An Abstract of the Thesis of

Neven Orhanovic for the degree of Doctor of Philosophy in Electrical and Computer Engineering presented on October 1, 1993

Title: Time Domain Simulation of Maxwell's Equations by the Method of Characteristics

Abstract approved: ____________________________

Vijai K. Tripathi

A numerical method based on the method of characteristics for hyperbolic systems of partial differential equations in four independent variables is developed and used for solving time domain Maxwell's equations. The method uses the characteristic hypersurfaces and the characteristic conditions to derive a set of independent equations relating the electric and magnetic field components on these hypersurfaces. A discretization scheme is developed to solve for the unknown field components at each time step. The method retains many of the good features of the original method of characteristics for hyperbolic systems in two independent variables, such as optimal time step, good behavior near data discontinuities and the ability to treat general boundary conditions. The method is exemplified by calculating the time domain response of a few typical planar interconnect structures to Gaussian and unit step excitations. Although the general emphasis is on interconnect problems, the method is applicable to a number of other transient electromagnetic field problems governed by Maxwell's equations. In addition to the method of characteristics a finite difference scheme, known in mathematic circles as the modified Richtmyer scheme, is applied
to the time domain solution of Maxwell's equations. Both methods should be useful for efficient full wave analysis of three dimensional electromagnetic field problems.
Time Domain Simulation of Maxwell's Equations
by the Method of Characteristics

by

Neven Orhanović

A THESIS
submitted to
Oregon State University

in partial fulfillment of
the requirements for the
degree of

Doctor of Philosophy

Completed October 1, 1993
Commencement June 1994
Table of Contents

1 Introduction .......................................................... 1
   1.1 Interconnects .................................................. 1
   1.2 Interconnect Analysis Methods ................................. 2
      1.2.1 Analysis methods for planar microwave structures ....... 6
      1.2.2 Finite Difference and Finite Element Methods ........... 9
   1.3 Numerical Methods for Electromagnetic Problems .......... 10
   1.4 Finite Difference Methods for Time-Domain Maxwell's Equations .... 11
      1.4.1 Boundary Conditions .................................... 12
      1.4.2 Stability criteria; Courant-Friedricks-Lewy Condition .... 13
   1.5 Method of Characteristics .................................... 14

2 Relevant Partial Differential Equation Theory .................. 17
   2.1 Introductory Remarks on Partial Differential Equations ....... 17
   2.2 First Order Partial Differential Equations in Two Independent Variables 18
      2.2.1 Geometrical Interpretation of First Order PDEs; Monge cones 18
      2.2.2 Characteristic and Focal Curves .......................... 19
   2.3 Theory of Linear and Quasi-Linear Partial Differential Equations of First Order 23
2.3.1 Characteristic Curves .............................................. 23
2.3.2 Initial Value Problem ............................................... 25
2.3.3 Remarks on Differentiation in $n$ Dimensions .................. 27
2.3.4 Characteristic Manifold ............................................. 30
2.4 Partial Differential Equations of Higher Order .................... 31
2.4.1 Systems of Partial Differential Equations ....................... 31
2.4.2 Systems of First Order with Two Independent Variables; Character- 
istics ................................................................. 32
2.4.3 Systems of First Order with $n$ Independent Variables ........ 34
2.5 Properties of Characteristic Curves .................................. 36

3 Application of the Method of Characteristics to Maxwell's Equa-
3.1 Problem formulation .................................................. 37
3.2 Method of Characteristics in Three Space Dimensions ............. 42
3.3 Numerical Solution ..................................................... 47
3.4 Boundary Conditions ................................................... 56
3.5 Richtmyer's Modified Finite Difference Scheme .................... 61

4 Application of the Method to Interconnect Problems .................. 63

5 Conclusion ................................................................. 86

Bibliography ............................................................... 88
List of Figures

1.1 Examples of planar transmission line structures. ....................... 3
1.2 Examples of microstrip discontinuities. ............................... 5

3.1 Characteristic hypersurface for two space dimensions. ............... 48
3.2 Grid nodes and notation on the hypersurface for two space dimensions. 52
3.3 Basic cell for field calculations in three dimensions. ................. 54
3.4 Field calculation at boundary between two different regions. ....... 55
3.5 Field calculation for structure boundary points. ...................... 57

4.1 Microstrip line structure of Example 1. .................................. 64
4.2 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics. 65
4.3 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics. 66
4.4 Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme. . . . 66
4.5 Distribution of $E_z$ at $t = t_2$ obtained by the Richtmyer scheme. . . . 67
4.6 Time variation of $E_z$. ....................................................... 67
4.7 90° microstrip bend structure of Example 2. .......................... 68
4.8 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics. 69
4.9 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics. 70
4.10 Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics. 70
4.11 Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme. . . . . 71
4.12 Distribution of $E_z$ at $t = t_2$ obtained by the modified Richtmyer scheme. 71
4.13 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics. 72
4.14 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics. 73
4.15 Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics. 73
4.16 Time variation of $E_z$. . . . . . . . . . . . . . . . . . . . . . . . . . . . 74
4.17 Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme. . . . 74
4.18 Distribution of $E_z$ plane at $t = t_2$ obtained by the Richtmyer scheme. 75
4.19 Microstrip step discontinuity of Example 3. . . . . . . . . . . . . . . . 75
4.20 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics. 76
4.21 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics. 77
4.22 Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics. 77
4.23 Time variation of $E_z$. . . . . . . . . . . . . . . . . . . . . . . . . . . . 78
4.24 Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme. . . . 78
4.25 Distribution of $E_z$ at $t = t_2$ obtained by the Richtmyer scheme. . . . 79
4.26 Microstrip T-junction of Example 4. . . . . . . . . . . . . . . . . . . . 80
4.27 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics. 81
4.28 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics. 81
4.29 Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics. 82
4.30 Time variation of $E_z$. . . . . . . . . . . . . . . . . . . . . . . . . . . . 82
4.31 Microstrip cross-over of Example 5. . . . . . . . . . . . . . . . . . . . 83
4.32 Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics.

4.33 Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.

4.34 Time variation of $E_z$. 

---

---
Time Domain Simulation of Maxwell's Equations by the Method of Characteristics

Chapter 1

Introduction

1.1 Interconnects

As the signal frequencies in today's electrical circuits increase the conductors connecting the circuit terminals no longer behave as ideal electrical connections (short circuits) but rather themselves become electrical circuits. These connecting conductors, also called interconnects or interconnections, significantly affect the propagating electrical signals and can have serious impact on the behavior of the whole circuit. These interconnects can typically be found in a large number of electronic products, such as printed circuit boards (PCBs), multichip modules (MCMs), integrated circuits (ICs) and packages.

The present trend toward increased packaging density in digital circuits and the implementation of high speed devices have led to increasing demands for the characterization of interconnects. The planar geometry used in electronic technology usually allows for the interconnects to be modeled as planar multiconductor transmission lines. Parallel conductors suspended or embedded in dielectric media have found numerous applications in microwave and digital networks (Fig. 1.1). Transmission line effects on these interconnecting conductors start to appear in situations where the rise or fall times of the digital signals become comparable to the propagation time along the conductors. Signals propagating on these lines suffer distortion which may degrade the performance of the connected circuits. Line coupling and mismatched
terminations at the source and load end produce crosstalk and reflections which can result in false switching of digital systems. Together with timing delay problems, crosstalk and reflections are major concerns to circuit designers.

Interconnects are also becoming increasingly important in the design of integrated circuits and multichip modules. As clock speeds increase and the signal rise times decrease, while simultaneously the complexities and input/output counts of Silicon and GaAs chips increase, the numbers of interconnects between chips increases. At the same time the interchip spacing must decrease because of the speed-of-light propagation constraints as well as a few additional considerations. As a result, increasing numbers of interconnects, each carrying very fast signal waveforms, must be packed onto very small hybrid or chip-on-board substrates. This trend is already creating problems for the designers of chip packages, substrates, and circuit boards in which the considerations of electromagnetic compatibility and interference are becoming of paramount importance. The understanding, or lack thereof, of electromagnetic crosstalk between signals, skin effect problems, ringing, reflections on the signal lines, and the delivery of clean signals to the chips makes the difference between fully functional and totally unreliable digital signal and data processors.

In the future, a digital designer will need to model and simulate the complete electromagnetic behavior of high frequency, high density, chips, printed circuit boards and substrates, so that the designs at all levels will be verifiable before they are fabricated; experience has demonstrated that electromagnetic performance deficiencies or defects are difficult, if not impossible, to correct after fabrication.

1.2 Interconnect Analysis Methods

A rigorous interconnect analysis is a complicated task, especially if the response is to be evaluated at high frequencies (in the gigahertz region). Interconnects are typically embedded in an inhomogeneous medium (Fig. 1.1) or have considerable conductor losses. This means that the waves propagating on the interconnect are not of
Figure 1.1: Examples of planar transmission line structures.
the transverse electromagnetic (TEM) nature. At high frequencies, where the cross sectional dimensions of the interconnect structure becomes comparable to the wavelengths in the signal spectrum, higher order modes (non-TEM) can propagate. The analysis is further complicated by having to include the effects of line discontinuities: bends T-junctions, crossovers, vias (Fig. 1.2). Also, in order to evaluate an interconnect response terminating networks (typically nonlinear) have to be considered simultaneously with the interconnect structure.

Fortunately, the problem of high frequency signal transmission has existed in a closely related area — the area of microwave and millimeter-wave engineering — for a few decades. The most commonly used signal transmission media at microwave frequencies are microstrip lines, strip lines, coplanar lines, slot lines, fin lines and waveguides. A large amount of work has been done in the analysis and characterization of these structures and most of this work can be directly applied to today's interconnect problems. The common property of all these structures, together with any macroscopic electromagnetic system, is that their behavior is governed by Maxwell's equations. A solution based on complete Maxwell's equations is often referred to as a full-wave solution.

Many interconnect analyses rely on certain approximations in order to reduce the complexity present in a complete solution of Maxwell's equations. These approximations usually fall into two categories. In the first, one assumes that the interconnect is infinite in length in order to reduce the problem to two dimensions, which only requires consideration of the structure's cross section. The limitation of this assumption is that the analyses cannot be applied to the characterization of three-dimensional discontinuities such as corners, vias, and wire bonds which are often encountered in hybrid and integrated circuits. The second assumption is a TEM quasi-static approximation, which assumes that the propagating mode is TEM mode. Under this assumption the solution of Maxwell's equations reduces to the electrostatic problem of the solution of Poisson's equation. The results obtained from such techniques are valid only at low frequencies and become less accurate with increasing frequency. As
Figure 1.2: Examples of microstrip discontinuities.
frequency. As the transverse dimensions of the structure being analyzed approach an appreciable fraction of a wavelength, the accuracy of such methods decreases. Another consideration in interconnect analysis must be the propagation of higher order modes and radiation effects which arise at higher frequencies. In order to accurately analyze three dimensional discontinuities and other interconnects at higher frequencies, one must solve Maxwell's equations in three dimensions.

1.2.1 Analysis methods for planar microwave structures

The problem of interconnect analysis is closely related to the analysis of planar microwave structures and most of the existing microwave analysis methods apply directly to the analysis of interconnects. Microstrip and other planar structures and discontinuities have been the objects of investigation for more than two decades. In the microwave area, efficient numerical modeling of spatial three dimensional discontinuities is still the bottleneck of accurate large scale simulation of complex microwave integrated circuits. In general, these circuits are composed of cascaded sections of complexly shaped planar transmission lines deposited on a multilayered dielectric substrate mixed with frequent discontinuities. A number of methods have been developed in the past to characterize microwave circuit discontinuities. Some of these methods result in closed formula descriptions based partly on quasi-static calculations and partly on full-wave analyses and measurement results. Most of the available closed form expressions have been implemented in microwave CAD packages, but many do not fulfill the requirements on accuracy, usable parameter range, and frequency range for the design of modern microwave and millimeter-wave circuits. Numerous numerical methods also exist and some are described below.

Numerical methods for interconnect and microwave circuit analysis can be classified in terms of the basic problem they solve into steady state or frequency domain methods (e.g. [2]) and transient or time domain methods. They can also be categorized by the amount of preprocessing they require. Some methods require little or no analytical preprocessing and can easily be adapted to solve any kind of elec-
tromagnetic problem. Other methods require considerable analytical preprocessing and are more problem dependent. The methods can also be classified in terms of the approach to the problem. Some methods are based on direct numerical solution of governing integral or partial differential equations (usually derived from Maxwell's equations). Others approach the problem by modeling the structure of interest with a better understood lumped/distributed electrical circuit. A numerical method is then derived to solve for the behavior of this more familiar electrical model. A classical example of this latter approach is the Transmission Line Matrix (TLM) method.

The transmission line matrix (TLM) method was introduced by Johns and Beurle in 1971 [3] for solving two-dimensional waveguide problems. The method was soon extended for solving the time dependent Maxwell equations in three dimensions [4]. Later the method was reformulated to make it more accurate and efficient [5] than the first methods. The basis for the TLM method is the Huygens principle which shows that a wavefront can be considered as consisting of a number of secondary radiators giving rise to spherical wavelets. The envelope of these wavelets forms a new wavefront which gives rise to new wavelets, and so on. The TLM method implements Huygens’ model with a mesh of nodes that are connected with transmission line segments. There are two types of nodes, series and shunt, and it can be shown that there is an analogy between the voltages and currents on these nodes and the components of the electric and magnetic fields of Maxwell's equations [7]. The inductive, capacitive, and resistive properties of the transmission lines correspond to the permeability, permittivity, and conductivity of the space being modeled. Boundary conditions are represented as different transmission line terminations. The analysis is performed by exciting one or more of the nodes by an ideal voltage impulse (Dirac delta distribution) and calculating the propagation of this impulse through the mesh of transmission lines. The resulting train of impulses at the output node carries information about the original analyzed structure. This response is than Fourier transformed to obtain an approximation for the field transfer function between two nodes in the structure. Some characteristics of the TLM method are that the propagation velocity in the TLM mesh depends on the direction of propagation and the frequency and that the
boundary conditions used for modeling lossy conductors are valid only in a relatively narrow frequency range.

Among other commonly used frequency domain microwave analysis methods are the Mode Matching Method (e.g., [8]) and the Spectral Domain Approach (SDA) (e.g., [9]). These methods have been frequently utilized for planar microwave structures, however, their application is virtually limited to the cases where the circuit discontinuity fits into an orthogonal coordinate system. An alternative method is the Method of Lines [10]. The method of lines is a space-frequency domain method where the two spatial variables which correspond to the substrate plane are discretized, while the remaining variable perpendicular to the substrate plane is treated analytically. The advantage of this technique is its easy formulation, the simple convergence behavior and that there are no specially suited expansion functions necessary. Furthermore it requires only a two-dimensional discretization scheme and hence requires less computer memory than the finite difference, finite element and TLM methods. However, the method is currently applicable only to rectangular shaped circuits and for circuits of arbitrary shape difficulties arise with satisfying all the boundary conditions. This shortcoming is eliminated by the Space Spectral Domain Approach (SSDA) [11] which uses a combination of the one-dimensional MOL and the one-dimensional SDA together with a set of continuous basis functions which satisfy the boundary conditions. By introducing specially suited basis functions one of the advantages of the two-dimensional MOL is eliminated. The above frequency domain methods have successfully been used for determining the resonant frequencies of complexly shaped three dimensional microwave circuit structures. For the analysis of arbitrarily shaped transmission line discontinuities the Transmission Line Matrix, Finite Element (FE) or Finite Difference (FD) methods offer a higher degree of flexibility.

Another class of methods for analyzing planar line discontinuities are the orthogonal series expansion techniques which use a combination of exact field solutions for one port problems to obtain the solution of the planar discontinuity problem.

Perhaps the most general approach to the solution of interconnect or microwave
problems is the direct numerical solution of the frequency or time domain Maxwell's equations. Among the most versatile and most widely used of these methods are the finite element and finite difference methods.

1.2.2 Finite Difference and Finite Element Methods

The two most commonly used classes of numerical methods for solving problems described by partial differential equations, occurring in a wide range of disciplines, are the finite difference and finite element methods.

Finite difference methods are discrete techniques where the domain of interest is represented by a set of points or nodes and information between these points is commonly obtained using Taylor series expansions. The basic concepts are quite simple. The domain of solution of the given PDE is first subdivided by a net with a finite number of mesh points. The partial derivatives at each point are then replaced by finite difference approximations. A number of these approximations can be derived through the use of Taylor series expansions resulting in a large number of finite difference schemes.

In contrast to the finite difference schemes, in the finite element method the domain of interest is divided into subdomains commonly referred to as finite elements. The unknown function is represented within each element by an interpolating polynomial which is continuous along with its derivatives to a specified order within the element. These interpolation functions are variously denoted as shape functions, basis functions, or just interpolation functions, depending upon the discipline in which the method is being applied. Although points or nodes play a role in finite element theory, the emphasis is directed more toward the interpolation functions.

While the finite difference schemes can be represented using Taylor series in a relatively straightforward manner, the theory behind the finite element method uses concepts from functional analysis and variational methods in order to formulate the algebraic equations that are analogous to the finite difference formulas. In addition,
one must overcome the conceptual problem of assembling information obtained on
the element by element basis into a global representation of the problem. Several
avenues lead to the same finite element formulation. A conceptually simple, yet
mathematically rigorous approach can be formulated using the method of weighted
residuals (MWR). Among the MWR family of methods, the Galerkin, subdomain,
and collocation schemes are most commonly encountered in engineering practice. The
most commonly used types of basis functions are the Lagrangian bases, serendipity
bases, and Hermitian bases.

The two classes of methods are related and finite element equations can often
be interpreted in terms of weighted average finite difference approximations. The two
approaches do not always generate schemes of the same order of accuracy. Moreover,
the order of accuracy is only one indicator of computational performance and, in fact,
solutions obtained using the finite element and finite difference methods on the same
grid can be quite different.

1.3 Numerical Methods for Electromagnetic Problems

Besides just calculating the field solution, full-wave numerical methods can serve a
number of other important purposes. They can be used as:

- an aid for deeper understanding of circuit behavior;
- an aid for the development and validation of CAD-oriented models;
- a tool for circuit performance optimization.

More specifically, one can use full-wave numerical methods for:

- accurate modeling of transmission structures, discontinuities and passive mi-
crowave elements;
- study of radiation from discontinuities/microstrip circuits:
  - estimation of radiation loss;
  - spurious electromagnetic coupling between discontinuities.
- design of novel structures with desired electrical characteristics;
• study of external effects (thermal, deviations in material constants and dimensions) on electrical performance;
• generation of lookup tables for CAD applications.

Some advantages of full-wave numerical analysis methods are that they can give results to any desired accuracy up to any frequency by using an appropriate mesh discretization of the geometry — the only limiting factor being the available computer resources. On the other hand, it is important to keep in mind that the quasi-static methods, in regimes where they are applicable, generally require less computational expenditure to yield the desired result.

1.4 Finite Difference Methods for Time-Domain Maxwell’s Equations

The two curl equations of Maxwell represent a hyperbolic linear system of partial differential equations (PDEs) in four independent variables. A large number of finite difference methods for solving linear and quasi-linear hyperbolic systems of PDEs in four independent variables exists in the mathematical literature. All of them have been well studied by mathematicians. Of the numerous existing methods for solving these equation only a few are commonly used by electrical engineers. The most widely used finite difference method is known to the microwave engineering community as Yee’s method, after Kane S. Yee who applied it to the scattering of electromagnetic waves from conducting surfaces [12]. This method is so common in the field of time domain electromagnetic calculation (microwaves, antennas, wave propagation, etc.) that is often referred to as “the” finite difference method. The basic characteristics of Yee’s differencing scheme is that different components of the electric and magnetic fields ($E$ and $H$ fields, respectively) are calculated at different nodes of the mesh, i.e., only one field component is calculated at a given point (node). Also, the $E$-field components are not calculated at the same time as the $H$-field components but at times separated by half a time step, in a leapfrog fashion.
1.4.1 Boundary Conditions

For the purpose of time domain modeling of an electromagnetic structure using a numerical technique one needs to confine the structure of interest within a certain domain and perform the calculations only in this domain of interest. The behavior of the structure outside this domain is then described by prescribing the boundary conditions on the boundary of the domain of interest. The given boundary conditions, together with the initial conditions and the governing hyperbolic system of partial differential equations then determine the solution. A problem of this type is called an initial boundary value problem (IBVP).

For electromagnetic problems the boundary conditions consist of two relations between the field components which typically describe electric walls, magnetic walls, absorbing boundaries, or excitations (in the form of given electric or magnetic field components). Electric and magnetic walls cause wave reflection and if these boundary conditions are used in field calculations, the analyzed structures need to be made very large in order to separate out the scattered pulses. Absorbing boundary conditions are therefore essential for an efficient finite difference solution. The freedom of specifying various boundary conditions depends on the particular numerical method. For example, in Yee's finite difference method the boundary conditions for electric and magnetic walls are simple to model while absorbing boundary conditions pose a serious problem for the method. This problem is typically circumvented in the microwave literature in two ways. In the first approach, absorbing boundary conditions are modeled by solving the problem twice for each absorbing boundary, once with a vanishing tangential electric field (electric wall) and once with a vanishing tangential magnetic field (magnetic wall). The results of the two solutions are then averaged to give the desired approximation [14]. In the second approach, absorbing boundary conditions are modeled by forcing the fields at the boundaries to have the same values as at a distance $\Delta x$ before the boundary at the time $\Delta x/v_p$. Here $\Delta x$ is the mesh spacing and $\Delta x/v_p$ is the time that the wave needs to propagate along the distance $\Delta x$. This second approach gives sufficient results only if the velocity of the wave is
dispersionless and the wave propagates in a direction perpendicular to the wall.

1.4.2 Stability criteria; Courant-Friedrichs-Lewy Condition

The necessary condition for the stability of a finite difference method is determined by the Courant-Friedrichs-Lewy (CFL) condition which, in simplified terms, states that the domain of dependence of the hyperbolic partial differential equation must be completely contained within the domain of dependence of the finite difference scheme. One can compare this necessary CFL condition with the sufficient stability condition for a particular differencing scheme and see how close the sufficient condition for stability is to the necessary condition. This gives a measure of "quality" of a finite difference method by showing how close a difference scheme is to an optimal scheme. This reasoning can be quantified in the following way (for details see [16]). Let the mesh size in all \( m \) space dimensions be equal to \( \Delta x \) and let the time increment (time step size) be \( \Delta t \). The sufficient stability condition can then be written as

\[
\frac{\Delta t}{\Delta x} \leq r_1,
\]

where \( r_1 \) is determined by the differencing scheme (for a given hyperbolic system).

Similarly, the necessary CFL condition can be written as

\[
\frac{\Delta t}{\Delta x} \leq r_2.
\]

One can then define the factor \( q \) by

\[
q = \frac{r_1}{r_2},
\]

where \( q \leq 1 \). \( q = 1 \) then gives an optimal scheme.

We now focus on the hyperbolic system of partial differential equations obtained from the two Maxwell's curl equations. For a rectangular grid with the grid size in all three space dimensions equal to \( \Delta x \) and a point \( P \) located in a homogeneous, isotropic, linear medium characterized by the constants \( \mu = \mu_0 \mu_r \) and \( \epsilon = \epsilon_0 \epsilon_r \) the CFL condition gives \( r_2 = \sqrt{\mu \epsilon} \). As an example, the sufficient stability condition in
Yee’s differencing scheme is (e.g., [12])

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{\sqrt{3}} \sqrt{\mu \varepsilon} = r_1.$$  \hspace{1cm} (1.4)

and, therefore, \( q = r_1/r_2 = 1/\sqrt{3} \).

1.5 Method of Characteristics

The method of characteristics is a standard mathematical technique for solving hyperbolic systems of partial differential equations in two independent variables. It is well known that there is a family of characteristic curves, or characteristics, associated with each solution of a two-variable system of hyperbolic equations. For each of these curves the system of equations defines an interior operator along the curve, i.e., for each characteristic curve a differential operator exists which contains derivatives only in the direction of the characteristic curve. This means that along each characteristic curve the system of hyperbolic partial differential equations defines (is equivalent to) an ordinary differential equation. This system of ordinary differential equations is then solved along the corresponding characteristics. This is done analytically or numerically (by finite difference schemes). The method has been applied for the analysis of lossy uniform and nonuniform transmission lines terminated in nonlinear elements [18].

The method of characteristics has many interesting properties. One of these properties is that it gives physical insight into the problem being solved. The intersections of a family of characteristic curves with a time = constant plane represent the wavefronts. It can be shown (e.g., [19]) that all information (discontinuities in the initial data and its derivatives) propagates along the characteristics. A consequence of this is that a numerical solution obtained by the method of characteristics is very accurate near discontinuities, which is not the case with most other numerical methods. The domain of dependence for a particular point is determined (bounded) by the outermost characteristics through that point. Therefore the time step in a finite difference scheme obtained by the discretization of the characteristic equations along
the characteristics is optimal, i.e., the factor \( q \) defined above is equal to 1.

For hyperbolic systems with more than two independent variables there is an infinite set of bicharacteristic curves associated with each solution of the system and these curves generate a family of characteristic hypersurfaces. For each of these bicharacteristic curves the system of equations gives a relation between the derivatives of the dependent variables along the curve and the derivatives in any other direction lying in the characteristic hypersurface containing it. These relations between the derivatives are analogous to the characteristic conditions, involving derivatives in only one direction, obtained from hyperbolic systems in two independent variables. The properties associated with the characteristic curves now apply to the characteristic hypersurfaces.

One would like to extend the method of characteristics to problems in more space dimensions (more than two independent variables) while keeping the good properties of the method for two-variable systems. Precisely this idea was the motivation for the Thesis.

Unfortunately, a direct extension of the method of characteristics to hyperbolic systems in more than two independent variables is not possible. This is because the bicharacteristic relations for more variable problems are weaker than the corresponding relations for two variable problems, in that they contain derivatives in more directions instead of one. On the other hand, in more-variable problems there are an infinity of bicharacteristics through each point instead of the finite number of characteristics in two-variable problems. For example, in the case of three independent variables a single infinity of bicharacteristics forms the characteristic hypersurface. For three independent variables, one can still obtain a solution based on relations along the bicharacteristics by using the fact that there are an infinity of these relations available to compensate for their weaker form [20].

The purpose of this Thesis is to introduce a new numerical method based on the characteristic equations for hyperbolic systems in four independent variables which
retains most of the properties of the method of characteristics for hyperbolic systems with two independent variables and apply it to the problem of transient full-wave interconnect analysis. In particular the goal is to develop an optimal discretization scheme \((q = 1)\) as well as the ability to treat a large class of boundary conditions given by two general relations between the field components.

The method developed here is quite general and could be extended to a number of general electromagnetic problems. However, in this Thesis we concentrate on its application to the analysis of interconnect discontinuities.

The Thesis is organized as follows. First, a summary of the theory of partial differential equations is presented in Chapter 2. The Chapter focuses mostly on hyperbolic equations and systems of equations and introduces the notation, terminology, and derivations needed for Chapter 3, making the Thesis a complete unit. Chapter 3 represents the crux of the Thesis. Here the theory of Chapter 2 is used to develop a numerical method based on the method of characteristics for solving the hyperbolic system of partial differential equations in four independent variables obtained from Maxwell’s equations. The method is then exemplified in Chapter 4 by applying it to a few interconnect discontinuity problems. Finally, Chapter 5 gives the concluding remarks and outlines the possible directions of future research.
Chapter 2

Relevant Partial Differential Equation Theory

This chapter presents an outline of partial differential equation (PDE) theory that is related to the material in this Thesis. It introduces some of the terminology that is used in later chapters, and contributes to its completeness.

2.1 Introductory Remarks on Partial Differential Equations

A partial differential equation is a relation of the form

\[ F(x, y, \ldots, u, u_x, u_y, \ldots, u_{xx}, u_{xy}, \ldots) = 0, \quad (2.1) \]

where \( F \) is a function of the variables \( x, y, \ldots, u, u_x, u_y, \ldots, u_{xx}, u_{xy}, \ldots \). A function \( u(x, y, \ldots) \) of the independent variables \( x, y, \ldots \) is sought such that equation (2.1) is identically satisfied in these independent variables if \( u(x, y, \ldots) \) and its partial derivatives

\[
\begin{align*}
    u_x &= \frac{\partial u}{\partial x}, & u_y &= \frac{\partial u}{\partial y}, & \ldots, \\
    u_{xx} &= \frac{\partial^2 u}{\partial x^2}, & u_{yy} &= \frac{\partial^2 u}{\partial y^2}, & \ldots, \\
    & \vdots
\end{align*}
\]

are substituted in \( F \). Such a function \( u(x, y, \ldots) \) is called a solution (integral, integral surface) of the partial differential equation (2.1). One may be interested in not only a single or particular solution but in the totality of solutions of 2.1. If further conditions are imposed in addition to (2.1), we may look for individual solutions.
The order of the highest derivative occurring in (2.1) is called the order of the PDE.

If the function $F$ is linear in the variables $u, u_x, u_y, \ldots, u_{xx}, u_{xy}, \ldots$, with the coefficients depending only on the independent variables $x, y, \ldots$, the PDE is called linear. If $F$ is linear in the highest order derivatives (say the $n$-th), with the coefficients depending on $x, y, \ldots$ and possibly on $u$ and its partial derivatives up to order $n - 1$, the PDE is called quasi-linear.

In the case of only two independent variables $x, y$, the solution $u(x, y)$ of the partial differential equation (2.1) may be visualized geometrically as a surface, an integral surface in the $x, y, u$-space.

### 2.2 First Order Partial Differential Equations in Two Independent Variables

#### 2.2.1 Geometrical Interpretation of First Order PDEs; Monge cones

Geometrical intuition is of great help in the theory of integration of first order partial differential equations for a function $u(x, y)$ of two independent variables. In addition, the same intuitive reasoning used for PDEs with two independent variables can often be extended to the case of equations with more independent variables.

We consider the partial differential equation

$$F(x, y, u, p, q) = 0,$$  \hspace{1cm} (2.2)

with $F_p^2 + F_q^2 \neq 0$ and the abbreviation $p = u_x, q = u_y$. For every integral surface through the point $P$ with coordinates $x, y, u$ the quantities $p$ and $q$, which determine the position of the tangent plane at this point, must satisfy condition (2.2). The tangent plane of the integral surface at the point $P$ is restricted to positions which belong to the manifold characterized by equation (2.2). For a given point $P : (x, y, u)$, this manifold is in general a one parameter family (for example for $p^2 + q^2 = 1$ the
family is \( p = \cos(\lambda), q = \sin(\lambda) \) with the parameter \( \lambda \) of planes. If \( F \) is linear in \( p \) and \( q \), then this family of possible tangent planes forms an axial pencil of planes through a straight line called the Monge axis. For the general case of \( F \) this family of planes forms a cone, the Monge cone. Thus, in the \( x, y, u \)-space the partial differential equation is represented geometrically by a "cone field", just as an ordinary differential equation of first order is represented by a direction field. To find a solution means to find a surface which at each of its points touches the corresponding cone.

2.2.2 Characteristic and Focal Curves

Monge cones can also be represented by means of a relation for their generating lines instead of the relation \( F = 0 \) for their tangent planes. To do this analytically, we first represent the Monge cone \( F = 0 \) parametrically by considering \( p \) and \( q \) as functions of a parameter \( \lambda \). A generating line of the cone is then the limit of the line of intersection of the tangent planes belonging to the parameters \( \lambda \) and \( \lambda + h \), respectively, as \( h \to 0 \).

If we consider \( x, y, u \) along a fixed generator as functions of the distance \( \sigma \) from the vertex of the cone, then we obtain the equations

\[
\frac{du}{d\sigma} = p(\lambda) \frac{dx}{d\sigma} + q(\lambda) \frac{dy}{d\sigma} \tag{2.3}
\]

and

\[
0 = p'(\lambda) \frac{dx}{d\sigma} + q'(\lambda) \frac{dy}{d\sigma}. \tag{2.4}
\]

By differentiating \( F = 0 \) with respect to \( \lambda \) we also find

\[
F_p p'(\lambda) + F_q q'(\lambda) = 0. \tag{2.5}
\]

Therefore the relation

\[
dx : dy : du = F_p : F_q : (pF_p + qF_q) \tag{2.6}
\]

holds for the generators of the cone. This relation may be regarded as the representation of the Monge cone dual to that given by the partial differential equation (2.2).
The directions of the generators of the Monge cone are called *characteristic directions*. For quasi-linear partial differential equations the Monge cones degenerate into a pencil of planes and the generators become a straight line. Each point of the \(x, y, u\) space then has only one characteristic direction belonging to it. For the general PDE (2.2) we have a one-parameter family of characteristic direction at each point. Space curves having a characteristic direction at each point are called *focal curves* or *Monge curves*. The conditions (2.6) for the focal curves can be written in the form

\[
\frac{dx}{ds} = F_p, \quad \frac{dy}{ds} = F_q, \quad \frac{du}{ds} = pF_p + qF_q
\]

by introducing a suitable parameter \(s\) along them. The last of these three partial differential equations is called the strip condition. It states that the functions \(x(s), y(s), u(s), p(s), q(s)\) not only define a space curve, but simultaneously a plane tangent to it at every point. A configuration consisting of a curve and a family of tangent planes to this curve is called a *strip*. This system of three ordinary differential equations (2.7) and the relation \(F(x, y, u, p, q) = 0\) represent an underdetermined system. Each solution of this system yields a focal strip.

Focal strips which are embedded in integral surfaces are called *characteristic strips*. Every integral surface \(u(x, y)\) must have focal curves since at every point the integral surface is tangent to a Monge cone, and therefore contains a characteristic direction. The field formed by these characteristic directions yields the corresponding focal curves as its integral curves on the integral surface. The requirement that a focal curve be embedded in an integral surface leads to two additional ordinary differential equations for the quantities \(p\) and \(q\) as functions of \(s\). (Embedding means that in the neighborhood of the projection of the focal curve on the \(x, y\)-plane \(u\) is a single-valued, twice continuously differentiable function of \(x\) and \(y\).)

To find these differential equations on a specific integral surface \(u = u(x, y)\), on which the quantities \(p\) and \(q\) may also be considered as specific given functions of \(x, y\), we note that the differential equations

\[
\frac{dx}{ds} = F_p, \quad \frac{dy}{ds} = F_q
\]
define a one-parameter family of curves on the surface, along which

\[
\frac{du}{ds} = u_x \frac{dx}{ds} + u_y \frac{dy}{ds}
\]  

(2.9)

and therefore

\[
\frac{du}{ds} = pF_p + qF_q
\]  

(2.10)

holds. Thus our curves form a family of Monge curves and generate the integral surface. By differentiating the partial differential equation (2.2) first with respect to \(x\) and then with respect to \(y\), we obtain the relations

\[
F_{pp} + F_{qq} + F_{up} + F_{x} = 0, \\
F_{pp} + F_{qq} + F_{uq} + F_{y} = 0,
\]  

(2.11)

which hold identically on our integral surface. Since \(F_p = dx/ds, F_q = dy/ds, p_y = q_x\), for Monge (focal) curves given in terms of the parameter \(s\) the above two equations become

\[
\frac{dp}{ds} + F_up + F_x = 0, \quad \frac{dq}{ds} + F_uq + F_y = 0.
\]  

(2.12)

Thus, if a Monge curve is embedded in an integral surface, the coordinates \(x, y, u\) of its points and the quantities \(p\) and \(q\) satisfy, along that curve, the following system of five ordinary differential equations

\[
\frac{dx}{ds} = F_p, \quad \frac{dy}{ds} = F_q, \quad \frac{du}{ds} = pF_p + qF_q, \\
\frac{dp}{ds} = -(pF_u + F_x), \quad \frac{dq}{ds} = -(qF_u + F_y).
\]  

(2.13)

This system is called the characteristic system of differential equations belonging to (2.2).

If we now reverse the process and disregard the fact that this system of ordinary differential equations was obtained by considering a given integral surface, we may use the system as a starting point without reference to solutions of (2.2). Since there is an irrelevant additive constant in the parameter \(s\), the system defines a four-parameter family of curves: \(x(s), y(s), u(s)\) and corresponding tangent planes \(p(s), q(s)\), i.e., a family of strips.
We note that the function $F$ is an integral of our characteristic system of differential equations. The word "integral" is used here in the sense of a function $\phi(x_1, x_2, \ldots, x_n)$ of the independent variables $x_i$ which has a constant value along each curve which solves the system

$$\frac{dx_i}{ds} = a_i(x_1, x_2, \ldots, x_n) \quad (i = 1, 2, \ldots, n). \quad (2.14)$$

To see that $F$ is an integral of (2.13) we differentiate 2.2 with respect to $s$ to get

$$\frac{dF}{ds} = F_p \frac{dp}{ds} + F_q \frac{dq}{ds} + F_u \frac{du}{ds} + F_x \frac{dx}{ds} + F_y \frac{dy}{ds}. \quad (2.15)$$

Because of the characteristic differential equations the expression on the right vanishes identically in $s$.

We now single out from the four-parameter family of solutions of the characteristic differential equations a three-parameter family by using the condition that, along these solutions, $F$ should have the constant value zero (from the original PDE). Every solution of the characteristic differential equations which also satisfies the equation $F = 0$ is called a characteristic strip; a space curve $x(s), y(s), u(s)$ bearing such a strip is called a characteristic curve.

The most important result of the theory of first order partial differential equations is the equivalence of the problems of integrating the partial differential equation (2.2) and the characteristic system of ordinary differential equations (2.13). In other words, the integration of a first order partial differential equation can be reduced to that of the corresponding characteristic system of ordinary differential equations.

In the following sections we restrict our discussion only to the special case of quasi-linear partial differential equations.
2.3 Theory of Linear and Quasi-Linear Partial Differential Equations of First Order

2.3.1 Characteristic Curves

We consider the quasi-linear partial differential equation

\[ \sum_{i=1}^{n} a_i u_{x_i} = a, \]  

(2.16)

where the coefficients \( a_i \) and \( a \) are continuously differentiable functions of the variables \( x_1, x_2, \ldots, x_n, u \), and \( \sum_{i=1}^{n} a_i^2 \neq 0 \). In order to study the quasi-linear equation (2.16) we first look at the corresponding linear equation, where the coefficients \( a_i \) are functions of the independent variables \( x_1, x_2, \ldots, x_n \) only.

The equation (2.16) states geometrically that at every point of the \( x, u \)-space on the surface \( u = u(x_1, x_2, \ldots, x_n) \) the characteristic directions

\[ dx_1 : dx_2 : \cdots : dx_n : du = a_1 : a_2 : \cdots : a_n : a \]  

(2.17)

are tangent to the surface. In the case of two independent variables, these directions coincide with directions of the Monge axes of (2.16).

In the \( n + 1 \)-dimensional \( x, u \)-space we determine \( n + 1 \) curves

\[ x_i = x_i(s, t_1, t_2, \ldots, t_{n-1}), \quad (i = 1, 2, \ldots, n) \]

\[ u = u(s, t_1, t_2, \ldots, t_{n-1}) \]  

(2.18)

of the parameters \( s, t_1, t_2, \ldots, t_{n-1} \) by means of the system of ordinary differential equations

\[ \frac{dx_i}{ds} = a_i(x_1, x_2, \ldots, x_n), \quad (i = 1, 2, \ldots, n) \]

\[ \frac{du}{ds} = a(x_1, x_2, \ldots, x_n, u). \]  

(2.19)

The \( (n - 1) \)-parameter family of curves given by this system of ordinary differential equations (2.19) is called the family of characteristic curves of the PDE (2.16); the
projection of a characteristic curve on the $x$-space is called a \textit{characteristic base curve.} The equations (2.19) are called the \textit{characteristic differential equations.}

These characteristic curves in the $x,u$-space are defined by (2.19) without reference to specific solutions of the partial differential equation (2.16).

The connection between characteristic curves and integral surfaces is given by the following theorem:

On every integral surface $u = u(x_1, x_2, \ldots, x_n)$ of the partial differential equation there exists an $(n - 1)$-parameter family of characteristic curves which generate the integral surface. Conversely, every surface $u = u(x_1, x_2, \ldots, x_n)$ generated by such a family is an integral surface. Moreover, if a characteristic curve has a point in common with an integral surface, then it lies entirely on the surface.

The general case where the partial differential equation (2.16) is quasi-linear can be reduced to a homogeneous PDE with an additional independent variable $x_{n+1}$. We introduce $u = x_{n+1}$ as a new independent variable and allow the desired solution to be defined in the implicit form

$$\phi(x_1, x_2, \ldots, x_{n+1}) = 0, \quad (2.20)$$

or more generally, in terms of a constant $c$ in the form

$$\phi(x_1, x_2, \ldots, x_{n+1}) = c. \quad (2.21)$$

The problem is now reduced to finding $\phi$. Taking the partial derivatives of (2.21) gives

$$\phi_{x_i} + \phi_{x_{n+1}} u_{x_i} = 0 \quad (i = 1, 2, \ldots, n). \quad (2.22)$$

Multiplying the above equations by $a_i$ and adding gives

$$\sum_{i=1}^{n} a_i \phi_{x_i} + \phi_{x_{n+1}} \sum_{i=1}^{n} a_i u_{x_i} = 0. \quad (2.23)$$

After using $\sum_{i=1}^{n} a_i u_{x_i} = a$ we get

$$\sum_{i=1}^{n} a_i \phi_{x_i} + a \phi_{x_{n+1}} = 0. \quad (2.24)$$
Therefore we have the following partial differential equation for $\phi$:

$$\sum_{\nu=1}^{n+1} a_{\nu} \phi_{x_{\nu}} = 0, \quad (2.25)$$

where $a_{n+1} = \alpha(x_1, \ldots, x_n, u)$. However, the equation (2.25) need not hold identically in $x_1, \ldots, x_{n+1}$ because it was derived from only those sets of values for which the relation $\phi = 0$, or $\phi = c$, holds. Thus, from this point of view (2.25) is not yet a linear homogeneous partial differential equation. But if instead of considering a single solution of the original partial differential equation we consider a one-parameter family depending on the parameter $c$ and given by $\phi = c$, then equation (2.25) must hold for all values $x_1, x_2, \ldots, x_{n+1}$; i.e., it is really a linear partial differential equation. If we select

$$x_1, x_2, \ldots, x_{n+1} \quad (2.26)$$

arbitrarily and take the value $c$ given by $\phi(x_1, x_2, \ldots, x_{n+1}) = c$, then since (2.25) must hold for this value of $c$, it holds identically in $x_1, x_2, \ldots, x_{n+1}$.

Conversely, by finding a solution $\phi$ of (2.25) and setting $\phi = c$, we obtain a one-parameter family of solutions of (2.16).

Thus there is a one-to-one correspondence between the solutions of (2.25) and one-parameter families of solutions of the original equation (2.16). This shows that the integration of the general quasi-linear partial differential equation (2.16) is equivalent to the integration of the system of ordinary differential equations

$$\frac{dx_i}{ds} = a_i, \quad \frac{du}{ds} = a. \quad (2.27)$$

2.3.2 Initial Value Problem

From the characteristic curves defined by the characteristic equations we can now construct the integral surface by solving the following initial value problem (or Cauchy's problem): In $(n+1)$-dimensional $x, u$-space let an $(n-1)$-dimensional initial manifold $C$ be given by the continuously differentiable functions

$$x_i = x_i(t_1, t_2, \ldots, t_{n-1}), \quad (i = 1, 2, \ldots, n)$$
of the independent parameters \( t_1, t_2, \ldots, t_{n-1} \). The set of equations (2.28) defines an \((n - 1)\)-dimensional surface in \(n\)-dimensional space and prescribes the values of the function \( u \) on this surface. We assume that the rank of the matrix \( \frac{\partial x_i}{\partial t_j} \) is \( n - 1 \). We also assume that the projection \( C_0 \) of this manifold on to the \( x \)-space is free of double points, i.e., different points of \( C_0 \) correspond to different sets of values \( t_1, t_2, \ldots, t_{n-1} \). In the neighborhood of \( C_0 \) we seek a solution \( u(x_1, x_2, \ldots, x_n) \) of the partial differential equation which passes through \( C \), i.e., which goes over into \( u(t_1, t_2, \ldots, t_{n-1}) \) when the quantities \( x_i \) are replaced by \( x_i(t_1, t_2, \ldots, t_{n-1}) \). We solve this initial value problem in the following way: For a given set of values \( t_1, t_2, \ldots, t_{n-1} \) we find solutions

\[
x_i = x_i(s, t_1, t_2, \ldots, t_{n-1}) \quad (i = 1, 2, \ldots, n) \quad (2.29)
\]

\[
u = u(s, t_1, t_2, \ldots, t_{n-1}) \quad (2.30)
\]

of the ordinary characteristic differential equations (2.19) which at \( s = 0 \) coincide with the prescribed functions of \( t_1, t_2, \ldots, t_{n-1} \). We now express the quantities \( s, t_1, \ldots, t_{n-1} \) in terms of \( x_1, x_2, \ldots, x_n \) (by means the equations (2.29)) and substitute them into \( u = u(s, t_1, t_2, \ldots, t_{n-1}) \) so that \( u \) appears as a function of \( x_1, x_2, \ldots, x_n \). This introduction of the quantities \( x_1, x_2, \ldots, x_n \) as new independent variables is certainly possible if the Jacobian

\[
\Delta = \frac{\partial(x_1, x_2, \ldots, x_n)}{\partial(s, t_1, \ldots, t_{n-1})} = \begin{vmatrix}
\frac{\partial x_1}{\partial s} & \cdots & \frac{\partial x_n}{\partial s} \\
\frac{\partial x_1}{\partial t_1} & \cdots & \frac{\partial x_n}{\partial t_1} \\
\vdots & & \\
\frac{\partial x_1}{\partial t_{n-1}} & \cdots & \frac{\partial x_n}{\partial t_{n-1}}
\end{vmatrix} \quad (2.31)
\]

does not vanish along \( C \), i.e., for \( s = 0 \). Because of (2.19), the elements of the first row can be expressed along \( C \) by the relations \( \frac{\partial x_i}{\partial s} = a(x_1, x_2, \ldots, x_n, u) \); here prescribed initial values are to be substituted for the \( x_i \) and \( u \) as functions of \( t_1, t_2, \ldots, t_{n-1} \).
Therefore, the Jacobian (2.31) is identical with

\[
\Delta = \begin{vmatrix}
    a_1 & \cdots & a_n \\
    \frac{\partial x_1}{\partial t_1} & \cdots & \frac{\partial x_n}{\partial t_1} \\
    \vdots \\
    \frac{\partial x_1}{\partial t_{n-1}} & \cdots & \frac{\partial x_n}{\partial t_{n-1}}
\end{vmatrix}.
\] (2.32)

Under the assumption \(\Delta \neq 0\) we obtain from \(u(s,t_1,\ldots,t_{n-1})\) a function \(u(x_1,x_2,\ldots,x_n)\). The equation \(du/ds = a\) becomes

\[
\sum_{i=1}^{n} u_{x_i} \frac{dx_i}{ds} = \sum_{i=1}^{n} a_i u_{x_i} = a.
\] (2.33)

\(u(x_1,x_2,\ldots,x_n)\) is therefore a solution of the partial differential equation (2.16). Thus, assuming \(\Delta \neq 0\), the initial value problem possesses a uniquely determined solution.

2.3.3 Remarks on Differentiation in \(n\) Dimensions

Consider a function \(u(x_1,x_2,\ldots,x_n)\) of the independent variables \(x_1,x_2,\ldots,x_n\) which has continuous partial derivatives. At the point \(P\), with coordinates \(x_1,x_2,\ldots,x_n\), a vector \(a = (a_1,a_2,\ldots,a_n)\) may be given such that

\[
a_1^2 + a_2^2 + \cdots + a_n^2 \neq 0.
\] (2.34)

Through the point \(P\) we construct a straight line whose points are given in terms of the parameter \(s\) by the expressions

\[
x_1 + a_1 s, \quad x_2 + a_2 s, \quad \cdots, \quad x_n + a_n s.
\] (2.35)

Then

\[
\frac{\partial u}{\partial s} = \sum_{i=1}^{n} a_i u_{x_i}.
\] (2.36)

is defined as the derivative of the function \(u\) with respect to \(s\) or as the derivative of \(u\) in the "direction" given by the vector \(a\). At every point, the symbol

\[
\frac{\partial}{\partial s} = \sum_{i=1}^{n} a_i \frac{\partial}{\partial x_i}
\] (2.37)
denotes differentiation in the direction of the vector \( a \).

In \( n \)-dimensional space consider a \((n - 1)\)-dimensional surface \( S : \phi(x_1, x_2, \ldots, x_n) \) and a function \( u(x_1, x_2, \ldots, x_n) \) with continuous derivatives in a neighborhood of \( S \). Let \( P \) be a point of \( S \) for which

\[
\sum_{i=1}^{n} \phi_{x_i}^2 \neq 0, \quad (2.38)
\]

and let \( a \neq 0 \) be an arbitrary vector. We consider the derivative of \( u \) on \( S \) in the direction given by \( a \):

\[
\frac{\partial u}{\partial s} = \sum_{i=1}^{n} a_i u_{x_i}. \quad (2.39)
\]

If the equations

\[
a_i = \lambda \phi_{x_i}, \quad (2.40)
\]

hold, then (2.39) is called the derivative in the direction of the normal. If in addition \( \sum_{i=1}^{n} a_i^2 = 1 \), so that

\[
\frac{\partial u}{\partial s} = \sum_{i=1}^{n} \frac{\phi_{x_i}}{\sqrt{\sum_{i=1}^{n} \phi_{x_i}^2}} u_{x_i}, \quad (2.41)
\]

then we speak of the normal derivative of \( u \) at \( P \).

If the vector \( a \) is tangent to \( S \) at \( P \), and therefore perpendicular to the normal at \( P \), i.e., if

\[
\sum_{i=1}^{n} a_i \phi_{x_i} = 0, \quad (2.42)
\]

then

\[
\frac{\partial u}{\partial s} = \sum_{i=1}^{n} a_i u_{x_i}, \quad (2.43)
\]

is called a tangential derivative, or an inner derivative in \( S \) and is said to “lie on the surface \( S \)”. On the other hand, if

\[
\sum_{i=1}^{n} a_i \phi_{x_i} \neq 0, \quad (2.44)
\]

\( \frac{\partial u}{\partial s} \) is called an outward derivative and is said to “lead out of \( S \”).

For example, the expressions

\[
\phi_{x_i} \frac{\partial}{\partial x_k} - \phi_{x_k} \frac{\partial}{\partial x_i} \quad (2.45)
\]
for each pair of indices $i \neq k$ represent derivatives within the surface.

The inner derivatives of $u$ on the surface depend only on the distribution of the values of $u$ on the surface itself; they are, therefore, known if the values of $u$ on the surface $S$ are known. To see this, in the neighborhood of $S$ we introduce, instead of $x_1, x_2, \ldots, x_n$, the variables $\xi_1, \xi_2, \ldots, \xi_n$ such that $\xi_2, \ldots, \xi_n$ are $n - 1$ independent parameters in $S$ and $\xi_1 = \phi$. Then

$$u_{xi} = u_\phi \phi_{xi} + \sum_{k=2}^{n} u_{\xi_k} \xi_k x_i \tag{2.46}$$

The directional derivative

$$\sum_{i=1}^{n} a_i u_{xi} = u_\phi \sum_{i=1}^{n} a_i \phi_{xi} + \sum_{k=2}^{n} u_{\xi_k} \sum_{i=1}^{n} a_i \xi_k x_i \tag{2.47}$$

is therefore known, under the condition $\sum_{i=1}^{n} a_i \phi_{xi} = 0$, if the values $u(0, \xi_2, \ldots, \xi_n)$ of $u$ on $S$ are given.

From $n - 1$ mutually independent inner derivatives of $u$ lying on the surface $S$ (e.g., $\phi_{xi} \partial u / \partial x_i - \phi_{x_k} \partial u / \partial x_i$, for $\phi_{x_k} \neq 0$, $i = 1, 2, \ldots, n - 1$) and a single outward derivative (e.g. $u_{x_n}$) all the partial derivatives of $u$ can be obtained by forming linear combinations. Therefore all the derivatives $u_{xi}$ are known if the function $u$ and one outward derivative of $u$ are given on $S$.

For example, if $n = 2$ and $x_1 = x, x_2 = y$, then $S$ is a curve in the $x,y$-plane which may be represented by two functions $x(\tau), y(\tau)$ of a parameter $\tau$. In this case the condition for inner differentiation (2.42) is simply

$$a_1 \frac{dy}{d\tau} - a_2 \frac{dx}{d\tau} = 0, \tag{2.48}$$

or

$$a_1 = \lambda \frac{dx}{d\tau}, \quad a_2 = \lambda \frac{dy}{d\tau} \tag{2.49}$$

where $\lambda$ is an arbitrary constant.
2.3.4 Characteristic Manifold

The formulation of the initial value problem is modified here by relating previous statements to \( n \)-dimensional \( x \)-space. Let an \((n - 1)\)-dimensional basic manifold \( B \) be given in this space by the relation

\[
\phi(x_1, x_2, \ldots, x_n) = 0. 
\tag{2.50}
\]

Previously the initial manifold was represented by the \( n \) coordinates \( x_i \) as functions of \( n - 1 \) parameters \( t_1, t_2, \ldots, t_{n-1} \). Assigning functional values to the points of this manifold \( B \) it is enlarged to the \( x, u \)-manifold \( C \).

Without discussing the actual solution of the initial value problem, we pose the following question: Consider an initial manifold \( B \) with given values \( u \). Assume that the partial differential equation

\[
\sum_{i=1}^{n} a_i u_{x_i} = a \tag{2.51}
\]

is satisfied in some arbitrary small neighborhood of \( B \) by a function \( u(x_1, x_2, \ldots, x_n) \) with the given initial values. What does this partial differential equation assert along the initial manifold \( B \) for the function \( u \)?

At a point of the initial manifold \( B \) on which the initial function \( u \) is given, a particular direction of differentiation

\[
\frac{\partial}{\partial s} = \sum_{i=1}^{n} a_i \frac{\partial}{\partial x_i} \tag{2.52}
\]

in \( n \)-dimensional \( x \)-space is is defined by the characteristic equations \( dx_i / ds = a_i \).

Now the partial differential equation simply states

\[
\frac{du}{ds} = a, \tag{2.53}
\]

i.e., it establishes the value of the characteristic derivative of \( u \) along \( B \) (since the right side is known on \( B \)).

We have the following alternatives: At the considered point of \( B \), either (i) the equation

\[
\gamma = \sum_{i=1}^{n} a_i \phi_{x_i} \neq 0 \tag{2.54}
\]
holds, or \( (ii) \) the equation
\[
\gamma = \sum_{i=1}^{n} a_i \phi_{x_i} = 0
\] (2.55)
holds.

If equation (2.54) holds, then the characteristic direction leads out of the manifold \( B \) at this point. Equation (2.53), and therefore the PDE (2.51), yields an outward derivative of \( u \); all the first derivatives of \( u \) at the considered point of \( B \) are thus determined by the value of \( u \) on \( B \) alone and by the partial differential equation.

If equation (2.55), called the characteristic condition holds, then \( \partial u / \partial s \) is an inner derivative in \( B \), and therefore already known from the assignment of \( u \) on \( B \). Relation (2.53) thus represents a restriction on the assignment of \( u \) on \( B \); this restrictive condition must be satisfied if a solution \( u \) of the partial differential equation is to exist in the neighborhood of \( B \) with the given initial values on \( B \). If the two relations (2.53) and (2.55) are satisfied at every point \( P \) of \( B \), they characterize \( B \) together with the covering \( u \) as a characteristic basic manifold.

In other words: At the point \( P \) of the given basic manifold \( \phi = 0 \) on which the values of \( u \) are arbitrarily prescribed, either the partial differential equation determines the corresponding derivatives of \( u \) in a unique way or it puts a restriction on the given initial values of \( u \).

2.4 Partial Differential Equations of Higher Order

2.4.1 Systems of Partial Differential Equations

Consider a partial differential equations of the second order:
\[
F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) = 0 \tag{2.56}
\]
for a function \( u(x, y) \). The substitution \( u_x = p, u_y = q \) leads to a system of three first order partial differential equations for three functions \( u, p, q \):
\[
F(x, y, u, p, q, p_x, p_y, q_y) = 0,
\]
Every solution \( u, p, q \) of this system yields \( u \) as a solution of the PDE (2.56), and conversely, every solution \( u \) of (2.56) leads to a set of solutions \( u, u_x, u_y \) of (2.57). Thus, a partial differential equation of the second order is equivalent to a system of three partial differential equations of the first order. The converse, however, is not true.

Therefore, we may restrict ourselves to the treatment of systems of partial differential equations of first order.

### 2.4.2 Systems of First Order with Two Independent Variables; Characteristics

We write a system of \( m \) equations for a function vector \( u \) with the components \( u^1, u^2, \ldots, u^m \) in the form

\[
L_i[u] = \sum_{j=1}^{m} a^{ij} u^j_x + \sum_{j=1}^{m} b^{ij} u^j_y + d^i \quad (i = 1, 2, \ldots, m),
\]

(2.58)

where the elements \( a^{ij}, b^{ij} \) constitute \( m \) by \( m \) matrices \( A \) and \( B \), respectively.

We assume that at least one of these, say \( B \), is nonsingular, i.e., \(|B| \neq 0\). We also assume that the coefficients possess continuous derivatives. The terms \( d^i \) may depend on the unknown functions in a nonlinear way; in this case we call the above system semi-linear.

In matrix notation we may write

\[
L[u] = Au_x + Bu_y + d.
\]

(2.59)

We now consider the equation \( L[u] = 0 \) and pose the problem related to Cauchy's initial value problem: From given initial values of the vector \( u \) on a curve \( C: \phi(x, y) = 0 \) with \( \phi_x^2 + \phi_y^2 \neq 0 \), determine the first derivatives \( u_{xi} \) on \( C \) so that \( L[u] = 0 \) is satisfied in the neighborhood of \( C \).
First we realize that on $C$ the interior derivative $u_y \phi_x - u_x \phi_y$ is known. As a consequence on $C$ we have the relations
\[ u_y^i = -r u_x^i + \frac{f_i}{\phi_x}, \]  
where $f_i$ are the values of the known interior derivatives of $u^i$ on $C$ and $r = -\phi_y/\phi_x$. The last term in the above equations is known on $C$. Substituting these relations into the partial differential equations gives
\[ L_i[u] = \sum_{j=1}^{n} (a^{ij} - r b^{ij}) u_x^i + d^i + \sum_{j=1}^{n} b^{ij} \frac{f_j}{\phi_x}, \quad (i = 1, 2, \ldots, m), \]  
a system of linear partial differential equations for the $m$ derivatives $u_x^i$ on $C$. Hence a necessary and sufficient condition for the unique determinacy of all the first derivatives along $C$ is
\[ Q = |a^{ij} - r b^{ij}| = |A - r B| \neq 0. \]  
$Q$ is called the characteristic determinant of the system (2.58).

If $Q \neq 0$ along the curves $\phi = \text{const.}$, then these curves are called free. Each of these curves can be continued into an integral strip in the neighborhood of $C$. The initial values for Cauchy’s problem are chosen arbitrarily.

If $\tau(x, y)$ is a real solution of the algebraic equation $Q = 0$ of order $n$ for $\tau$, then the curves $C$, defined by the ordinary differential equation
\[ dx : dy = \tau, \quad \text{or} \quad Q \left( x, y, \frac{dx}{dy} \right) = 0, \]  
define the characteristic curves. For characteristic curves the continuation of the initial values into an integral strip is generally not possible.

If the equations $Q = 0$ does not possess real roots $\tau$, then all curves are free; continuation into an strip of initial values is always possible and unique. The system is then called elliptic. In the opposite case, i.e., when $Q = 0$ possesses $n$ distinct real roots, the system is called totally hyperbolic.

If $\tau$ is a real root (maybe the only one) of (2.62), we can solve along $C$ the
system of linear homogeneous equations for the vector \( l = (l_1, l_2, \ldots, l_m) \):

\[
\sum_{i=1}^{m} (a^{ij} - \tau b^{ij}) = 0 \quad \text{or} \quad l(A - \tau B) = 0. \tag{2.64}
\]

Then the linear, "characteristic", combination \( \sum_{i=1}^{m} l^i L_i[u] = IL[u] = 0 \) of the partial differential equations (2.58) can be written in the characteristic normal form

\[
IL[u] = IB(u_r + \tau u_x) + \frac{1}{\phi_x} IBf = 0, \tag{2.65}
\]

where all the unknowns are differentiated in the same direction, i.e., along the characteristic curve corresponding to \( \tau \).

Therefore in the hyperbolic case, i.e., when \( m \) families of characteristic curves exist, we can replace the system (2.58) by an equivalent one, in which each equation contains differentiation only in one, characteristic, direction.

### 2.4.3 Systems of First Order with \( n \) Independent Variables

A linear system with \( n \) variables can be written in the form

\[
L_i[u] = \sum_{\nu=1}^{n} a^{ij\nu} u_{x^\nu}^i + b^i = 0 \quad (i = 1, 2, \ldots, n), \tag{2.66}
\]

with \( a^{ij\nu} \) depending on \( x \), and \( b^i \) depending on \( x \) and possibly also on \( u \). Using matrix notation and the abbreviation \( u_{x^\nu} = u^\nu \), the above equation can be written in the form

\[
L[u] = \sum_{\nu=1}^{n} A^\nu u^\nu + b = 0, \tag{2.67}
\]

where \( A^\nu \) are \( m \) by \( m \) matrices.

We again consider a surface \( C: \phi(x_1, x_2, \ldots, x_n) = 0 \) with \( \text{grad}(\phi) \neq 0 \), and say \( \phi_n \neq 0 \). On \( C \) we consider the characteristic matrix

\[
A = \sum_{\nu=1}^{n} A^\nu \phi_\nu, \tag{2.68}
\]

and the characteristic determinant or the characteristic form

\[
Q(\phi_1, \phi_2, \ldots, \phi_n) = |A|. \tag{2.69}
\]
Initial values of a vector $u$ may be given on $C$. Then we have:

If $Q \neq 0$ on $C$, then the system (2.66) uniquely determines all derivatives $u_\nu$ along $C$ from arbitrarily given initial values; in this case the surface $C$ is called free.

If $Q = 0$ along $C$, we call $C$ a characteristic surface. Then a characteristic linear combination of the operators $L_i$ in (2.66) exists such that that in $\Lambda$ the differentiation of the vector $u$ on $C$ is interior; $\Lambda[u] = 0$ establishes a relationship between the initial data, and hence these data cannot be chosen arbitrarily.

To prove these statements, we first use the fact that $u_\nu \phi_n - u_n \phi_\nu$ is an interior derivative of $u$ on $C$. Hence $u_\nu$ is known on $C$ from the data if only one outgoing derivative, say $u_n$, is known ($\phi_n \neq 0$ was assumed). Multiplying (2.67) by $\phi_n$ gives

$$
\phi_n L[u] = \sum_{\nu=1}^n A^\nu u_\nu \phi_\nu + \sum_{\nu=1}^n A^\nu (u_\nu \phi_n - u_n \phi_\nu) + b
$$

$$
= \sum_{\nu=1}^n A^\nu \phi_\nu u_n + I = 0
$$

(2.70)

where $I$ is an interior differential operator on $u$ in $C$. Hence, under the the assumption $|A| = Q \neq 0$, the system of linear partial differential equations (2.66) for the vector $u_n$ determines $u_n$ uniquely.

On the other hand, if $Q = 0$, then there exists a null vector $1$ of the matrix $A$ such that $1^T A = 0$. Multiplying (2.66) by $1^T$ gives the equations

$$
1^T \phi_n L[u] = 1^T I = 0,
$$

(2.71)

expressed by an interior differential operator on the data along $C$; this operator $1^T I$ does not contain $u_n$. Therefore, $1^T I = 0$ is a differential relation which restricts the initial values of $u$ on $C$.

The characteristic equation $Q = 0$ has the form of a partial differential equation of first order for $\phi(x_1, x_2, \ldots, x_n)$. If it is satisfied identically in $x_1, x_2, \ldots, x_n$, and not only under the condition $\phi = 0$, then the whole family of surfaces $\phi = \text{const.}$ consists of characteristic surfaces.

Now we have the following classification: If the homogeneous algebraic equation
\( Q = 0 \) in the quantities \( \phi_1, \phi_2, \ldots, \phi_n \) cannot be satisfied by any real set of values (except \( \phi_r = 0 \)), then the characteristics cannot exist, and the system is called \textit{elliptic}.

If, in the extreme contrast to the elliptic case, the equation \( Q = 0 \) possesses \( m \) different real solutions \( \phi_n \) for arbitrary prescribed values \( \phi_1, \ldots, \phi_{n-1} \) (or if a corresponding statement is true after a suitable coordinate transformation), then the system is called \textit{totally hyperbolic}. An important theorem, which will not proved here, states that for hyperbolic systems Cauchy’s problem is always solvable.

\textbf{2.5 Properties of Characteristic Curves}

Characteristic curves \( C \) have the following properties, each of which can be used as a definition:

1) Along a characteristic curve the partial differential equation (or for systems, a linear combination of the partial differential equations) represents an interior differential equation.

1’) Initial data on a characteristic curve cannot be prescribed freely, but must satisfy a compatibility condition if these data are to be extended into “integral strips”.

2) Discontinuities of a solution cannot occur except along characteristics.

3) Characteristics are the only possible “branch lines” of solutions, i.e., lines for which the same initial value problem may have several solutions.
Chapter 3

Application of the Method of Characteristics to Maxwell’s Equations

3.1 Problem formulation

The behavior of arbitrary macroscopic electrical structures in the presence of electric and magnetic fields is governed by Maxwell’s equations\(^1\). These equations are the fundamental equations of classical electrodynamics and they can be used to explain and predict the behavior of all macroscopic electromagnetic phenomena. Maxwell’s equations can be written in the form

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \]

\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \]

\[ \nabla \cdot \mathbf{D} = \rho, \]

\[ \nabla \cdot \mathbf{B} = 0, \]

where \( \rho \) is the volume density of free charge, \( \mathbf{J} \) is the current density and the vectors \( \mathbf{E}, \mathbf{H}, \mathbf{B}, \mathbf{D} \) are resulting field vectors.

The above four equations are not independent. The two divergence equations can be derived from the two curl equations and the equation of continuity (charge conservation)

\[ \nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}. \]

\(^1\)After James Clerk Maxwell (1831–1879).
In Maxwell’s equations (3.1)–(3.4) one may think of the volume free charge density \( \rho \) and the volume current density \( J \) as known functions (sources) and the fundamental field vectors \( E, D, B, H \) as twelve unknowns (each having three components). But the four field vectors are also related through the constitutive relations of the medium. For a linear, isotropic, homogeneous medium these relations are:

\[
B = \mu H, \quad (3.6)
\]

\[
D = \varepsilon E, \quad (3.7)
\]

where the constants \( \mu = \mu_0 \mu_r \) and \( \varepsilon = \varepsilon_0 \varepsilon_r \) are properties of the medium. The two curl equations (3.1)–(3.2) and the two constitutive relations and (3.6)–(3.7) provide four independent equations relating the fields at every point\(^2\). Often the current density \( J \) is not specified as a known function but is related to the electric field \( E \). For interconnect problems it suffices to take this relationship to be

\[
J = \sigma E, \quad (3.8)
\]

where \( \sigma \) is the conductivity of the medium. This linear relationship is not required by the theory described below and our method could readily be generalized to arbitrary \( J-E \) relationships.

Substituting the two constitutive relations (3.6)–(3.7) and the expression for the current density (3.8) into the curl equations (3.1)–(3.2) gives

\[
\nabla \times E = -\mu \frac{\partial H}{\partial t}, \quad (3.9)
\]

\[
\nabla \times H = \sigma E + \varepsilon \frac{\partial E}{\partial t}, \quad (3.10)
\]

or, expressed as components in the Cartesian coordinate system,

\[
\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial z} = -\mu \frac{\partial H_x}{\partial t}, \quad (3.11)
\]

\[
\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\mu \frac{\partial H_y}{\partial t}, \quad (3.12)
\]

\[
\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial x} = -\mu \frac{\partial H_z}{\partial t}, \quad (3.13)
\]

\(^2\)Equation (3.7) includes the information given in the continuity equation (3.5) in its derivation.
For practical purposes one must start the field computation at some finite start time and perform the computation in a finite region of space. The fields before the start time are then described by prescribed initial conditions (ICs) and the behavior of the circuit outside the region of interest is taken into account by prescribing the boundary conditions (BCs) at the structure boundary. The initial conditions are given throughout the the domain \( D \) (structure of interest) as

\[ E(x,y,z,0) = e_0(x,y,z), \]
\[ H(x,y,z,0) = h_0(x,y,z) \quad (x,y,z) \in D, \quad (3.17) \]

where \( e_0 \) and \( h_0 \) are known vector functions (vector fields). The boundary conditions relate the field components on the domain boundary \( \partial D \). They are given by two relations of the form

\[ F_1(E(x,y,z,t),H(x,y,z,t)) = 0, \]
\[ F_2(E(x,y,z,t),H(x,y,z,t)) = 0, \quad (x,y,z) \in \partial D. \quad (3.18) \]

Our initial boundary value problem (IBVP) is then described by the six partial differential equations (3.11)–(3.16) together with the initial and boundary conditions (3.17) and (3.18).

In order to write the equations (3.11)–(3.16) in a form more convenient for mathematical treatment, we use the notation

\[ (E_x, E_y, E_z, H_x, H_y, H_z) = (u_1, u_2, u_3, u_4, u_5, u_6) \quad (3.19) \]

and

\[ (x,y,z,t) = (x_1, x_2, x_3, x_4). \quad (3.20) \]
Using the above notation in the curl equations (3.11)-(3.16) gives

\[
\frac{\partial u^3}{\partial x_2} - \frac{\partial u^2}{\partial x_3} = -\mu \frac{\partial u^4}{\partial x_4},
\]

\[
\frac{\partial u^1}{\partial x_3} - \frac{\partial u^3}{\partial x_1} = -\mu \frac{\partial u^5}{\partial x_4},
\]

\[
\frac{\partial u^2}{\partial x_1} - \frac{\partial u^1}{\partial x_2} = -\mu \frac{\partial u^6}{\partial x_4},
\]

\[
\frac{\partial u^6}{\partial x_2} - \frac{\partial u^5}{\partial x_3} = \sigma u^1 + \epsilon \frac{\partial u^1}{\partial x_4},
\]

\[
\frac{\partial u^4}{\partial x_3} - \frac{\partial u^6}{\partial x_1} = \sigma u^2 + \epsilon \frac{\partial u^2}{\partial x_4},
\]

\[
\frac{\partial u^5}{\partial x_1} - \frac{\partial u^4}{\partial x_2} = \sigma u^3 + \epsilon \frac{\partial u^3}{\partial x_4}.
\]

The above equations can be written in matrix form as

\[
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0
\end{bmatrix}
\frac{\partial \mathbf{u}}{\partial x_1}
+ 
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\frac{\partial \mathbf{u}}{\partial x_2}
+
\begin{bmatrix}
\epsilon & 0 & 0 & 0 & 0 & 0 \\
0 & \epsilon & 0 & 0 & 0 & 0 \\
0 & 0 & \epsilon & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu
\end{bmatrix}
\frac{\partial \mathbf{u}}{\partial x_3}
+ 
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\frac{\partial \mathbf{u}}{\partial x_4}
\]
where $\mathbf{u} = [u^1, u^2, u^3, u^4, u^5, u^6]^T$.

By introducing the matrices

$$A_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (3.28)$$

$$A_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad A_4 = \begin{bmatrix} \epsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & \epsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & \epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \end{bmatrix}, \quad (3.29)$$

$$B = \begin{bmatrix} \sigma & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma \end{bmatrix} \quad (3.30)$$
equation (3.27) becomes
\[ \sum_{k=1}^{4} A_k u_k + Bu = 0. \] (3.31)

With the notation (3.19)-(3.20) the initial and boundary conditions (3.17) and (3.18) become
\[ u(x_1, x_2, x_3, 0) = u_0(x_1, x_2, x_3) \quad (x_1, x_2, x_3) \in D \] (3.32)
and
\[ F_1(u) = 0, \]
\[ F_2(u) = 0, \quad (x_1, x_2, x_3) \in \partial D, x_4 > 0. \] (3.33)
where \( D \) is our domain of interest, \( \partial D \) is the boundary of \( D \), \( u_0 \) is a known vector function and \( F_1 \) and \( F_2 \) are vector operators relating the field components at the boundaries.

3.2 Method of Characteristics in Three Space Dimensions

Therefore, the problem to be solved is
\[ L(u) = \sum_{k=1}^{4} A_k u_k + Bu = 0, \] (3.34)
together with the initial and boundary conditions given by (3.32) and (3.33).

The above vector equation represents a hyperbolic system of six partial differential equations in four independent variables. It is seen that (3.34) has the same form as equation (2.67). We now use the theory presented in in Chapter 2 to find the numerical solution of (3.34).

The first step is to find the characteristic hypersurface
\[ \phi(x_1, x_2, x_3, x_4) = 0 \] (3.35)
and a vector
\[ l = [l^1, l^2, l^3, l^4, l^5, l^6]^T, \] (3.36)
such that the operator
\[ \Lambda(u) = \mathbf{1}^T \mathbf{L}(u) \tag{3.37} \]
is an interior operator on the hypersurface \( \phi = 0 \). From Chapter 2 we expect six linearly independent 4 vectors, resulting in six independent interior partial differential equations on \( \phi = 0 \).

According to Chapter 2 the function \( \phi \) satisfies
\[ |\mathbf{A}| = 0, \tag{3.38} \]
where
\[ \mathbf{A} = \sum_{k=1}^{4} \mathbf{A}^k \phi_{x_k} \tag{3.39} \]
and \( |\mathbf{A}| \) is the characteristic determinant of (3.34).

By using the matrices \( \mathbf{A}_k \) from (3.28)-(3.29) in the above equation we find that
\[ \mathbf{A} = \sum_{k=1}^{4} \mathbf{A}_k \phi_{x_k} = \begin{bmatrix} \epsilon \phi_4 & 0 & 0 & 0 & \phi_3 & -\phi_2 \\ 0 & \epsilon \phi_4 & 0 & -\phi_3 & 0 & \phi_1 \\ 0 & 0 & \epsilon \phi_4 & \phi_2 & -\phi_1 & 0 \\ 0 & -\phi_3 & \phi_2 & \phi_4 & 0 & 0 \\ \phi_3 & 0 & -\phi_2 & 0 & \mu \phi_4 & 0 \\ -\phi_2 & \phi_1 & 0 & 0 & 0 & \mu \phi_4 \end{bmatrix}, \tag{3.40} \]
where \( \phi_{x_i} = \phi_i \). Therefore, \( \phi \) must satisfy
\[ \begin{vmatrix} \epsilon \phi_4 & 0 & 0 & 0 & \phi_3 & -\phi_2 \\ 0 & \epsilon \phi_4 & 0 & -\phi_3 & 0 & \phi_1 \\ 0 & 0 & \epsilon \phi_4 & \phi_2 & -\phi_1 & 0 \\ 0 & -\phi_3 & \phi_2 & \phi_4 & 0 & 0 \\ \phi_3 & 0 & -\phi_2 & 0 & \mu \phi_4 & 0 \\ -\phi_2 & \phi_1 & 0 & 0 & 0 & \mu \phi_4 \end{vmatrix} = 0. \tag{3.41} \]
The above characteristic condition yields

$$\sum_{k=1}^{3} \phi_k^2 - \mu \epsilon \phi_4^2 = 0. \quad (3.42)$$

For the case where $\epsilon$ and $\mu$ are not functions of position (homogeneous medium) the solution of the above partial differential equation is

$$\phi(x_1, x_2, x_3, x_4) = \sum_{k=1}^{3} (x_k - x_k^0)^2 - \frac{1}{\mu \epsilon} (x_4 - x_4^0)^2. \quad (3.43)$$

and the equation of the characteristic hypersurface through the point $P$ with coordinates $(x_1^0, x_2^0, x_3^0, x_4^0)$ is

$$\phi(x_1, x_2, x_3, x_4) = \sum_{k=1}^{3} (x_k - x_k^0)^2 - \frac{1}{\mu \epsilon} (x_4 - x_4^0)^2 = 0. \quad (3.44)$$

This equation represents a four-dimensional hypercone with the vertex at the point $P$. In the general case where $\epsilon$ and $\mu$ are arbitrary functions of position the characteristic hypersurface will be a “distorted” hypercone whose behavior in the neighborhood of $P$ can be calculated numerically.

Based on Subsection (2.4.3), vectors $l$ are solutions of

$$l^T A = A^T l = 0. \quad (3.45)$$

Equation (3.45) gives the following relationships between the components of $l$:

$$l^1 = \frac{1}{\epsilon \phi_4} \left( - \phi_3 l^5 + \phi_2 l^6 \right) \quad (3.46)$$

$$l^2 = \frac{1}{\epsilon \phi_4} \left[ - \frac{\phi_3}{\phi_1} \left( \phi_2 l^5 + \phi_3 l^6 \right) - \phi_1 l^6 \right] \quad (3.47)$$

$$l^3 = \frac{1}{\epsilon \phi_4} \left[ \frac{\phi_2}{\phi_1} \left( \phi_2 l^5 + \phi_3 l^6 \right) + \phi_1 l^5 \right] \quad (3.48)$$

$$l^4 = - \frac{1}{\phi_1} \left( \phi_2 l^5 + \phi_3 l^6 \right) \quad (3.49)$$

The vector $n = (\phi_1, \phi_2, \phi_3, \phi_4)$ of partial derivatives of $\phi$ defines a normal vector of the hypersurface $\phi = 0$. There are infinitely many normal vectors at the vertex $P$ of the hypercone, all satisfying the characteristic condition (3.42). A particular
choice of $\mathbf{n}$ defines a particular tangential plane through the vertex $P$ and with (3.37) and (3.45) defines a particular interior operator $A$ on the hypersurface. Here we choose the following six linearly independent normal vectors (whose projections on the $x_1, x_2, x_3$-space are in the directions of the coordinate axes):

$$
\begin{align*}
\mathbf{n}_1 &= (-\sqrt{\mu/\epsilon}, 0, 0, 1/\epsilon) \\
\mathbf{n}_2 &= (+\sqrt{\mu/\epsilon}, 0, 0, 1/\epsilon) \\
\mathbf{n}_3 &= (0, -\sqrt{\mu/\epsilon}, 0, 1/\epsilon) \\
\mathbf{n}_4 &= (0, +\sqrt{\mu/\epsilon}, 0, 1/\epsilon) \\
\mathbf{n}_5 &= (0, 0, -\sqrt{\mu/\epsilon}, 1/\epsilon) \\
\mathbf{n}_6 &= (0, 0, +\sqrt{\mu/\epsilon}, 1/\epsilon)
\end{align*}
$$

Using (3.49) these normal vectors result in the following six $1$ vectors:

$$
\begin{align*}
\mathbf{l}_1 &= \begin{bmatrix} 0 \\ \eta t^6 \\ -\eta t^5 \\ 0 \\ t^5 \\ t^6 \end{bmatrix}, & \mathbf{l}_2 &= \begin{bmatrix} 0 \\ -\eta t^6 \\ -\eta t^5 \\ 0 \\ t^5 \\ t^6 \end{bmatrix}, & \mathbf{l}_3 &= \begin{bmatrix} -\eta t^6 \\ 0 \\ \eta t^4 \\ t^4 \\ t^5 \\ t^6 \end{bmatrix}, \\
\mathbf{l}_4 &= \begin{bmatrix} \eta t^6 \\ 0 \\ \eta t^5 \\ -\eta t^4 \\ -\eta t^4 \\ -\eta t^5 \end{bmatrix}, & \mathbf{l}_5 &= \begin{bmatrix} \eta t^4 \\ 0 \\ 0 \\ t^4 \\ t^5 \\ t^6 \end{bmatrix}, & \mathbf{l}_6 &= \begin{bmatrix} -\eta t^5 \\ 0 \\ 0 \\ -t^4 \\ -t^4 \\ 0 \end{bmatrix}
\end{align*}
$$

where $\eta = \sqrt{\mu/\epsilon}$. For more convenient notation we arrange these vectors into columns
of the matrix \( L \) as

\[
L = \begin{bmatrix}
0 & 0 & -\eta l^6 & \eta l^6 & \eta l^5 & -\eta l^5 \\
\eta l^5 & -\eta l^6 & 0 & 0 & -\eta l^4 & -\eta l^4 \\
-\eta l^5 & -\eta l^5 & \eta l^4 & \eta l^4 & 0 & 0 \\
0 & 0 & l^4 & -l^4 & l^4 & -l^4 \\
l^5 & -l^5 & 0 & 0 & l^5 & l^5 \\
l^5 & l^5 & l^5 & l^5 & 0 & 0
\end{bmatrix}. \tag{3.58}
\]

With the choice \( l^4 = l^5 = l^6 = 1 \) (3.58) becomes

\[
L = \begin{bmatrix}
0 & 0 & -\eta & \eta & \eta & -\eta \\
\eta & -\eta & 0 & 0 & -\eta & -\eta \\
-\eta & -\eta & \eta & \eta & 0 & 0 \\
0 & 0 & 1 & -1 & 1 & -1 \\
1 & -1 & 0 & 0 & 1 & 1 \\
1 & 1 & 1 & 1 & 0 & 0
\end{bmatrix}. \tag{3.59}
\]

Equation (3.37) then gives

\[
1_i^T L(u) = \Lambda_i(u) = 1_i^T \sum_{k=1}^{3} A_{ik} u_{x_k} + 1_i^T B u = 0, \tag{3.61}
\]

where \( i = 1, 2, \ldots, 6 \).
Substituting the six vectors $l_i$ from (3.59) into the above equations finally leads to the six independent equations

\[ \Lambda_1(u) = \eta u_1^6 + \eta u_2^5 - u_1^3 + u_2^2 - \eta u_3^4 - u_1^1 - \eta u_3^4 + u_1^1 + \eta \sigma(u^2 - u^3) = 0, \]  
\[ \Lambda_2(u) = -\eta u_1^6 + \eta u_2^5 + u_1^3 + u_2^2 - \eta u_3^4 + u_1^1 + \eta u_3^4 - u_1^1 + \eta \sigma(-u^2 - u^3) = 0, \]  
\[ \Lambda_3(u) = -\eta u_1^6 + u_2^2 + \eta u_2^1 - u_2^3 + \eta u_3^4 + u_1^1 - \eta u_3^4 - u_2^3 + \eta \sigma(-u^1 + u^3) = 0, \]  
\[ \Lambda_4(u) = -\eta u_1^6 + u_2^2 - \eta u_2^1 + \eta u_3^4 - u_2^3 - u_1^1 + \eta u_3^4 + u_2^3 + \eta \sigma(u^1 + u^3) = 0, \]  
\[ \Lambda_5(u) = -\eta u_1^6 - u_2^1 - \eta u_2^1 + \eta u_3^4 + \eta u_3^4 - u_2^3 + u_1^1 + \eta \sigma(u^1 - u^2) = 0, \]  
\[ \Lambda_6(u) = -\eta u_1^6 - u_2^1 + \eta u_2^1 - u_2^3 - \eta u_3^4 + \eta u_3^4 + u_2^3 + u_1^1 + \eta \sigma(-u^1 - u^2) = 0, \]

where all the $\Lambda_k (k = 1, 2, \ldots, 6)$ are interior operators on the characteristic hypersurface $\phi = 0$.

It is important to note that the functions $u = u(x_1, x_2, x_3)$ in the above equations are evaluated on a particular characteristic hypersurface $\phi = 0$ and, thus, are functions of $x_1, x_2, x_3$ only.

### 3.3 Numerical Solution

Equations (3.62)–(3.67) are the characteristic equations of (3.34) obtained for the six normal vectors (3.50)–(3.55). Each of these normal vectors defines a plane tangent to the characteristic hypersurface $\phi$ for which the corresponding operator in (3.62)–(3.67) is also an interior operator. For the case of two space variables this is illustrated in Fig. 3.1(a). A tangent plane touches the characteristic hypersurface along a line called bicharacteristic ray.

Using a first order approximation for the derivatives in (3.62)–bicharacteristic rays $\overline{PR_i}$ ($i = 1, \ldots, 6$) and evaluating the remaining tangential derivatives at the points $S_1, \ldots, S_6$ gives

\[ \Lambda_1(u) \approx \frac{1}{\Delta x_1} \left[ \eta(u_P^6 - u_{R_1}^6) + \eta(u_P^5 - u_{R_1}^5) - (u_P^3 - u_{R_1}^3) + (u_P^2 - u_{R_1}^2) \right] \]
Figure 3.1: Characteristic hypersurface for two space dimensions.
\[-(\eta u_{x_2}^4 - u_{x_2}^1 - \eta u_{x_3}^4 + u_{x_3}^1)s_1 + \eta \sigma (u^2 - u^3)p = 0,\]

\[\Lambda_2(u) \approx \frac{1}{-\Delta x_2} \left[ -(\eta(u_p^6 - u_{R_2}^6)) + \eta(u_p^5 - u_{R_2}^5) + (u_p^3 - u_{R_2}^3) + (u_p^2 - u_{R_2}^2) \right] \]

\[(-\eta u_{x_2}^4 - u_{x_2}^1 + \eta u_{x_3}^4 - u_{x_3}^1)s_2 + \eta \sigma (-u^2 - u^3)p = 0,\]

\[\Lambda_3(u) \approx (-\eta u_{x_1}^4 + u_{x_1}^2)s_3 + \frac{1}{-\Delta x_3} \left[ \eta(u_p^6 - u_{R_3}^6) + \eta(u_p^4 - u_{R_3}^4) + (u_p^3 - u_{R_3}^3) \right] \]

\[(-u_p^1 - u_{R_3}^1) - (u_{x_1}^4 + u_{x_3}^2)s_3 + \eta \sigma (-u^1 + u^3)p = 0,\]

\[\Lambda_4(u) \approx (-\eta u_{x_1}^5 + u_{x_1}^2)s_4 + \frac{1}{-\Delta x_4} \left[ -(\eta(u_p^6 - u_{R_4}^6)) + \eta(u_p^4 - u_{R_4}^4) - (u_p^3 - u_{R_4}^3) \right] \]

\[(-u_p^1 - u_{R_4}^1) + (u_{x_1}^5 + u_{x_3}^2)s_4 + \eta \sigma (u^1 - u^3)p = 0,\]

\[\Lambda_5(u) \approx (-\eta u_{x_1}^6 - u_{x_1}^3 - \eta u_{x_2}^6 + u_{x_2}^3)s_5 + \frac{1}{-\Delta x_5} \left[ \eta(u_p^5 - u_{R_5}^5) + \eta(u_p^4 - u_{R_5}^4) \right] \]

\[(-u_p^1 - u_{R_5}^1) + (u_{x_1}^6 - u_{x_3}^1)s_5 + \eta \sigma (u^1 - u^3)p = 0,\]

\[\Lambda_6(u) \approx (-\eta u_{x_1}^6 - u_{x_1}^3 + \eta u_{x_2}^6 - u_{x_2}^3)s_6 + \frac{1}{-\Delta x_6} \left[ -(\eta(u_p^5 - u_{R_6}^5)) + \eta(u_p^4 - u_{R_6}^4) \right] \]

\[+(u_p^1 - u_{R_6}^1) + \eta \sigma (-u^1 + u^3)p = 0. \quad (3.68)\]

The notation is illustrated in Fig. 3.1(b) for the case of two space dimensions. Here \(u_{R_i}^\nu\) denotes the values of \(u^\nu\) at the point \(R_i\). Similarly, the notation \((u_{x_i}^\nu)^R_i\) means \(u_{x_i}^\nu\) evaluated at \(R_i\). The values \(\Delta x_i\) are the distances from \(R_i\) to the projection of the point \(P\) on the \((x_1, x_2, x_3)\)-plane.

Substituting \(\Delta x_i = \Delta x\) in the above equations and solving for \(u_P\) gives

\[u_P = \frac{1}{4F} \left\{ u_{R_3}^4 + u_{R_4}^4 + u_{R_5}^4 + u_{R_6}^4 \right. \]
\[+ \Delta x((u_{x_1}^2)s_3 - (u_{x_1}^2)s_4 - (u_{x_2}^2)s_3 - (u_{x_3}^2)s_4) + u_{R_6}^2 - u_{R_5}^2 \]
\[+ u_{R_4}^3 - u_{R_3}^3 + \Delta x((u_{x_1}^3)s_5 - (u_{x_1}^3)s_6 - (u_{x_2}^3)s_5 - (u_{x_3}^3)s_6) \]
\[+ \eta \left[ -u_{R_5}^4 - u_{R_4}^4 + u_{R_5}^4 + u_{R_4}^4 \right. \]
\[- \Delta x((u_{x_1}^5)s_3 - (u_{x_1}^5)s_4 + (u_{x_2}^5)s_3 + (u_{x_3}^5)s_4) - (u_{R_6}^5 - u_{R_5}^5) \]
\[+ u_{R_4}^6 - u_{R_3}^6 - \Delta x((u_{x_1}^6)s_5 - (u_{x_1}^6)s_6 - (u_{x_2}^6)s_6 - (u_{x_3}^6)s_6) \left. \right\}, \quad (3.69)\]
\[ u_p^2 = \frac{1}{4F} \{ \Delta x((u_{x1}^1)s_1 - (u_{x2}^1)s_2 - (u_{x3}^1)s_3 - (u_{x3}^1)s_2) + u_{R_6}^1 - u_{R_6}^1 \\
+ u_{R_1}^2 + u_{R_2}^2 + u_{R_5}^2 + u_{R_6}^2 \\
+ u_{R_2}^3 - u_{R_1}^3 + \Delta x(-(u_{x1}^3)s_5 - (u_{x1}^3)s_6 + (u_{x2}^3)s_5 - (u_{x2}^3)s_6) \\
+ \eta \left[ -\Delta x((u_{x1}^4)s_2 - (u_{x2}^4)s_1 - (u_{x3}^4)s_2 - (u_{x3}^4)s_1) + u_{R_6}^4 - u_{R_5}^4 \\
+ u_{R_1} + u_{R_2} - u_{R_5} - u_{R_6} \\
- (u_{R_2}^6 - u_{R_1}^6) - \Delta x((u_{x1}^6)s_6 + (u_{x1}^6)s_5 - (u_{x2}^6)s_6 + (u_{x2}^6)s_5) \right] \} \right\}, \tag{3.70} \]

\[ u_p^3 = \frac{1}{4F} \{ \Delta x(-(u_{x1}^3)s_1 - (u_{x2}^3)s_2 + (u_{x3}^3)s_3 - (u_{x3}^3)s_2) + u_{R_4}^3 - u_{R_3}^1 \\
+ u_{R_2}^3 - u_{R_1}^3 + \Delta x(-(u_{x1}^3)s_3 - (u_{x1}^3)s_4 + (u_{x2}^3)s_3 - (u_{x2}^3)s_4) \\
+ \eta \left[ -\Delta x((u_{x1}^4)s_2 + (u_{x2}^4)s_1 + (u_{x3}^4)s_2 + (u_{x3}^4)s_1) - (u_{R_4}^4 - u_{R_3}^4) \\
+ u_{R_2}^5 - u_{R_1}^5 - \Delta x(-(u_{x1}^5)s_3 - (u_{x1}^5)s_4 - (u_{x2}^5)s_3 - (u_{x2}^5)s_4) \\
- u_{R_1}^6 - u_{R_2}^6 + u_{R_3}^6 + u_{R_4}^6 \right] \} \right\}, \tag{3.71} \]

\[ u_p^4 = \frac{1}{4\eta} \left\{ -(u_{R_3}^1 - u_{R_4}^3 + u_{R_5}^1 + u_{R_4}^1) \\
- \Delta x((u_{x1}^2)s_3 - (u_{x1}^2)s_4 - (u_{x3}^2)s_3 - (u_{x3}^2)s_4) + u_{R_6}^2 - u_{R_5}^2 \\
- (u_{R_4}^3 - u_{R_3}^3) + \Delta x((u_{x1}^3)s_5 - (u_{x1}^3)s_6 - (u_{x2}^3)s_5 - (u_{x2}^3)s_6) \\
+ \eta \left[ u_{R_3}^4 + u_{R_4}^4 + u_{R_5}^4 + u_{R_6}^4 + \right] \\
+ \Delta x((u_{x1}^5)s_3 - (u_{x1}^5)s_4 + (u_{x3}^5)s_3 + (u_{x3}^5)s_4) - (u_{R_6}^5 - u_{R_5}^5) \\
- (u_{R_4}^6 - u_{R_3}^6) + \Delta x((u_{x1}^6)s_5 + (u_{x1}^6)s_6 + (u_{x2}^6)s_5 + (u_{x2}^6)s_6) \right\} \right\}, \tag{3.72} \]

\[ u_p^5 = \frac{1}{4\eta} \left\{ \Delta x((u_{x1}^1)s_1 - (u_{x2}^1)s_2 - (u_{x3}^1)s_3 - (u_{x3}^1)s_2) - (u_{R_6}^1 - u_{R_5}^1) \\
+ u_{R_1}^2 + u_{R_2}^2 - u_{R_5}^2 - u_{R_6}^2 \\
+ u_{R_2}^3 - u_{R_1}^3 - \Delta x(-(u_{x1}^3)s_5 - (u_{x1}^3)s_6 + (u_{x2}^3)s_5 - (u_{x2}^3)s_6) \\
+ \eta \left[ +\Delta x((u_{x2}^4)s_1 - (u_{x2}^4)s_2 + (u_{x3}^4)s_1 + (u_{x3}^4)s_2) - (u_{R_4}^4 - u_{R_5}^4) \\
+ u_{R_1} + u_{R_2} + u_{R_5} + u_{R_6} \\
- (u_{R_2}^6 - u_{R_1}^6) + \Delta x((u_{x1}^6)s_5 + (u_{x1}^6)s_6 + (u_{x2}^6)s_5 - (u_{x2}^6)s_6) \right\} \right\}, \tag{3.73} \]
\[ u_p^6 = \frac{1}{4\eta} \left\{ \Delta x((u_{x_1}^6)_i + (u_{x_2}^6)_i - (u_{x_3}^6)_i + (u_{x_3}^1)_i + u_{R_4}^1 - u_{R_3}^1 \right. \\
- (u_{R_2}^1 - u_{R_1}^1) + \Delta x(-(u_{x_2}^6)_i + (u_{x_2}^1)_i) + (u_{x_3}^6)_i + (u_{x_3}^1)_i \right. \\
- u_{R_1}^3 - u_{R_2}^3 + u_{R_3}^3 + u_{R_4}^3 \\
+ \eta \left[ + \Delta x((u_{x_2}^4)_i + (u_{x_2}^1)_i + (u_{x_3}^4)_i - (u_{x_2}^4)_i - (u_{R_4}^4 - u_{R_3}^4) \\
- (u_{R_2}^4 - u_{R_1}^4) + \Delta x((u_{x_1}^6)_i + (u_{x_1}^1)_i + u_{x_3}^6)_i - (u_{x_3}^6)_i \right. \\
+ u_{R_1}^6 + u_{R_2}^6 + u_{R_3}^6 + u_{R_4}^6 \right\}, \tag{3.74} \] 

where \( F = 1 + \eta \sigma \Delta x. \)

So far the discretization was performed in the directions of the bicharacteristic rays on the characteristic hypersurfaces. The remaining tangential derivatives at the points \( S_1, \ldots, S_6 \) still need to be discretized. We do this by calculating these derivatives using a method following Richtmyer [16]. The scheme is described below.

Using the grid of Fig. 3.2 and the notation \( U^p_j = u(j_1\Delta x, j_2\Delta x, j_3\Delta x, n\Delta t) \), we define the operators \( \nu \) and \( \delta_p \) by

\[ \nu U^p_j = \frac{1}{8} \sum_{i \in \Omega} U^p_i \quad \Omega = \{ i : |i_k - j_k| = 1/2, \quad k = 1, 2, 3 \}, \tag{3.75} \]

and

\[ \delta_p U^p_j = \frac{1}{4} \left( \sum_{i \in \Omega_1} U^p_i - \sum_{i \in \Omega_2} U^p_i \right), \tag{3.76} \]

\[ \Omega_1 = \{ i : |i_k - j_k| = 1/2, \quad k = 1, 2, 3; \quad k \neq p; \quad i_p = j_p + \frac{1}{2} \}, \tag{3.77} \]

\[ \Omega_2 = \{ i : |i_k - j_k| = 1/2, \quad k = 1, 2, 3; \quad k \neq p; \quad i_p = j_p - \frac{1}{2} \}, \tag{3.78} \]

where \( i = (i_1, i_2, i_3) \), \( j = (j_1, j_2, j_3) \) and \( e_k \) is a unit vector in three dimensional space with the \( k \)th entry unity.

Now we discretize (3.34) as

\[ \frac{1}{\Delta x} \left( \sum_{p=1}^{3} A_p \delta_p U^p_j \right) + \frac{1}{\Delta t/2} A_4 (U^{p+1/2}_j - \nu U^p_j) + B U^{p+1/2}_j = 0, \tag{3.79} \]

which gives

\[ U^{p+1/2}_j = \left( I + \frac{\Delta t}{2} A_4^{-1} B \right)^{-1} \left[ \nu U^p_j - \frac{1}{2} A_4^{-1} \left( \sum_{p=1}^{3} \frac{\Delta t}{\Delta x} A_p \delta_p U^p_j \right) \right] \tag{3.80} \]
Figure 3.2: Grid nodes and notation on the hypersurface for two space dimensions.
where \( I \) is the identity matrix. The above equation is used for the calculation of \( U_j^{n+1/2} \). The partial derivatives at \((j + \Delta d_r, n + 1/2)\) (points \( S_i \) in Fig. 3.2 or Fig. 3.3) are then calculated from these \( U \) values. To do this we define another difference operator \( \delta_{p,r,d} \) with

\[
\delta_{p,r,d} U_j^n = \frac{1}{2} \left( \sum_{i \in \Omega_1} U_i^n - \sum_{i \in \Omega_2} U_i^n \right), \quad p \neq r. \tag{3.81}
\]

\[
\Omega_1 = \{ i : |i_k - j_k| = 1/2, k = 1, 2, 3; k \neq p; k \neq r; i_p = j_p + \frac{1}{2}, i_r = j_r + d \}, \tag{3.82}
\]

\[
\Omega_2 = \{ i : |i_k - j_k| = 1/2, k = 1, 2, 3; k \neq p; k \neq r; i_p = j_p - \frac{1}{2}, i_r = j_r + d \}, \tag{3.83}
\]

where \( p, r = 1, 2, 3 \) and \( d = -1/2, 1/2 \). The above operator defines numerical differentiation in the \( x_p \) direction at the point which is displaced from \( j \) by \( d \) in the \( x_r \) direction. The six possible \((r,d)\) pairs correspond to the points \( S_i \) \((i = 1, \ldots, 6)\) in Fig. 3.3.

The tangential partial derivatives at the points \( S_i \) are then calculated as

\[
(u_{x_p})_{j+\Delta d_r}^{n+1/2} = \delta_{p,r,d} U_j^{n+1/2} \tag{3.84}
\]

where \((p, r = 1, 2, 3), r \neq p, d = -1/2, 1/2 \).

But \( \Delta t \) and \( \Delta x \) are related by the equation of the hypersurface (3.44) which implies \( \Delta t = \sqrt{\mu \epsilon \Delta x} \). Using this relation in (3.80) together with the matrices \( A_k \) as given by (3.28)–(3.30) results in the following equations for the components of \( U_j^{n+1/2} \):

\[
U_j^{1,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x/2} \left[ \nu U_j^{1,n} + \frac{\eta}{2} \left( \delta_3 U_j^{5,n} - \delta_3 U_j^{5,n} \right) \right], \tag{3.85}
\]

\[
U_j^{2,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x/2} \left[ \nu U_j^{2,n} + \frac{\eta}{2} \left( \delta_3 U_j^{4,n} - \delta_3 U_j^{4,n} \right) \right], \tag{3.86}
\]

\[
U_j^{3,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x/2} \left[ \nu U_j^{3,n} + \frac{\eta}{2} \left( \delta_3 U_j^{5,n} - \delta_3 U_j^{5,n} \right) \right], \tag{3.87}
\]

\[
U_j^{4,n+1/2} = \nu U_j^{4,n} + \frac{1}{2\eta} (\delta_3 U_j^{2,n} - \delta_2 U_j^{3,n}), \tag{3.88}
\]

\[
U_j^{5,n+1/2} = \nu U_j^{5,n} + \frac{1}{2\eta} (\delta_1 U_j^{3,n} - \delta_3 U_j^{1,n}), \tag{3.89}
\]

\[
U_j^{6,n+1/2} = \nu U_j^{6,n} + \frac{1}{2\eta} (\delta_2 U_j^{3,n} - \delta_1 U_j^{2,n}). \tag{3.90}
\]
Figure 3.3: Basic cell for field calculations in three dimensions.
The basic grid cell for this two-step algorithm is shown in Fig. 3.3.

In summary, for a point $P$ within the domain $D$ at the time step $n + 1$ the numerical procedure is as follows:

1. Use equations (3.85)–(3.90) to calculate the values $U_{j}^{n+1/2}$ from the known values $U_{i}^{n}$.
2. Use (3.84) to calculate the tangential partial derivatives at the points $S_{i}$ ($i = 1, \ldots, 6$).
3. Use (3.69)–(3.74) to calculate the field components at the point $P$.

For nodes which are on boundaries between two different media equations (3.62)–(3.67) need to be discretized taking into account the discontinuity in the characteristic hypersurface at the region interface. This is done by solving equations (3.68) with $\Delta x_{1}, \ldots, \Delta x_{6}$ corresponding to the different media. The spacing between the nodes (grid size) changes from region to region according to $\Delta t = \sqrt{\mu c\Delta x}$. Since the points $R_{i}$ of the boundary nodes will not fall onto the nodes of the neighboring grid, field values in neighboring region need to be obtained by interpolation (Fig. 3.4).

![Figure 3.4: Field calculation at boundary between two different regions.](image-url)
3.4 Boundary Conditions

The boundary conditions for our problem are prescribed by the two equations (3.33) relating the electric and magnetic field components at any time. Written in terms of the \( u \) vector components these equations are

\[
\begin{align*}
    f_1(u^1, u^2, u^3, u^4, u^5, u^6) &= 0, \\
    f_2(u^1, u^2, u^3, u^4, u^5, u^6) &= 0 \quad (x_1, x_2, x_3) \in \partial D,
\end{align*}
\]

where \( f_1 \) and \( f_2 \) are known functions. In typical applications these equations represent either known excitations or absorbing boundary conditions. The excitations are usually given in the form of prescribed tangential components of the electric or magnetic fields as functions of time boundary conditions can be described by specifying the ratio of the two pairs of electric and magnetic field components (e.g., \( E_y/H_z = \eta_e \), \( E_x/H_y = -\eta_e \) for a boundary whose normal is in the direction [and orientation] of the \( x \)-axis, where \( \eta_e \) is the characteristic impedance of external dielectric medium.) Translating these statements into our notation implies that (for our application) the BCs have the linear form

\[
\begin{align*}
    a_{11}u^1 + a_{12}u^2 + \ldots + a_{16}u^6 &= b_1(t), \\
    a_{21}u^1 + a_{22}u^2 + \ldots + a_{26}u^6 &= b_2(t), \quad (x_1, x_2, x_3) \in \partial D,
\end{align*}
\]

where the coefficients next to the two normal components of the fields are zero.

Equations (3.93) represent a system of two equations with four unknowns. In order to calculate the fields at a boundary point \( P \), these equations need to be used together with two other equations relating the tangential field components in the neighborhood of \( P \). These additional equations can be derived from (3.61) with a suitable choice of \( \lambda \) vectors.

For a bicharacteristic ray \( PR_i \) equation (3.61) defines an interior operator on a characteristic hypersurface through \( P \) (Figure 3.5). Equations (3.56)–(3.57) show that there are two degrees of freedom in the choice of a vector \( \lambda \), i.e., there are two
linearly independent \( l \) vectors for a given bicharacteristic ray passing through \( P \). We can use these two linearly independent \( l \) vectors in (3.61) to obtain two independent characteristic equations for the tangential field components in the neighborhood of \( P \).

![Diagram of field calculation for structure boundary points.](image)

**Figure 3.5:** Field calculation for structure boundary points.

For the \( l \) vectors of the bicharacteristic rays \( \overline{PR}_i (i = 1, \ldots, 6) \) we choose

\[
\begin{align*}
    l_{11} &= \begin{bmatrix} 0 \\ \eta \\ 0 \\ 0 \\ 1 \end{bmatrix}, \\
    l_{12} &= \begin{bmatrix} 0 \\ \eta \\ 0 \\ 0 \\ 0 \end{bmatrix}, \\
    l_{21} &= \begin{bmatrix} 0 \\ -\eta \\ 0 \\ 0 \\ 1 \end{bmatrix}, \\
    l_{22} &= \begin{bmatrix} 0 \\ -\eta \\ 0 \\ 0 \\ -1 \end{bmatrix},
\end{align*}
\]

(3.94)
where the first index indicates the bicharacteristic ray \((i = 1, \ldots, 6)\) and the second index \((j = 1, 2)\) indicates the two choices of 1 on this ray. Substituting these vectors into (3.61) leads to the twelve operators

\[
\begin{align*}
\Lambda_{11} &= u_{x_1}^2 + \eta u_{x_1}^6 - u_{x_2}^1 - \eta u_{x_3}^4 + \eta \sigma u^2 = 0, \\
\Lambda_{12} &= -u_{x_1}^3 + \eta u_{x_1}^5 + u_{x_3}^1 - \eta u_{x_2}^4 - \eta \sigma u^3 = 0, \\
\Lambda_{21} &= u_{x_1}^2 - \eta u_{x_1}^6 - u_{x_2}^1 + \eta u_{x_3}^4 - \eta \sigma u^2 = 0, \\
\Lambda_{22} &= -u_{x_1}^3 - \eta u_{x_1}^5 - u_{x_3}^1 + \eta u_{x_2}^4 + \eta \sigma u^3 = 0, \\
\Lambda_{31} &= u_{x_1}^2 + \eta u_{x_2}^6 - u_{x_2}^1 - \eta u_{x_3}^5 - \eta \sigma u^1 = 0, \\
\Lambda_{32} &= -\eta u_{x_1}^5 + \eta u_{x_2}^4 + u_{x_2}^3 - \eta u_{x_3}^2 + \eta \sigma u^3 = 0, \\
\Lambda_{41} &= u_{x_1}^2 - \eta u_{x_2}^6 - u_{x_2}^1 + \eta u_{x_3}^5 + \eta \sigma u^1 = 0, \\
\Lambda_{42} &= \eta u_{x_1}^5 - \eta u_{x_2}^4 + u_{x_2}^3 - \eta u_{x_3}^2 - \eta \sigma u^3 = 0, \\
\Lambda_{51} &= -u_{x_1}^3 - \eta u_{x_2}^6 + u_{x_3}^1 + \eta u_{x_3}^5 + \eta \sigma u^1 = 0, \\
\Lambda_{52} &= u_{x_2}^3 - \eta u_{x_1}^5 - u_{x_3}^2 + \eta u_{x_3}^4 - \eta \sigma u^2 = 0, \\
\Lambda_{61} &= -u_{x_1}^3 + \eta u_{x_2}^6 + u_{x_3}^1 - \eta u_{x_3}^5 - \eta \sigma u^1 = 0,
\end{align*}
\]
\[ \Lambda_{\varepsilon_2} = u_{x_2}^3 + \eta u_{x_1}^6 - u_{x_3}^2 - \eta u_{x_2}^4 + \eta \sigma u^2 = 0. \]  

(3.108)

The tangential fields components at a boundary point \( P \) are now determined by the two boundary conditions (3.93) and two of the above equations (e.g., for a boundary whose normal is in the direction and orientation of the \( x_1 \)-axis, the bicharacteristic ray \( \overline{PR_i} \) is inside the structure and, therefore, the first two equations determine the fields).

Discretizing the above equations along their corresponding bicharacteristic rays gives

\[
(1 + \Delta \varepsilon \eta x) u_P^2 + \eta u_P^6 = u_R^2 + \eta u_R^6 + \Delta x (u_{x_2}^1 + \eta u_{x_2}^4), \]  

(3.109)

\[
-(1 + \Delta \varepsilon \eta x) u_P^3 + \eta u_P^5 = -u_R^3 + \eta u_R^5 + \Delta x (-u_{x_2}^1 + \eta u_{x_2}^4), \]  

(3.110)

\[
(1 + \Delta \varepsilon \eta x) u_P^2 - \eta u_P^6 = u_R^2 - \eta u_R^6 - \Delta x (u_{x_2}^1 - \eta u_{x_2}^4), \]  

(3.111)

\[
-(1 + \Delta \varepsilon \eta x) u_P^3 - \eta u_P^5 = -u_R^3 - \eta u_R^5 - \Delta x (-u_{x_2}^1 - \eta u_{x_2}^4), \]  

(3.112)

\[
-(1 + \Delta \varepsilon \eta x) u_P^1 + \eta u_P^6 = -u_R^1 + \eta u_R^6 + \Delta x (-u_{x_2}^1 + \eta u_{x_2}^5), \]  

(3.113)

\[
(1 + \Delta \varepsilon \eta x) u_P^3 + \eta u_P^4 = u_R^3 + \eta u_R^4 + \Delta x (u_{x_3}^2 + \eta u_{x_3}^6), \]  

(3.114)

\[
-(1 + \Delta \varepsilon \eta x) u_P^1 - \eta u_P^6 = -u_R^1 - \eta u_R^6 - \Delta x (-u_{x_2}^1 - \eta u_{x_2}^5), \]  

(3.115)

\[
(1 + \Delta \varepsilon \eta x) u_P^3 - \eta u_P^4 = u_R^3 - \eta u_R^4 - \Delta x (u_{x_3}^2 - \eta u_{x_3}^6), \]  

(3.116)

\[
(1 + \Delta \varepsilon \eta x) u_P^1 + \eta u_P^5 = u_R^1 + \eta u_R^5 + \Delta x (u_{x_2}^1 + \eta u_{x_2}^6), \]  

(3.117)

\[
-(1 + \Delta \varepsilon \eta x) u_P^2 + \eta u_P^4 = -u_R^2 + \eta u_R^4 + \Delta x (-u_{x_2}^3 + \eta u_{x_2}^6), \]  

(3.118)

\[
(1 + \Delta \varepsilon \eta x) u_P^1 - \eta u_P^5 = u_R^1 - \eta u_R^5 - \Delta x (u_{x_2}^1 - \eta u_{x_2}^6), \]  

(3.119)

\[
-(1 + \Delta \varepsilon \eta x) u_P^2 - \eta u_P^4 = -u_R^2 - \eta u_R^4 - \Delta x (-u_{x_2}^3 - \eta u_{x_2}^6). \]  

(3.120)

For every boundary point two of the above equations are used together with the boundary conditions (3.93) to calculate the tangential field components. The remaining two normal components are then calculated from discretized versions of the appropriate two equations in (3.21)-(3.26). The method is described below for
a point which is on a boundary whose normal is in the direction of the $x_1$-axis, as shown in Fig. 3.5.

For the point $P$ shown in Fig. 3.5 equations (3.109) and (3.110) are used. First the values $U_j^{n+1/2}$ are calculated for four points inside the structure using (3.85)–$u_{x_2}^1$, $u_{x_3}^1$, $u_{x_2}^4$, and $u_{x_3}^4$ are then calculated at the point $S_1$ from

$$(u_{x_p})_{j+de_r}^{n+1/2} = \delta_{p,r,d} U_j^{n+1/2},$$

(3.121)

where $p = 2, 3, r = 1$, and $d = -1/2$ and $\delta_{p,r,d}$ is the finite difference operator defined by (3.81). After these calculations the right hand sides of equations (3.109) and (3.110) are known and these equations are used together with the boundary conditions at the point $P$

$$a_{12} u_p^2 + a_{13} u_p^3 + a_{15} u_p^5 + a_{16} u_p^6 = b_1^p(t),$$

$$a_{22} u_p^2 + a_{23} u_p^3 + a_{25} u_p^5 + a_{26} u_p^6 = b_2^p(t),$$

(3.122)

to solve for $u_p^2$, $u_p^3$, $u_p^5$, and $u_p^6$.

The above procedure is used to calculate the tangential derivatives at nearby boundary points at the time step $n + 1$ from the values at the previous time step $n$. The remaining two normal field components $u_1$ and $u_4$ are calculated in the following way.

Equations (3.21)–(3.26) are discretized in the form

$$U_j^{1,n+1} = \frac{1}{1 + \eta\sigma\Delta x} \left[ U_j^{1,n} + \frac{\eta}{2} (\delta_3 U_j^{6,n+1} - \delta_2 U_j^{5,n+1}) \right],$$

(3.123)

$$U_j^{2,n+1} = \frac{1}{1 + \eta\sigma\Delta x} \left[ U_j^{2,n} + \frac{\eta}{2} (\delta_3 U_j^{4,n+1} - \delta_1 U_j^{6,n+1}) \right],$$

(3.124)

$$U_j^{3,n+1} = \frac{1}{1 + \eta\sigma\Delta x} \left[ U_j^{3,n} + \frac{\eta}{2} (\delta_1 U_j^{5,n+1} - \delta_2 U_j^{4,n+1}) \right],$$

(3.125)

$$U_j^{4,n+1} = U_j^{4,n} + \frac{1}{2\eta} (\delta_3 U_j^{2,n+1} - \delta_2 U_j^{3,n+1}),$$

(3.126)

$$U_j^{5,n+1} = U_j^{5,n} + \frac{1}{2\eta} (\delta_1 U_j^{3,n+1} - \delta_2 U_j^{1,n+1}),$$

(3.127)

$$U_j^{6,n+1} = U_j^{6,n} + \frac{1}{2\eta} (\delta_2 U_j^{1,n+1} - \delta_1 U_j^{2,n+1}),$$

(3.128)
where \( \delta^0_{p}U_{j}^{i,n} = U_{j+e_p}^{i,n} - U_{j-e_p}^{i,n} \).

Equations (3.123) and (3.123) are then used to calculate the remaining two field components \( u_1 \) and \( u_4 \).

Points on other boundaries are treated in a similar manner.

### 3.5 Richtmyer’s Modified Finite Difference Scheme

As was mentioned in the introductory chapter, a large number of finite difference schemes for solving hyperbolic systems of linear equations in three space variables exist in the mathematical literature. One of these methods is often referred to as the Modified Richtmyer Scheme [16]. For two dimensional field problems this method has been implemented in [17]. Here we apply the modified Richtmyer scheme to Maxwell’s equations in three space dimensions. The method is used in the examples of the next chapter for result verification.

Using the difference notation of previous sections for our model equation

\[
L(u) = \sum_{k=1}^{4} A_k u_{x_k} + Bu = 0, \tag{3.129}
\]

this scheme can be written as

\[
U_{j}^{n+1/2} = \left( I + \frac{\Delta t}{2} A_4^{-1} B \right)^{-1} \left[ \nu U_{j}^{n} - \frac{1}{2} A_4^{-1} \left( \sum_{p=1}^{3} \frac{\Delta t}{\Delta x} A_p \delta_p U_{j}^{n} \right) \right], \tag{3.130}
\]

\[
U_{j}^{n+1} = \left( I + \frac{\Delta t}{2} A_4^{-1} B \right)^{-1} \left[ U_{j}^{n} - A_4^{-1} \left( \sum_{p=1}^{3} \frac{\Delta t}{\Delta x} A_p \delta_p U_{j}^{n+1/2} \right) \right], \tag{3.131}
\]

where the operators \( \nu \) and \( \delta_p \) are defined by equations (3.75) and (3.76), respectively.

The stability condition for Richtmyer’s method is given by the equation

\[
\Delta t \leq \sqrt{\mu \varepsilon \Delta x}. \tag{3.132}
\]

Substituting the matrices \( A_k \) and \( B \) from (3.28)–(3.30) and using the maximal time step \( \Delta t = \sqrt{\mu \varepsilon \Delta x} \) into (3.130)–(3.131) gives the two step algorithm

\[
U_{j}^{1,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x} \left[ \nu U_{j}^{1,n} + \frac{\eta}{2} \left( \delta_2 U_{j}^{5,n} - \delta_3 U_{j}^{5,n} \right) \right], \tag{3.133}
\]
\[ U_j^{2,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x} \left[ \nu U_j^{2,n} + \frac{\eta}{2} \left( \delta_3 U_j^{4,n} - \delta_1 U_j^{5,n} \right) \right], \quad (3.134) \]

\[ U_j^{3,n+1/2} = \frac{1}{1 + \eta \sigma \Delta x} \left[ \nu U_j^{3,n} + \frac{\eta}{2} \left( \delta_1 U_j^{5,n} - \delta_2 U_j^{4,n} \right) \right], \quad (3.135) \]

\[ U_j^{4,n+1/2} = \nu U_j^{4,n} + \frac{1}{2\eta} \left( \delta_3 U_j^{2,n} - \delta_2 U_j^{3,n} \right), \quad (3.136) \]

\[ U_j^{5,n+1/2} = \nu U_j^{5,n} + \frac{1}{2\eta} \left( \delta_1 U_j^{3,n} - \delta_3 U_j^{1,n} \right), \quad (3.137) \]

\[ U_j^{6,n+1/2} = \nu U_j^{6,n} + \frac{1}{2\eta} \left( \delta_2 U_j^{1,n} - \delta_1 U_j^{2,n} \right), \quad (3.138) \]

\[ U_j^{1,n+1} = \frac{1}{1 + \eta \sigma \Delta x} \left[ U_j^{1,n} + \frac{\eta}{2} \left( \delta_2 U_j^{5,n+1/2} - \delta_3 U_j^{5,n+1/2} \right) \right], \quad (3.139) \]

\[ U_j^{2,n+1} = \frac{1}{1 + \eta \sigma \Delta x} \left[ U_j^{2,n} + \frac{\eta}{2} \left( \delta_3 U_j^{4,n+1/2} - \delta_1 U_j^{4,n+1/2} \right) \right], \quad (3.140) \]

\[ U_j^{3,n+1} = \frac{1}{1 + \eta \sigma \Delta x} \left[ U_j^{3,n} + \frac{\eta}{2} \left( \delta_1 U_j^{5,n+1/2} - \delta_2 U_j^{4,n+1/2} \right) \right], \quad (3.141) \]

\[ U_j^{4,n+1} = U_j^{4,n} + \frac{1}{2\eta} \left( \delta_3 U_j^{2,n+1/2} - \delta_2 U_j^{3,n+1/2} \right), \quad (3.142) \]

\[ U_j^{5,n+1} = U_j^{5,n} + \frac{1}{2\eta} \left( \delta_1 U_j^{3,n+1/2} - \delta_3 U_j^{1,n+1/2} \right), \quad (3.143) \]

\[ U_j^{6,n+1} = U_j^{6,n} + \frac{1}{2\eta} \left( \delta_2 U_j^{1,n+1/2} - \delta_1 U_j^{2,n+1/2} \right), \quad (3.144) \]

where \( U_j^{i,m} \) stands for the \( i \)-th component of the vector \( U_j^m \).
In this chapter the method developed in the previous chapter is applied to a few interconnect structures using unit step or Gaussian excitations. For each example the method is compared with Richtmyer's modified finite difference scheme described in Section 3.5.

The first example presents a simple microstrip structure. Half of the structure is shown in Fig. 4.1. The signal conductor is 0.6 mm wide and 50 μm thick with a conductivity of 10⁷ S/m. We choose a symmetric excitation for the structure located on the x = 0 boundary. Because of the symmetry, only one half of the structure is analyzed, with the symmetry plane at y = b = 1 mm modeled by magnetic wall boundary conditions (Hx = 0, Hz = 0 on this boundary). The structure is excited along the x = 0 boundary with the z-component of the electric field uniformly distributed underneath the strip and the time variation described by a narrow Gaussian pulse. The boundary conditions on this plane are given by

\[
E_y(0, y, z, t) = 0,
\]
\[
E_z(0, y, z, t) = \begin{cases} 
  e^{-(t-t_0)^2/(2T^2)}, & 1 - w/2 \leq y \leq b, \quad 0 \leq z \leq h, \\
  0, & \text{otherwise},
\end{cases}
\]

where \( t_0 = 3.75 \text{ ps} \) is the pulse delay, \( T_\sigma = 1.5 \text{ ps} \) is the pulse width parameter, \( b = 1 \text{ mm} \) is the width of the structure, \( h = 0.635 \text{ mm} \) is the height of the strip above the ground plane and \( w/2 = 0.3 \text{ mm} \) is the half-width of the strip. The ground plane is modeled by a perfectly conducting wall described by \( E_x = 0, E_y = 0 \). The
remaining boundaries are modeled as absorbing walls obtained by requiring that the ratio of the orthogonal electric and magnetic field components be equal to the wave impedance of the neighboring medium. For example the boundary conditions on the \( y = 0 \) plane are described by

\[
\frac{E_x}{H_y} = \begin{cases} 
\eta, & 0 \leq x \leq a, \ 0 \leq z \leq h, \\
\eta_0, & 0 \leq x \leq a, \ h \leq z \leq c,
\end{cases}
\]

\[
\frac{E_y}{-H_z} = \begin{cases} 
\eta, & 0 \leq x \leq a, \ 0 \leq z \leq h, \\
\eta_0, & 0 \leq x \leq a, \ h \leq z \leq c,
\end{cases}
\]

where \( a = 2 \text{mm} \) is the length of the structure, \( c = 1.5 \text{mm} \) is the structure height, \( \eta_0 = \sqrt{\mu_0/\epsilon_0 \epsilon_r} = 120.34 \Omega \) is the wave impedance of the dielectric substrate and \( \eta_0 = \sqrt{\mu_0/\epsilon_0} = 376.73 \Omega \) is the wave impedance of free space air above the substrate). The remaining absorbing boundaries are modeled in a similar manner.

The resulting space distributions of the \( z \)-component of the electric field on the \( z = 0.5 \text{mm} \) plane at two different times \( t_1 = 4 \text{ps} \) and \( t_2 = 8 \text{ps} \) are shown in
Figures 4.2 and 4.3.

The same structure is analyzed using the modified Richtmyer algorithm. The spatial distribution of $E_z$ in the same plane is shown in Figures 4.4 and 4.5.

Finally, the time responses obtained by the two methods are compared Fig. 4.6. The responses are plotted for two points under the signal trace located at (0.4, 0.8, 0.5) mm and (1.2, 0.8, 0.5) mm.

In the second example we analyze a microstrip bend discontinuity. Figure 4.7 shows a 90° microstrip bend structure along with the dimensions and the substrate dielectric constant. The thickness of the signal conductor is 50 μm and the conductivity is $10^7$ S/m. In this example there is no symmetry plane so the whole structure needs to be analyzed. The structure is first excited with a unit step input. The excitation is located on the $x = 0$ plane in the form of a uniformly distributed $z$-component of the electric field in the region under the strip. The boundary conditions for this plane
Figure 4.3: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.

Figure 4.4: Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme.
Figure 4.5: Distribution of $E_z$ at $t = t_2$ obtained by the Richtmyer scheme.

Figure 4.6: Time variation of $E_z$. 

are given by

\[ E_y(0, y, z, t) = 0, \]

\[ E_z(0, y, z, t) = \begin{cases} 
U(t), & y_1 \leq y \leq y_2, \ 0 \leq z \leq h, \\
0, & \text{otherwise},
\end{cases} \]

where \( U(t) \) is a unit step function, \( y_1 = 0.15 \text{ mm} \) and \( y_2 = 0.35 \text{ mm} \) are the locations of the strip edges, and \( h = 0.635 \text{ mm} \) is the height of the dielectric substrate. The remaining boundaries are modeled as absorbing walls, as described in the previous example.

The response obtained by the method of characteristics is shown in Figures 4.8–4.10 in the form of the space distribution of the z-component of the electric field under the strip for three different times, \( t_1 = 2 \text{ ps} \), \( t_2 = 4 \text{ ps} \) and \( t_3 = 6 \text{ ps} \). The output is taken on the plane \( z = 0.2 \text{ mm} \). In Figure 4.8 the unit step waveform is propagating towards the bend. It is seen that the amplitude of the electric field is greater near the edges of the strip than at the strip center. Figure 4.9 is a snapshot at the moment...
when the wavefront is at the edge of the first strip. Finally, in Figure 4.10 one can see how the wave propagating in the $x$-direction is rapidly dampened as it continues through the part of substrate where the strip is not present. The wavefront in this figure has just reached the end of the structure.

![Graphical representation](image)

Figure 4.8: Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics.

The step response of the same structure obtained by the modified Richtmyer scheme is shown in Figures 4.11–4.12. Oscillatory behavior near the boundaries where the field distribution has a discontinuity is easily visible. The oscillations, however, are rapidly dampened as one moves away from the boundary.

The same bend structure is next excited by a Gaussian excitation on the $x = 0$ plane given by

$$
E_y(0, y, z, t) = 0,
$$

$$
E_z(0, y, z, t) = \begin{cases} 
    e^{-\frac{(t-t_0)^2}{(2T_0^2)}}, & y_1 \leq y \leq y_2, 0 \leq z \leq h, \\
    0, & \text{otherwise}, 
\end{cases}
$$

where $t_0 = 1.6\,\text{ps}$ and $T_\sigma = 0.67\,\text{ps}$. The space distribution of the response on the
Figure 4.9: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.

Figure 4.10: Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics.
Figure 4.11: Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme.

Figure 4.12: Distribution of $E_z$ at $t = t_2$ obtained by the modified Richtmyer scheme.
$z = 0.2 \text{ mm}$ plane obtained by the method of characteristics is shown in Figures 4.13–4.15.

![Graph showing $E_z(t_1)$]  

**Figure 4.13:** Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics.

The time responses of the two methods are compared in Fig. 4.16. The outputs are taken at two points located at $(0.2, 0.25, 0.2)$

The results obtained by the Richtmyer scheme are shown in Figures 4.17 and 4.18.

As the third example we analyze the microstrip step discontinuity shown in Fig. 4.19. Because of the symmetry, only one half of the structure is analyzed and this half is shown in the Figure. The face at $y = b = 1 \text{ mm}$ is modeled by magnetic wall boundary conditions. The thickness and conductivity of the conductor are the same as in the previous examples. The structure is excited by a Gaussian pulse on the $x = 0$ plane given by

$$E_y(0, y, z, t) = 0,$$
Figure 4.14: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.

Figure 4.15: Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics.
Figure 4.16: Time variation of $E_z$.

Figure 4.17: Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme.
Figure 4.18: Distribution of $E_z$ plane at $t = t_2$ obtained by the Richtmyer scheme.

Figure 4.19: Microstrip step discontinuity of Example 3.
\[ E_z(0, y, z, t) = \begin{cases} 
\frac{e^{-((t-t_0)^2/(2T_e^2))}}{0.7 \text{ mm} \leq y \leq 1 \text{ mm}, \ 0 \leq z \leq 0.635 \text{ mm}}, \\
0, \quad \text{otherwise}, 
\end{cases} \]

where \( t_0 = 7.5 \text{ ps} \) and \( T_e = 3 \text{ ps} \).

The space distribution of the \( z \) component of the electric field on the \( z = 0.5 \text{ mm} \) plane at is shown in Figures 4.20–4.22.

![Ez(t1) distribution](image)

**Figure 4.20:** Distribution of \( E_z \) at \( t = t_1 \) obtained by the method of characteristics.

The time responses obtained by the method of characteristics and that obtained by the modified Richtmyer scheme are shown in Fig. 4.23.

The response obtained by the modified Richtmyer scheme is also shown in Figures 4.24 and 4.25.

In the fourth example a microstrip T-junction discontinuity is analyzed. Figure 4.26 shows a microstrip “T” structure together with the dimensions and the substrate dielectric constant. The thickness of the signal conductor is 50 \( \mu \text{m} \) and the conductivity is \( 10^7 \text{ S/m} \). The structure is excited with a Gaussian input. The
Figure 4.21: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.

Figure 4.22: Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics.
Figure 4.23: Time variation of $E_z$.  

Figure 4.24: Distribution of $E_z$ at $t = t_1$ obtained by the Richtmyer scheme.
The time responses obtained by the method of characteristics and that obtained by the modified Richtmyer scheme are compared in Fig. 4.30. The outputs were taken at the points (0.2, 0.25, 0.2) mm and (0.55, 0.25, 0.2) mm.
Figure 4.26: Microstrip T-junction of Example 4.
Figure 4.27: Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics.

Figure 4.28: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.
Figure 4.29: Distribution of $E_z$ at $t = t_3$ obtained by the method of characteristics.

Figure 4.30: Time variation of $E_z$. 

In the final example we analyze the microstrip cross over shown in Fig. 4.31. The region under the strip on the $x = 0$ plane is excited with a unit step electric field $z$ component. The boundary conditions for this plane are described by

$$E_y(0, y, z, t) = 0,$$

$$E_z(0, y, z, t) = \begin{cases} U(t), & y_1 \leq y \leq y_2, 0 \leq z \leq h, \\ 0, & \text{otherwise}, \end{cases}$$

where $U(t)$ is a unit step function, $y_1 = 0.35\, \text{mm}$ and $y_2 = 0.65\, \text{mm}$ are the locations of the strip edges, and $h = 0.5\, \text{mm}$ is the height of the first substrate. The other boundaries are modeled as absorbing walls. Each strip is $0.1\, \text{mm}$ thick and has a conductivity of $10^7\, \text{S/m}$.

Figures 4.32–4.33 show the distribution of the electric field $z$-component on the plane $z = 0.8\, \text{mm}$ at the times $t_1 = 12\, \text{ps}$ and $t_2 = 24\, \text{ps}$.
Figure 4.32: Distribution of $E_z$ at $t = t_1$ obtained by the method of characteristics.

Figure 4.33: Distribution of $E_z$ at $t = t_2$ obtained by the method of characteristics.
The time variation of $E_z$ for two locations, $(1, 0.5, 0.8) \text{ mm}$ and $(1, 0.8, 0.8) \text{ mm}$, is shown in Fig. 4.34. The second waveform represents the crosstalk signal from the lower to the upper trace.

Figure 4.34: Time variation of $E_z$. 
Chapter 5

Conclusion

A numerical method based on the method of characteristics for hyperbolic systems of partial differential equations in four independent variables was developed and applied to the solution of time domain Maxwell's equations. The method was oriented towards interconnect analysis problems and exemplified on a few interconnect structures. It should, however, be useful for a number of other electromagnetic problems described by Maxwell's equations.

Since the method is based on the solution of a set of characteristic equations along the characteristic hypersurfaces, it possesses a number of good features present in the method of characteristics for two variable systems of equations. Some of the features of the method are that the grid size in a given region is determined by the propagation velocity of the medium and that the method results in an optimal discretization scheme in the sense it uses the maximal theoretically possible time step for a given mesh spacing. Also, it computes all the $E$ and $H$-field components at every grid point and in principle allows for the treatment of general boundary conditions at the boundary points given by the two operator equations (3.18). The method also retains relatively good accuracy near data discontinuities.

For other potential applications the method could easily be generalized in a number of different directions. Some of these directions are:

- extension to arbitrary $J = F(E)$ relationships (operators) and to nonisotropic media;
• extension of method to arbitrary operators in the boundary condition equations (3.18);

• development of different development schemes for the internal points and boundary points that would lead to simpler, more efficient algorithms.

In addition to the method of characteristics developed in this Thesis, Richtmyer's modified finite difference scheme was also applied to Maxwell's equations. The method was used in parallel with the method of characteristics for result comparison and verification. This method should also be useful for solving electromagnetic field problems occurring in other areas.
Bibliography


