\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} \tag{B.2}
\]

\[
\frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} \tag{B.3}
\]

The conservative form of the non-dimensionalized Maxwell’s equations as derived previously is

\[
\frac{\partial T}{\partial \tau} + X \frac{\partial P}{\partial x} + Y \frac{\partial Q}{\partial y} + J_\sigma = 0 \tag{B.4}
\]

Using the relations given in equations (B.1) - (B.3) and flux vector equation (B.4), the expression in equation (B.5) is obtained where coefficient terms \(X\), and \(Y\) are omitted.

\[
\frac{\partial T}{\partial \tau} + \xi_t \frac{\partial T}{\partial \xi} + \eta_t \frac{\partial T}{\partial \eta} + \xi_x \frac{\partial P}{\partial \xi} + \eta_x \frac{\partial P}{\partial \eta} + \xi_y \frac{\partial Q}{\partial \xi} + \eta_y \frac{\partial Q}{\partial \eta} + J_\sigma = 0 \tag{B.5}
\]
The conservative form of equation (B.5) is obtained by dividing it with the Jacobian of transformation, \( J \), and subsequently, using a similar manipulation as described in Appendix A. The first three terms are

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{J} \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi T}{J} \right) + \frac{\partial}{\partial \eta} \left( \eta T \right) \quad \text{(B.6)}
\]

The remaining derivatives in equation (B.4) are subjected to the similar procedure and the complete equation is described as

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{J} \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi T}{J} \right) + \frac{\partial}{\partial \eta} \left( \eta T \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi P}{J} \right) + \frac{\partial}{\partial \eta} \left( \eta P \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi Q}{J} \right) + \frac{\partial}{\partial \eta} \left( \eta Q \right) + \frac{J_\sigma}{J} = 0 \quad \text{(B.7)}
\]

Rearrange equation (B.7) to group the terms with respect to their derivatives

\[
\frac{\partial}{\partial \tau} \left( \frac{T}{J} \right) + \left[ \frac{\partial}{\partial \xi} \left( \frac{\xi T}{J} \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi P}{J} \right) + \frac{\partial}{\partial \xi} \left( \frac{\xi Q}{J} \right) \right] + \left[ \frac{\partial}{\partial \eta} \left( \eta T \right) + \frac{\partial}{\partial \eta} \left( \eta P \right) + \frac{\partial}{\partial \eta} \left( \eta Q \right) \right] + \frac{J_\sigma}{J} = 0 \quad \text{(B.8)}
\]

Subsequently, the terms in equation (B.8) are expressed as

\[
\frac{\partial T}{\partial \tau} + \bar{X} \frac{\partial P}{\partial \xi} + \bar{Y} \frac{\partial Q}{\partial \eta} + J_\sigma = 0 \quad \text{(B.9)}
\]

Where, \( \bar{T}, \bar{P}, \) and \( \bar{Q} \) are the flux vectors in the transformed coordinates and are defined as

\[
\bar{T} = \frac{T}{J} \quad \text{(B.10)}
\]

\[
\bar{P} = \frac{1}{J} \left( \xi_t T + \xi_x P + \xi_y Q + \xi_z R \right) \quad \text{(B.11)}
\]

\[
\bar{Q} = \frac{1}{J} \left( \eta_t T + \eta_x P + \eta_y Q + \eta_z R \right) \quad \text{(B.12)}
\]

\[
\bar{J}_\sigma = \frac{J_\sigma}{J} \quad \text{(B.13)}
\]
APPENDIX C

EIGEN EQUATIONS IN THREE DIMENSIONS

To obtain the eigenvalues and eigenvectors from the model equation in three dimension, a linearization procedure is required in the first step to represent the model equation in terms of flux vector $\bar{T}$. Next, the flux Jacobian matrices are derived. The eigenvalues and eigenvectors of the flux Jacobian matrices can be determined, subsequently, using any online mathematical calculator.

FLUX JACOBIAN MATRICES

Using a linearization procedure, the model equation is expressed in terms of flux vector $\bar{T}$.

$$\frac{\partial \bar{T}}{\partial \tau} + X \frac{\partial \bar{T}}{\partial \xi} + Y \frac{\partial \bar{T}}{\partial \eta} + Z \frac{\partial \bar{T}}{\partial \zeta} + \bar{J}_\sigma = 0$$ (C.1)

$$\frac{\partial \bar{T}}{\partial \tau} + \bar{A} \frac{\partial \bar{T}}{\partial \xi} + \bar{B} \frac{\partial \bar{T}}{\partial \eta} + \bar{C} \frac{\partial \bar{T}}{\partial \zeta} + \bar{J}_\sigma = 0$$ (C.2)

The following expression are derived using the procedure presented in [123].

$$\bar{P}^{n+1} = \bar{P}^n + \frac{\partial \bar{P}}{\partial \bar{T}} \Delta \bar{T} + O(\Delta \tau)^2$$ (C.3)

$$\bar{Q}^{n+1} = \bar{Q}^n + \frac{\partial \bar{Q}}{\partial \bar{T}} \Delta \bar{T} + O(\Delta \tau)^2$$ (C.4)

$$\bar{R}^{n+1} = \bar{R}^n + \frac{\partial \bar{R}}{\partial \bar{T}} \Delta \bar{T} + O(\Delta \tau)^2$$ (C.3)
In equations (C.3) – (C.5), the terms $\partial P/\partial T$, $\partial Q/\partial T$ and $\partial R/\partial T$ are defined as the Jacobian matrices and are given as

$$A = \frac{\partial P}{\partial T}$$

$$B = \frac{\partial Q}{\partial T}$$

$$C = \frac{\partial R}{\partial T}$$

(C.5)

The flux Jacobian matrix $\partial \vec{P}/\partial \vec{T}$ is obtained from

$$\frac{\partial \vec{P}}{\partial \vec{T}} = \frac{\partial (P_1, P_2, P_3, P_4, P_5, P_6)}{\partial (T_1, T_2, T_3, T_4, T_5, T_6)}$$

(C.6)

In the matrix form equation (C.6) is written as

$$\frac{\partial \vec{P}}{\partial \vec{T}} = \begin{bmatrix}
\frac{\partial P_1}{\partial T_1} & \frac{\partial P_1}{\partial T_2} & \frac{\partial P_1}{\partial T_3} & \frac{\partial P_1}{\partial T_4} & \frac{\partial P_1}{\partial T_5} & \frac{\partial P_1}{\partial T_6} \\
\frac{\partial P_2}{\partial T_1} & \frac{\partial P_2}{\partial T_2} & \frac{\partial P_2}{\partial T_3} & \frac{\partial P_2}{\partial T_4} & \frac{\partial P_2}{\partial T_5} & \frac{\partial P_2}{\partial T_6} \\
\frac{\partial P_3}{\partial T_1} & \frac{\partial P_3}{\partial T_2} & \frac{\partial P_3}{\partial T_3} & \frac{\partial P_3}{\partial T_4} & \frac{\partial P_3}{\partial T_5} & \frac{\partial P_3}{\partial T_6} \\
\frac{\partial P_4}{\partial T_1} & \frac{\partial P_4}{\partial T_2} & \frac{\partial P_4}{\partial T_3} & \frac{\partial P_4}{\partial T_4} & \frac{\partial P_4}{\partial T_5} & \frac{\partial P_4}{\partial T_6} \\
\frac{\partial P_5}{\partial T_1} & \frac{\partial P_5}{\partial T_2} & \frac{\partial P_5}{\partial T_3} & \frac{\partial P_5}{\partial T_4} & \frac{\partial P_5}{\partial T_5} & \frac{\partial P_5}{\partial T_6} \\
\frac{\partial P_6}{\partial T_1} & \frac{\partial P_6}{\partial T_2} & \frac{\partial P_6}{\partial T_3} & \frac{\partial P_6}{\partial T_4} & \frac{\partial P_6}{\partial T_5} & \frac{\partial P_6}{\partial T_6}
\end{bmatrix}$$

(C.7)
To obtain the elements of the matrix in equation (C.7), the flux vectors \( P, Q, \) and \( R \) are expressed in terms of the components of vector \( T \) as shown

\[
T = \begin{bmatrix} E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix}
\]

\[
P = \begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \end{bmatrix} = \begin{bmatrix} 0 \\ H_z \\ -H_y \\ 0 \\ -E_z \\ E_y \end{bmatrix} = \begin{bmatrix} 0 \\ T_6 \\ -T_5 \\ 0 \\ -T_3 \\ T_2 \end{bmatrix}
\]

\[
Q = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \\ Q_6 \end{bmatrix} = \begin{bmatrix} -H_z \\ 0 \\ H_x \\ E_z \\ 0 \\ -E_x \end{bmatrix} = \begin{bmatrix} -T_6 \\ 0 \\ T_4 \\ T_3 \\ 0 \\ -T_1 \end{bmatrix}
\]

\[
R = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \\ R_6 \end{bmatrix} = \begin{bmatrix} H_y \\ -H_x \\ 0 \\ -H_y \\ H_x \\ 0 \end{bmatrix} = \begin{bmatrix} T_5 \\ -T_4 \\ 0 \\ -T_2 \\ T_1 \\ 0 \end{bmatrix}
\]
From equations (A.14) and (A.15)

\[ T_1 = \frac{T_1}{f} \quad (C.9) \]

\[ P_1 = \frac{1}{f} [\xi_t T_1 + \xi_x P_1 + \xi_y Q_1 + \xi_z R_1] \quad (C.10) \]

Substitute the values from equations (C.9) and (C.10) in the first element of Jacobian matrix \( A \) as shown

\[ \frac{\partial P_1}{\partial T_1} = \frac{\partial}{\partial T_1} \left\{ \frac{1}{f} [\xi_t T_1 + \xi_x P_1 + \xi_y Q_1 + \xi_z R_1] \right\} \quad (C.11) \]

Using the values of \( P_1, Q_1, \) and \( R_1 \) from vectors in equation (C.8), following expression is obtained

\[ \frac{\partial P_1}{\partial T_1} = \frac{\partial}{\partial T_1} \left\{ \frac{1}{f} [\xi_t T_1 - \xi_y T_6 + \xi_z T_5] \right\} = \frac{\partial [\xi_t T_1 - \xi_y T_6 + \xi_z T_5]}{\partial T_1} \quad (C.12) \]

The resulting equation obtained after differentiation of equation (C.12) is

\[ \frac{\partial P_1}{\partial T_1} = \xi_t \quad (C.13) \]

Similarly, equations for finding elements of first row of matrix in (C.7) are given below

\[ \frac{\partial P_1}{\partial T_2} = \frac{\partial}{\partial T_2} \left\{ \frac{1}{f} [\xi_t T_1 - \xi_y T_6 + \xi_z T_5] \right\} = \frac{\partial [\xi_t T_1 - \xi_y T_6 + \xi_z T_5]}{\partial T_2} \quad (C.14) \]

\[ \frac{\partial P_1}{\partial T_2} = 0 \quad (C.15) \]
\[
\frac{\partial P_1}{\partial T_3} = \frac{\partial \left\{ \frac{1}{J} [\xi_1 T_1 - \xi_y T_6 + \xi_z T_5] \right\}}{\partial \left( \frac{T_3}{J} \right)} = \frac{\partial \left[ \xi_1 T_1 - \xi_y T_6 + \xi_z T_5 \right]}{\partial T_3} \tag{C.16} \\
\frac{\partial P_1}{\partial T_4} = 0 \tag{C.17} \\
\frac{\partial P_1}{\partial T_5} = \frac{\partial \left\{ \frac{1}{J} [\xi_1 T_1 - \xi_y T_6 + \xi_z T_5] \right\}}{\partial \left( \frac{T_5}{J} \right)} = \frac{\partial \left[ \xi_1 T_1 - \xi_y T_6 + \xi_z T_5 \right]}{\partial T_5} \tag{C.18} \\
\frac{\partial P_1}{\partial T_6} = 0 \tag{C.19} \\
\frac{\partial P_1}{\partial T_5} = \xi_z \tag{C.20} \\
\frac{\partial P_1}{\partial T_6} = \frac{\partial \left\{ \frac{1}{J} [\xi_1 T_1 - \xi_y T_6 + \xi_z T_5] \right\}}{\partial \left( \frac{T_6}{J} \right)} = \frac{\partial \left[ \xi_1 T_1 - \xi_y T_6 + \xi_z T_5 \right]}{\partial T_6} \tag{C.21} \\
\frac{\partial P_1}{\partial T_6} = -\xi_y \tag{C.22} \\
\frac{\partial P_1}{\partial T_6} = -\xi_y \tag{C.23} 
\]
In a similar manner, the other elements of the Jacobian matrix $A$, and subsequently, of matrices $B$, and $C$ can be determined. For a time-independent grid system, $\xi_t = 0$.

\[
A = \frac{\partial \bar{P}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \xi_z & -\xi_y \\
0 & 0 & 0 & -\xi_z & 0 & \xi_x \\
0 & 0 & 0 & \xi_y & -\xi_x & 0 \\
-\xi_z & \xi_y & 0 & 0 & 0 \\
\xi_z & 0 & -\xi_x & 0 & 0 & 0 \\
-\xi_y & \xi_x & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
B = \frac{\partial \bar{Q}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \eta_z & -\eta_y \\
0 & 0 & 0 & -\eta_z & 0 & \eta_x \\
0 & 0 & 0 & \eta_y & -\eta_x & 0 \\
-\eta_z & \eta_y & 0 & 0 & 0 \\
\eta_z & 0 & -\eta_x & 0 & 0 & 0 \\
-\eta_y & \eta_x & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
C = \frac{\partial \bar{R}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \zeta_z & -\zeta_y \\
0 & 0 & 0 & -\zeta_z & 0 & \zeta_x \\
0 & 0 & 0 & \zeta_y & -\zeta_x & 0 \\
-\zeta_z & \zeta_y & 0 & 0 & 0 \\
\zeta_z & 0 & -\zeta_x & 0 & 0 & 0 \\
-\zeta_y & \zeta_x & 0 & 0 & 0 & 0
\end{bmatrix}
\]

(C.24)
Obtain \( \bar{A} = \bar{X}A, \bar{Y} = \bar{Y}B \) and \( \bar{C} = \bar{Z}C \) using the material coefficient matrices defined in equation (4.54).

\[
\bar{A} = \frac{\partial \bar{P}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \frac{\xi_z}{\varepsilon} & -\frac{\xi_y}{\varepsilon} \\
0 & 0 & 0 & -\frac{\xi_z}{\varepsilon} & 0 & \frac{\xi_x}{\varepsilon} \\
0 & 0 & 0 & \frac{\xi_y}{\varepsilon} & -\frac{\xi_x}{\varepsilon} & 0 \\
0 & -\frac{\xi_z}{\mu} & \frac{\xi_y}{\mu} & 0 & 0 & 0 \\
\frac{\xi_z}{\mu} & 0 & -\frac{\xi_x}{\mu} & 0 & 0 & 0 \\
-\frac{\xi_y}{\mu} & \frac{\xi_x}{\mu} & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\bar{B} = \frac{\partial \bar{Q}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \frac{\eta_z}{\varepsilon} & -\frac{\eta_y}{\varepsilon} \\
0 & 0 & 0 & -\frac{\eta_z}{\varepsilon} & 0 & \frac{\eta_x}{\varepsilon} \\
0 & 0 & 0 & \frac{\eta_y}{\varepsilon} & -\frac{\eta_x}{\varepsilon} & 0 \\
0 & -\frac{\eta_z}{\mu} & \frac{\eta_y}{\mu} & 0 & 0 & 0 \\
\frac{\eta_z}{\mu} & 0 & -\frac{\eta_x}{\mu} & 0 & 0 & 0 \\
-\frac{\eta_y}{\mu} & \frac{\eta_x}{\mu} & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\bar{C} = \frac{\partial \bar{R}}{\partial \bar{T}} = \begin{bmatrix}
0 & 0 & 0 & 0 & \frac{\zeta_z}{\varepsilon} & -\frac{\zeta_y}{\varepsilon} \\
0 & 0 & 0 & -\frac{\zeta_z}{\varepsilon} & 0 & \frac{\zeta_x}{\varepsilon} \\
0 & 0 & 0 & \frac{\zeta_y}{\varepsilon} & -\frac{\zeta_x}{\varepsilon} & 0 \\
0 & -\frac{\zeta_z}{\mu} & \frac{\zeta_y}{\mu} & 0 & 0 & 0 \\
\frac{\zeta_z}{\mu} & 0 & -\frac{\zeta_x}{\mu} & 0 & 0 & 0 \\
-\frac{\zeta_y}{\mu} & \frac{\zeta_x}{\mu} & 0 & 0 & 0 & 0
\end{bmatrix}
\]
APPENDIX D

EIGEN EQUATIONS IN TWO DIMENSIONS

A similar procedure, presented in Appendix C, is used to derive the flux Jacobian matrices for a two dimensional model equation. The corresponding eigenvalues and eigenvectors are calculated using an online mathematical calculator.

FLUX JACOBIAN MATRICES

Using a linearization procedure, the model equation is expressed in terms of flux vector $\vec{T}$.

$$\frac{\partial \vec{T}}{\partial \tau} + \vec{X} \frac{\partial \vec{T}}{\partial \xi} + \vec{Y} \frac{\partial \vec{T}}{\partial \eta} + \vec{J}_\sigma = 0 \quad (D.1)$$

$$\frac{\partial \vec{T}}{\partial \tau} + \vec{A} \frac{\partial \vec{T}}{\partial \xi} + \vec{B} \frac{\partial \vec{T}}{\partial \eta} + \vec{J}_\sigma = 0 \quad (D.2)$$

The following expression are derived using the procedure presented in [123].

$$\vec{P}^{n+1} = \vec{P}^n + \frac{\partial \vec{P}}{\partial \vec{T}} \Delta \vec{T} + O(\Delta \tau)^2 \quad (D.3)$$

$$\vec{Q}^{n+1} = \vec{Q}^n + \frac{\partial \vec{Q}}{\partial \vec{T}} \Delta \vec{T} + O(\Delta \tau)^2 \quad (D.4)$$

In equations (D.3) – (D.4), the terms $\partial \vec{P} / \partial \vec{T}$, $\partial \vec{Q} / \partial \vec{T}$ and $\partial \vec{R} / \partial \vec{T}$ are defined as the Jacobian matrices and are given as

$$A = \frac{\partial \vec{P}}{\partial \vec{T}} \quad (D.5)$$

$$B = \frac{\partial \vec{Q}}{\partial \vec{T}}$$
The flux Jacobian matrix $\frac{\partial P}{\partial T}$ is obtained from

$$
\frac{\partial P}{\partial T} = \frac{\partial (\bar{P}_1, \bar{P}_2, \bar{P}_3)}{\partial (\bar{T}_1, \bar{T}_2, \bar{T}_3)}
$$

(D.6)

In the matrix form equation (C.5) is written as

$$
\begin{bmatrix}
\frac{\partial \bar{P}_1}{\partial \bar{T}_1} & \frac{\partial \bar{P}_1}{\partial \bar{T}_2} & \frac{\partial \bar{P}_1}{\partial \bar{T}_3} \\
\frac{\partial \bar{P}_2}{\partial \bar{T}_1} & \frac{\partial \bar{P}_2}{\partial \bar{T}_2} & \frac{\partial \bar{P}_2}{\partial \bar{T}_3} \\
\frac{\partial \bar{P}_3}{\partial \bar{T}_1} & \frac{\partial \bar{P}_3}{\partial \bar{T}_2} & \frac{\partial \bar{P}_3}{\partial \bar{T}_3}
\end{bmatrix}
$$

(D.7)

To obtain the elements of the matrix in equation (D.6), the flux vectors $P$, and $Q$, are expressed in terms of the components of vector $T$ as shown

$$
T = \begin{bmatrix}
E_z \\
H_x \\
H_y
\end{bmatrix} = \begin{bmatrix}
\bar{T}_1 \\
\bar{T}_2 \\
\bar{T}_3
\end{bmatrix}
$$

$$
P = \begin{bmatrix}
P_1 \\
P_2 \\
P_3
\end{bmatrix} = \begin{bmatrix}
-H_y \\
0 \\
E_z
\end{bmatrix} = \begin{bmatrix}
-T_3 \\
0 \\
T_1
\end{bmatrix}
$$

(D.8)

$$
Q = \begin{bmatrix}
Q_1 \\
Q_2 \\
Q_3
\end{bmatrix} = \begin{bmatrix}
H_x \\
E_z \\
0
\end{bmatrix} = \begin{bmatrix}
\bar{T}_2 \\
\bar{T}_1 \\
0
\end{bmatrix}
$$
From equations (B.10) and (B.11)

\[ T_1 = \frac{T_1}{J} \]  \quad (D.9)

\[ P_1 = \frac{1}{J} [\xi_t T_1 + \xi_x P_1 + \xi_y Q_1] \]  \quad (D.10)

Substitute the values from equations (D.9) and (D.10) in the first element of Jacobian matrix \( A \) as shown

\[ \frac{\partial P_1}{\partial T_1} = \frac{\partial \left( \frac{1}{J} [\xi_t T_1 + \xi_x P_1 + \xi_y Q_1] \right)}{\partial \left( \frac{T_1}{J} \right)} \]  \quad (D.11)

Using the values of \( P_1 \) and \( Q_1 \) from vectors in equation (D.8), following expression is obtained

\[ \frac{\partial P_1}{\partial T_1} = \frac{\partial \left( \frac{1}{J} [\xi_t T_1 - \xi_x T_3 + \xi_y T_2] \right)}{\partial \left( \frac{T_1}{J} \right)} = \frac{\partial \left[ \xi_t T_1 - \xi_x T_3 + \xi_y T_2 \right]}{\partial T_1} \]  \quad (D.12)

The resulting equation obtained after differentiation of equation (D.12) is

\[ \frac{\partial P_1}{\partial T_1} = \xi_t \]  \quad (D.13)

Similarly, equations for finding elements of first row of matrix in (D.7) are given below

\[ \frac{\partial P_1}{\partial T_2} = \frac{\partial \left( \frac{1}{J} [\xi_t T_1 - \xi_x T_3 + \xi_y T_2] \right)}{\partial \left( \frac{T_2}{J} \right)} = \frac{\partial \left[ \xi_t T_1 - \xi_x T_3 + \xi_y T_2 \right]}{\partial T_2} \]  \quad (D.14)

\[ \frac{\partial P_1}{\partial T_2} = \xi_y \]  \quad (D.15)
\[
\frac{\partial \vec{P}_1}{\partial T_3} = \frac{\partial \left\{ \frac{1}{J} \left[ \xi_t T_1 - \xi_x T_3 + \xi_y T_2 \right] \right\}}{\partial \left\{ \frac{T_3}{J} \right\}} = \frac{\partial \left[ \xi_t T_1 - \xi_x T_3 + \xi_y T_2 \right]}{\partial T_3}
\]

(D.16)

\[
\frac{\partial \vec{P}_1}{\partial T_2} = -\xi_x
\]

(D.17)

In a similar manner, the other elements of the Jacobian matrix \( A \), and subsequently, of matrix \( B \), can be determined. For a time-independent grid system, \( \xi_t = 0 \).

\[
A = \frac{\partial \vec{P}}{\partial \vec{T}} = \begin{bmatrix}
0 & \xi_y & -\xi_x \\
\xi_y & 0 & 0 \\
-\xi_x & 0 & 0
\end{bmatrix}
\]

(D.18)

\[
B = \frac{\partial \vec{Q}}{\partial \vec{T}} = \begin{bmatrix}
0 & \eta_y & -\eta_x \\
\eta_y & 0 & 0 \\
-\eta_x & 0 & 0
\end{bmatrix}
\]

(D.19)

Obtain \( \vec{A} = \vec{X} \vec{A} \), and \( \vec{Y} = \vec{Y} \vec{B} \) using the material coefficient matrices defined in equation (4.29).