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CONTRIBUTIONS TO
THE TIME DOMAIN-FINITE DIFFERENCE METHOD
FOR
THE MODELING OF MICROWAVE STRUCTURES

by

Ihn Seok Kim

A thesis presented to
The School of Graduate Studies and Research
of the University of Ottawa
in partial fulfillment of the requirement
for the degree of Doctor of Philosophy
in Electrical Engineering
Faculty of Engineering



Ihn Seok Kim, Ottawa, Ontario, Canada, 1990.



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He who ignores discipline despises himself, but whoever heeds correction gains understanding. Prov. 15:32

Dear Heavenly Father,

Thank you for giving us light, so we can recognize any object (discontinuity) in this world!

Thank you for giving us hyperbolic partial differential equations, especially Maxwell's equations, with which we can detect, model, and gather signals from very distant stars, and with which we can communicate between continents and with spacecrafts as they leave the solar system!

In our daily life, we can recognize Professors, friends, and families at a distance. Hyperbolic equations make our life much more interesting. Thank you for giving me a chance to study properties of the equations!

Thank you, Father!, for letting me work under guidance of a thoughtful supervisor, Professor Wolfgang Hoefler!

Lord! I would like to ask your blessing for all the persons who have prayed for me during this Ph.D. program, our parents, brothers and sisters, and friends. Please fill their emptiness with your merciful blessing! Thank you for providing me an opportunity, health, and capability to complete this challenging program!

In Jesus name, I pray. Amen!

ABSTRACT

In this thesis, the Time Domain-Finite Difference (TD-FD) approach based on Maxwell's time dependent curl equations has been investigated with the objective to develop a numerical model for simulation of electromagnetic (EM) wave propagation phenomena, and to obtain S-parameters of guided wave transmission structures. The numerical model formulated as initial boundary value problem has been developed for both CW (single frequency) and pulse (wide band) propagations.

The simulation property of EM field propagation is interpreted by considering the analogy between continuous and discrete characteristics of Maxwell's curl equations, the latter being derived from the leap-frog approximation scheme for local wave propagation. In an effort to relate the discrete wave propagation model to the continuous one, the geometrical meaning and the effects of the stability factor are introduced. The analysis of the leap-frog approximation under the plane wave condition shows that the TD-FD method is non-dissipative, which means that numerical energy is conserved during the simulated wave propagation. From the field distribution of numerical wave propagation, any physical parameters in the frequency domain can be extracted. This is done using the S-parameter extraction algorithm that has been developed for both the CW and pulse propagation cases.

To accurately model EM wave propagation by the numerical process, convergence criteria for checking the global errors in the numerical procedure are also introduced by considering the physical properties, phase linearity and matching condition (standing wave) along a lossless waveguide with uniform cross-section. The physical properties used

also confirm that Maxwell's equations can be separated into transverse and longitudinal parts in any uniform guide. The criteria serve as a basic building block for the analysis of more complex guiding structures.

In the formulation of a computational domain for EM wave propagation solutions, artificial matching boundary conditions (MBC) are necessary to make the domain compact. A new wideband MBC has been introduced. The MBC is based on the concept of the transition operator used in modern control theory.

An efficient local mesh refinement algorithm is also developed by using the concept of the characteristic and by enforcing boundary conditions for $\vec{E}$ and $\vec{H}$ fields at the interface of different mesh sizes.

Numerical analysis results are presented to validate the various procedures when combined into a complete model.

The objective of this study was to develop a TD-FD model of Maxwell's equations for EM wave propagation phenomena in continuous media. With this numerical model, almost all kinds of experiments can be done in complete freedom from experimental apparatus. Also, when probing the field distribution in an experiment, the numerical model provides excellent results without any field disturbance.

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The success of this study would not have been possible without the guidance and understanding of my supervisor, Professor Wolfgang Hoefer, who has encouraged me with his patience and good nature. I would also like to express my sincere gratitude to Professor Vaillancourt in the Mathematics Department for providing me with many valuable references and helpful discussions.

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This thesis is dedicated to my wife, Sookhe Kim, who encouraged me with God's wisdom at all the painful moments during the course of this study. She has also provided joyful and cheerful mood at the end of every evening with tea, humour, and numerical wave propagation phenomena.

Contents	Page
Prayer	iv
ABSTRACT.....	v
Acknowledgements.....	vii
Contents.....	viii
Index of Notation	X
1. Introduction	1
1.1 Purpuse.....	1
1.2 General theme	2
1.3 Contributions to the TD-FD method	4
1.4 Thesis summary.....	5
2. The Time Domain-Finite Difference Method As An S-Parameter Extraction Model	8
2.1 Introduction.....	8
2.2 Historical background of the method.....	9
2.3 Mathematical formulation.....	12
2.3.1 Partial differential equations.....	12
2.3.2 Finite difference aspects	16
2.4 Initial and boundary conditions	22
2.5 Error sources and remedies.....	25
2.5.1 Consistency	26
2.5.2 Stability.....	28
2.5.3 Spurious errors.....	29
2.6 Numerical solution procedure.....	30
2.6.1 CW case	31
2.6.2 Pulse case.....	34
2.7 Summary	37
3. Propagation Characteristics of the Numerical Wave.....	38
3.1 Introduction	38
3.2 Leap-frog scheme as a propagation model.....	39
3.3 Geometrical meaning of the stability factor	41
3.4 Numerical dispersion relation and anisotropy	44
3.5 Group velocity	51
3.6 Global error checking algorithm	56
3.6.1 CW case	57
3.6.2 Pulse case.....	58
3.7 Summary	61
4. Matching Boundary Condition	63
4.1 Introduction	63
4.2 One-way wave equation approximation approach	66

4.3	Transition operator matching boundary condition	74
4.4	Test of reflection property... ..	79
4.5	Absorbing material approach.....	82
4.6	Discussion	83
5.	Local Mesh Refinement Algorithm	85
5.1	Introduction	85
5.2	Mesh refinement algorithm.....	87
5.3	Example.....	93
5.4	Discussion	96
6.	Results of Numerical Analyses	97
6.1	Introduction	97
6.2	Qualitative observations.....	98
6.3	Analysis results	110
7.	Conclusions.....	122
7.1	Discussion	122
7.2	Future research direction.....	125
8.	Appendix.....	128
I	Anisotropy	128
II	Energy Conservation and Non-dissipativity.....	132
9.	References.....	137

Index of Notation

CAD	Computer Aided Design	1
EM	Electromagnetic	1
PDE	Partial Differential Equation	2
CW	Continuous Wave	4
TD-FD	Time Domain-Finite Difference	4
TE	Transverse Electric	7
EMP	Electromagnetic Pulse	10
CFL	Courant, Friedrichs, and Lewy	20
VAX	a trade name of a computer system.....	27
MBC	Matching Boundary Condition	63
SWR	Standing Wave Ratio	71
TLM	Transmission Line Matrix	85
DIAKOPTIC	a decomposition method for large scale computation	126
FDTLM	Finite Difference Transmission Line Matrix	127
$\vec{D}$	electric flux density (electric displacement) vector	8
$\vec{E}$ and $\vec{H}$	electric, magnetic field vector	8
c	speed of light	12
ϵ_0, μ_0	permittivity, permeability of vacuum	12
ϵ_r, μ_r	relative permittivity, permeability of matter	12
Z_0	characteristic impedance of free space	12
$R(x,y,z)$ and t	independent space and time variable	12
$\vec{U} = \vec{U}(R,t)$	dependent variable	13
$\vec{U}_t$	$\frac{\partial \vec{U}}{\partial t}$	15
$\vec{A}$	constitutive relation vector	13
$\vec{L}$	vector differential operator for Maxwell's two curl equations.....	13
$\vec{g}, \vec{b}$	initial, boundary data	13
Ω	domain of dependence	15
i, j, k	number of meshes in x, y , and z directions	17
$\Delta x, \Delta y, \Delta z$ and Δt	mesh size in x, y , and z directions and time step (or number of iteration)	18
$F^n(i,j,k)$	difference approximation of $F(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$	17
$\Delta \ell$	spatial mesh size	17
SF	stability factor	18
n_d	number of dimension.....	18
W, T	pulse width in space, time	23
f	frequency	24
λ, λ_0	wavelength in free space	44

L_f	leap-frog difference operator	27
$\hat{e}_i, \hat{h}_i$	transverse electric, magnetic field vector	31
β_i	propagation constant of the i_{th} mode	31
$E_{inc}, E_{ref}, E_{trans}$	electric fields for incident, reflected, transmitted	37
E_{tot}	total electric field	36
s, S	spectrum (frequency response), time domain sample	44
(i_o, j_o, k_o)	sampling position in the computaional domain	44
$\beta_x, \beta_y, \beta_z$	x-, y-, and z- components of propagation constant	45
β_o	free space propagation constant	45
v_{ph}	phase velocity for numerical dispersion analysis	45
c^*	phase velocity for numerical anisotropy analysis	50
v_g	group velocity	51
$\alpha_x, \alpha_y, \alpha_z$	wave propagation angles with respect to the cordinales x, y, and z, respectively	51
$Re\{\}$	taking real part of the quantity in the braces $\{\}$	57
Γ_o	reflection coefficient	57
S_{max}, S_{min}	maximum, minimum standing wave ratio	57
θ, A	phase, amplitude	60
$\vec{T}, \tau$	transition operator, time period	74
$\vec{K}$	inhomogeneous quantity for matching boundary condition calculation	77
σ_E, σ_H	electric, magnetic conductivity	83
NX	total number of $\Delta\ell$ in x coordinate	98
$a_w(t)$	amplitude component for anisotropy analysis	129
$\xi_i(\beta_i)$	amplification factor for the i_{th} eigen mode	134
$\vec{S}$	poynting vector	136

CHAPTER 1

Introduction

1.1 Purpose This study was originally triggered by an apparent need for the development of a good method or model to analyze generalized discontinuities in guided wave transmission problems[1-1]-[1-14]. To solve such discontinuity problems, a method must be general enough to model the complicated geometries (structures) of most realistic discontinuities. A literature review of research efforts into modeling discontinuities resulted in a list of references [1-1]-[1-14] that presented diverse ideas. There were few works which agreed with each other, and none of them was able to solve all problems of interest. Thus, this study was directed towards developing a versatile method or model to be implemented in a computer aided design (CAD) package with which general discontinuities could be analyzed.

Since the discontinuities could only be analyzed with a model or method that treats general electromagnetic (EM) wave propagation phenomena in terms of geometrical and physical factors (homogeneous and inhomogeneous) and for arbitrary wavefronts, it was essential to work with the time dependent form of Maxwell's equations

which govern the general macroscopic electromagnetic processes. In EM propagation theory, it is not possible to separate the geometry of the problems from the physics of the problem. Mathematically, electromagnetic phenomena are directly dependent upon boundary conditions imposed by the geometry, and the initial state of the electromagnetic fields and can be described with Maxwell's equations.

The power of Maxwell's equations lies in their generality of description, but in its analytical form the mathematical model is difficult to apply to the local geometry of most problems. Numerical methods readily approximate arbitrary geometries, since numbers can represent geometrical and physical features with complete generality. This study has thus been aimed at developing a numerical model for simulating EM wave scattering phenomena and to characterize discontinuities in guided wave transmission structures for the numerical computation of S-parameters using the time dependent Maxwell's equations. Thus, the focus of this thesis has been on a numerical approach which can accurately model the physical EM wave propagation phenomena instead of simply finding a numerical approximation to the solution of Maxwell's equations.

1.2 General theme EM wave scattering problems belong to the last of the three major categories of physical and engineering problems: equilibrium, eigenvalue, and propagation problems [1-15]. The propagation problem is the main subject of this thesis. Most problems of physics and engineering have been modeled by partial differential equations (PDEs). Propagation problems can be modeled mathematically with the hyperbolic form of systems of partial differential equations. Some examples of the fields in which these equations are important are fluid mechanics (weather prediction, aircraft and turbine design, oceanography, ...), geophysics (earth modeling, detecting minerals,

...), magnetohydrodynamics, elastics, and acoustics. Maxwell's two time dependent curl equations are hyperbolic equations.

Like in most instances involving hyperbolic equations, there is little hope of obtaining an analytical solution to Maxwell's equations, and thus one must envisage numerical approximations. Of these approximations, finite difference model is one of the most important. They are based on the idea of approximating partial derivatives with respect to both time and space with discrete differences. As long as the approximate model converges to the correct physical result when the discretization is very fine, the approximate model can be used to simulate EM wave propagation phenomena. This convergence will normally take place provided that the approximate model is *consistent* and *stable* [1-16],[1-17]. Since EM propagation problems are mathematically *initial boundary value problems*, any particular case of EM wave propagation problems can be formulated with Maxwell's two time dependent curl equations, together with certain auxiliary conditions. These conditions may include initial conditions, boundary conditions, radiation or matching boundary conditions, and symmetry conditions. Combining Maxwell's equations and the auxiliary conditions constitutes a mathematical problem for the determination of EM wave propagation behaviour. Developing a general model which can describe various waveguide discontinuities using the above mentioned procedure was the main object of this study.

Traditionally, EM wave scattering problems have been solved in the frequency domain. The frequency domain is an imaginary, hypothetical domain that is used to escape the complexity of solving electrical engineering problems in the time domain [1-18]. The Fourier transformation provides the transition between time and frequency domain analysis. There is no doubt that solving problems entirely in the time domain

(the real world) requires a high level of mathematical ability. A definite advantage of such solutions is that one keeps in touch with the physical quantities and phenomena during the solution process and thus maintains an improved conceptual understanding of problem detail. Since we have been educated in the frequency domain, transforming the time domain solutions into the frequency domain often helps us to better understand the significance of the result. Even though transient time domain solutions yield wideband characteristics in one calculation, CW applications have also been developed for handling single frequency characteristics in one calculation. Another advantage of the time domain technique is that it does not require any mode based calculating technique used in the frequency domain.

Time domain numerical approaches have become a popular research topic with the availability of a new generation of computers with huge memory capacities and parallel processing architectures. This means that the power of the TD-FD method [2-5] using Maxwell's equations can be fully demonstrated for the solution of EM wave propagation problems in the near future, since we have found that the method requires a large amount of computer storage. However, the two main objectives in this study are the extension of the method to the understanding of electromagnetic field propagation, and the extraction of microwave circuit parameters.

1.3 Contributions to the TD-FD method The new contributions in this study reside in the following features:

- (a) Refinement and reinterpretation of concepts employed in various areas of wave physics for a better understanding of the properties of the numerical model as

- applied to microwave engineering (Sections 2.3, 2.5 and Chapter 3),
- (b) Detailed study of the effect of the stability factor on numerical accuracy, dispersion and conservation of energy in the TD-FD algorithm, (Sections 3.3, 3.4, 3.5, 3.6, and Appendix II),
 - (c) A new local matching boundary condition with very wideband characteristics is introduced: this is achieved by introducing the transition operator concept used in modern control theory (Section 4.3),
 - (d) A local mesh refinement scheme is introduced to resolve strongly non-uniform field behaviour around a fine object or discontinuity with a mesh ratio 1:4 (Chapter 5),
 - (e) Some practical structures have been analyzed with the 2-D and 3-D TD-FD algorithms and results have been compared with data available in the literature (Chapter 6).

1.4 Thesis summary The content of this thesis is outlined as follows:

In Chapter 2, we review the TD-FD method which is still a relatively new method, and add the *characteristic* concept in an attempt to gain a deep understanding of the method. Errors affecting the method, and their remedies, are briefly introduced.

In Chapter 3, the view that the TD-FD model is not just a coarse mathematical approximation of a physical problem, but a physical model of a different kind with analyzable properties of its own, is discussed. The leap-frog approximation of Maxwell's equations is interpreted as a local numerical wave propagation model simulating real

EM wave propagation phenomena, but in a discrete mode. The explanation of this local discrete EM wave propagation model will be based on an analogy of the concept of the *characteristic* and the *domain of dependence* for the continuous case. We will show that these discrete numerical wave propagation phenomena are related to the stability factor of the method by introducing the geometrical meaning of the stability factor in a discrete computational domain. We will present the effect of the stability factor on the numerical dispersion characteristics and propose to use the upper limit value of the stability inequality for accurate and economical simulation. We will also introduce convergence criteria for analyzing guided wave transmission structures.

In Chapter 4, after reviewing the one-way wave equation approximation approach, the development of a new local wideband matching boundary condition, with which we can make the computational domain compact is introduced. This matching boundary condition is based on the transition operator concept of modern control theory and has been generated and tested with an infinitely long uniform homogeneous rectangular waveguide.

In Chapter 5, a new efficient mesh refinement algorithm to resolve fine boundary detail is presented. This algorithm has been developed from the mathematical paper by Berger and Oliger [5-3] and the test results show calculations are around 70 times faster than by just adapting a uniformly fine mesh for reasonable accuracy. Thus, the algorithm can save considerable computer resources and computational effort.

In Chapter 6, all the theories, algorithms, and considerations for the TD-FD method, developed in the previous chapters, are used to demonstrate the ability of the method to accurately characterize guided wave transmission line discontinuities. First, the simulation properties of the method in a standard rectangular waveguide will

be qualitatively illustrated for CW and pulse applications. Based on this qualitative observation, the method will be applied to various wave guide discontinuities in order to obtain their S-parameters.

Chapter 7 will summarize and conclude with a discussion of the limitations involved in the method. Future research directions will also be discussed.

In Appendix I, the anisotropy characteristic will be derived for TE mode propagation, with the results plotted in Fig. 3.4.4. Appendix II illustrates the advantage of the leap-frog approximation of Maxwell's equations for EM wave propagation problems by introducing the concept of non-dissipativity. During the derivation of the non-dissipativity property, the stability inequality is obtained as well. The numerical energy conservation property is explained with the non-dissipativity.

CHAPTER 2

The Time Domain - Finite Difference Method As An S-Parameter Extraction Model

2.1 Introduction In order to analyze EM wave propagation problems, a mathematical model for the propagation phenomena should be considered as a first step. Fortunately, Maxwell was able to predict EM propagation phenomena mathematically by adding the displacement current term $\frac{\partial \vec{D}}{\partial t}$ to Ampere's law and thus maintaining charge conservation. The displacement current term explains coupling phenomena as follows: a changing electric field causes changes in the magnetic field (Ampere's law) and a changing magnetic field causes changes in the electric field (Faraday's law). Thus, the electromagnetic field propagation in a bounded or unbounded domain is a physically alternatively coupled flow phenomenon of $\vec{E}$ and $\vec{H}$ fields. Hence, Maxwell's two time dependent curl equations serve as the basic mathematical model for macroscopic EM field propagation phenomena.

However, no generally valid analytical solution of the equations has been found mathematically for complex microwave structures, and numerical techniques have been

developed since computers have become available. In this chapter, the analytical development of a set of approximate Maxwell's equations for simulating EM field propagation phenomena in two cases (i.e., CW and pulse application) will be studied. The finite difference version of Maxwell's two time dependent curl equations is a function of both time and space. Hence, this technique is called Time Domain-Finite Difference (TD-FD) or Finite Difference-Time Domain (FD-TD) method; in this study, the former term will be used predominantly.

The first section presents the historical background of the TD-FD method. In Section 2.3, Maxwell's equations are reviewed from both the partial differential equation and finite difference equation point of view for a computer implementation as part of a modeling tool and for determining the field distribution associated with EM wave propagation. A numerical analysis based on hyperbolic partial differential equations should not be studied without considering the role of "characteristics" of the differential equations. Thus a preliminary concept of the characteristics is included in Section 2.3.1. To obtain a better understanding of the method, various error sources and their remedies are considered briefly in Section 2.4. Then, two separate procedures for S-parameter extraction from the field distribution in CW and pulse excitation cases will be demonstrated in Section 2.5. In Section 2.6, the numerical solution procedures for CW and pulse propagation will be presented in detail using the flow charts. This chapter will be concluded with some discussion of the method.

2.2 Historical background of the method Even though the finite differencing approximation theory for hyperbolic partial differential equations has not been well established in pure mathematics [2-1], approximation techniques have been used for

a long time, especially in the areas of weather prediction and fluid dynamics, before Yee [2-2] introduced the leap-frog approximation technique for Maxwell's two time dependent curl equations to the EM society in 1966. Yee's leap-frog algorithm is still used in the TD-FD analysis. Furthermore, Taylor, et. al. [2-3], attempted to solve the problem of pulse scattering by a cylindrical rod inside a cylindrical waveguide which was filled with a time-varying inhomogeneous lossy medium in two space dimensions, in 1969.

In the '70's, only a few papers appeared in the literature. Merewether [2-4] used the method in 1971 to predict the current induced on a thin metallic body of revolution excited by an electromagnetic pulse. In 1975, Taflové's CW approach [2-5] was introduced for finding the EM fields within an arbitrary dielectric scatterer of the order of one wavelength in diameter in unbounded space. In the same year, Longmire [2-6] credited Yee's algorithm as being "the fastest numerical way of solving Maxwell's equations". The technique was applied to airplanes for EMP coupling and scattering problems by Holland [2-7] in 1977 and by Kunz and Lee [2-8] in 1978.

During the 80's, many papers related to the method were published. The method has been applied to penetration problems [2-9], and to EMP coupling to lossy dielectric structures [2-10]. A simplified numerical procedure for the analysis of the EMP response of structures with dielectric or poorly conducting segments [2-11] appeared in 1980. In 1981, three papers describing algorithms used to increase the resolution for small objects or gaps were published by Holland and Kunz [2-12]-[2-14]. In 1982, Taflové suggested a hybrid technique combining the TD-FD method and the moment method for coupling and penetration problems [2-15] and Umashankar [2-16] used the technique to characterize the scattering from complex objects. Up to this point, CW application had dominated in scattering problems. Then, Mei's research group published the

algorithm for a computational mesh involving conforming boundaries [2-17]. In 1986, an experimental validation of the method was done by Kunz [2-18] and an application to eigenvalue problems by Choi and Hoefer [2-19] also appeared. In 1988, two new algorithms to obtain finer resolutions appeared: one using a contour integral scheme for narrow slots and lapped joints in a thick conducting screen, developed by Taflov et. al. [2-20], and the other, Turner, et. al. [2-21] evaluating a thin-slot formalism originated by Gilbert [2-14].

Specifically, the method was first applied in 1988 to guiding structures by Zhang and Mei [2-22], where a pulse excitation was used to provide wideband responses in the frequency domain. Then, in 1989, Wang et. al. applied the method to biomedical engineering [2-23], and two other papers characterizing the guiding structures, such as slot and coplanar lines excited with a Gaussian pulse were presented by Liang [2-24] and [2-25] at the AP-S and MTT-S symposia in San Jose and Los Angeles, respectively. Kim and Hoefer [2-26] studied the effects of the stability factor on the accuracy of 2-D TD-FD simulation. The use of a value close to the upper limit of the stability inequality was recommended for reasons of accuracy and economy. Britt [2-27] published a paper on a general application using pulse excitation in free space.

Even though it has been observed throughout the historical development that the method is versatile in terms of application, all applications have been performed in unbounded domains, (even for guiding structures which must have enclosures). Zhang, et. al. [2-22] claimed that their output data were not accurate enough for design. However, the references [2-22], [2-24] and [2-25] showed that it was possible to use the method for characterizing discontinuities of microwave and millimeter-wave integrated waveguiding structures. The present study is directed towards the analysis of discontinuities in millimeter-wave waveguides with enclosures.

2.3 Mathematical formulation

2.3.1 Partial differential equations Maxwell's two time dependent curl equations, is the mathematical model for EM propagation phenomena, are a system of first order hyperbolic partial differential equations.

In a source free region, Maxwell's curl equations are

$$\frac{\partial \vec{H}}{\partial t} = -\frac{c}{Z_o \cdot \mu_r} \nabla \times \vec{E}, \quad (2.3.1)$$

$$\frac{\partial \vec{E}}{\partial t} = \frac{Z_o \cdot c}{\epsilon_r} \nabla \times \vec{H}, \quad (2.3.2)$$

where $Z_o = \sqrt{\mu_o/\epsilon_o}$ is the characteristic impedance of free space, $c = \frac{1}{\sqrt{\mu_o\epsilon_o}}$ is the speed of light in free space, and $\vec{E}$ and $\vec{H}$ are the total field quantities as;

$$\vec{E} = \vec{E}^s + \vec{E}^i, \quad (2.3.3)$$

$$\vec{H} = \vec{H}^s + \vec{H}^i, \quad (2.3.4)$$

and the superscripts s and i indicate the scattered and incident fields; and where

$$\mu = \mu_o \mu_r = \mu_r \sqrt{\frac{\mu_o}{\epsilon_o}} \sqrt{\mu_o \epsilon_o} = \frac{Z_o \cdot \mu_r}{c},$$

$$\epsilon = \epsilon_o \epsilon_r = \epsilon_r \sqrt{\frac{\epsilon_o}{\mu_o}} \sqrt{\mu_o \epsilon_o} = \frac{\epsilon_r}{Z_o \cdot c}.$$

In the Cartesian coordinate system (x, y, z) , Maxwell's two curl equations can be expanded as :

$$\frac{\partial H_x}{\partial t} = \frac{c}{Z_o \cdot \mu_r} \cdot \left[\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right] \quad (2.3.5.a)$$

$$\frac{\partial H_y}{\partial t} = \frac{c}{Z_o \cdot \mu_r} \cdot \left[\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right] \quad (2.3.5.b)$$

$$\frac{\partial H_z}{\partial t} = \frac{c}{Z_o \cdot \mu_r} \cdot \left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right] \quad (2.3.5.c)$$

$$\frac{\partial E_x}{\partial t} = \frac{Z_o \cdot c}{\epsilon_r} \cdot \left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right] \quad (2.3.5.d)$$

$$\frac{\partial E_y}{\partial t} = \frac{Z_o \cdot c}{\epsilon_r} \cdot \left[\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right] \quad (2.3.5.e)$$

$$\frac{\partial E_z}{\partial t} = \frac{Z_o \cdot c}{\epsilon_r} \cdot \left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right] \quad (2.3.5.f)$$

In matrix notation, the equations can be written as:

$$\frac{\partial}{\partial t} \begin{vmatrix} \vec{E} \\ \vec{H} \end{vmatrix} = \begin{vmatrix} 0 & \frac{1}{\epsilon} \\ -\frac{1}{\mu} & 0 \end{vmatrix} \cdot \begin{vmatrix} \nabla \times & 0 \\ 0 & \nabla \times \end{vmatrix} \cdot \begin{vmatrix} \vec{E} \\ \vec{H} \end{vmatrix} \quad (2.3.6)$$

or in compact notation as:

$$\frac{\partial \vec{U}}{\partial t} = \vec{A} \cdot \vec{L} \cdot \vec{U} = \vec{A} \cdot \frac{\partial \vec{U}}{\partial \vec{R}}, \quad (2.3.7)$$

where

$$\vec{U} = \begin{vmatrix} \vec{E} \\ \vec{H} \end{vmatrix},$$

$$\vec{A} = \begin{vmatrix} 0 & \frac{1}{\epsilon} \\ -\frac{1}{\mu} & 0 \end{vmatrix},$$

$$\vec{L} = \begin{vmatrix} \nabla \times & 0 \\ 0 & \nabla \times \end{vmatrix},$$

and $\vec{R}$ is a position vector.

The initial condition of $\vec{U}$ is

$$\vec{U}(\vec{R}, t = 0) = f(\vec{R}) \quad (2.3.8.a)$$

and the boundary condition is

$$\vec{U}(\vec{R}, t) = \vec{b}(\vec{R}, t), \quad t \geq 0 \quad (2.3.8.b)$$

then the solution is

$$\vec{U}(\vec{R}, t) = \vec{g}(\vec{R} \pm ct) \quad (2.3.9)$$

where of course $\vec{g}(0)$ must be equal to $\vec{b}(0, 0)$. Two solutions for a pulse propagation are pictorially shown in Figs. 6.2.4(a) - (i), where the pulse excited in the middle of waveguide is split into two solutions like (2.3.9), one for a left moving wave and the other for a right moving wave.

Propagation problems are initial value problems within free boundaries that have an unsteady or transient nature. If a boundary value problem is combined with an initial value problem, then in mathematical parlance, such a problem is known as *initial boundary value problem* or *mixed initial value boundary value problem*. Fig. 2.3.1 illustrates the general propagation problem. We explain the problem for future reference as follows; the vector $\vec{U}$ at some point $\vec{x}$ at time $t \geq 0$ is determined completely by the initial data at time $t = 0$ line lying between the characteristic curves drawn from the point p to the initial line. The included region formed by the characteristic lines is called the domain of dependence of the point p. The situation is shown in Fig. 2.3.1 for the one-dimensional case. It is the right time to discuss the mixed initial boundary value problem. It is known that the solution in the region A, enclosed by the characteristics, is determined by the initial condition and that the extension of the solution into region B is determined by the boundary condition [2-28]. More generally, the number of unknown components of $\vec{U}$ that can properly be prescribed on a curve Γ_B is equal to the number of characteristics entering region B from Γ_B . In propagation problems, therefore, the

solution marches out from the initial state guided and modified in transit by the side boundary conditions.

Characteristics are the lines in the plane of the independent variables along which *signals* can propagate. In a source free case, characteristics of Maxwell's equations are the same as those of the homogeneous wave equation. The characteristics of the wave equation produce a conical surface in two space dimensions as shown in Fig. 2.3.2. The conical domain Ω in the two space dimensions becomes the triangle PAB in the one space dimension as illustrated in Fig. 2.3.2. The base of Ω is the interval AB (circle) on the x-axis from the apex (x^0, t^0) .

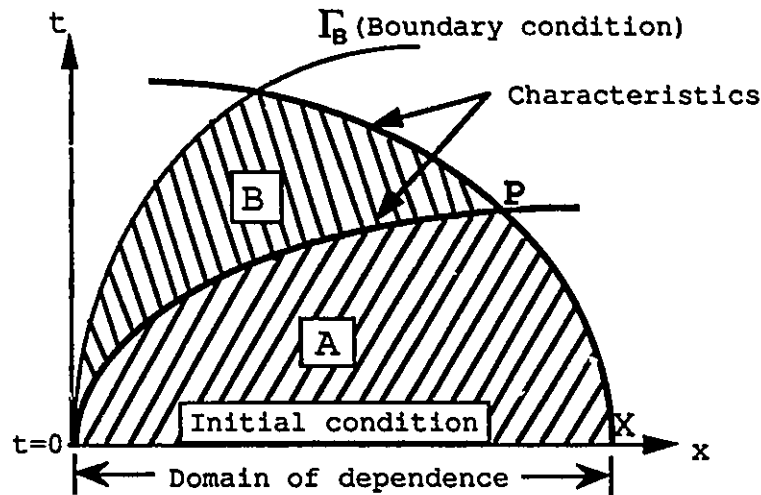


Fig. 2.3.1 Graphical representation of the general propagation problem.

The value of $\vec{U}$ at (x^n, t^0) depends only on the values of $\vec{U}$ and $\vec{U}_t$ on the interval AB and this interval is the domain of dependence of the solution at (x^0, t^0) . Thus they might represent the position of a wavefront in space as a function of time. A hyperbolic

equation possesses two families of real characteristics: one describes waves travelling to the left and the other waves travelling to the right. Physical systems that are governed by hyperbolic equations are ones in which signals propagate at a finite speed (speed of light in the case of Maxwell's equations) in a finite region.

$$(x_1 - x_{01})^2 + (x_2 - x_{02})^2 = (ct)^2 \quad (2.3.10)$$

In the one space dimensional case, the lines of $PA = \text{constant}$ and $PB = \text{constant}$ represent the two families of characteristics along which the signal propagates. An observer at point P is subject to the effects of what has happened in the horizontally crosshatched region, AB, but disturbances outside this region cannot be felt. This region is known, therefore, as the *domain of dependence* at point P. Similarly, a disturbance created at point P can be felt only in the vertically crosshatched region known as the *domain of influence*. It is important that numerical methods for solving hyperbolic equations recognize the importance of finite domains [2-29]. The functional analogy of the domain of dependence in this continuous case will be used to interpret numerical (TD-FD) wave propagation characteristics in a discretized computational domain in Chapter 3.

2.3.2 Finite difference aspects The approximate model for EM propagation problems may be obtained by replacing the continuous Maxwell's equations using the finite difference scheme as below at each nodal point where the solution function is to be found. The leap-frog finite difference scheme adopted by Yee [2-2] will be used for this study. We denote a space lattice point as

$$(i, j, k) = (i\delta x, j\delta y, k\delta z) \quad (2.3.11)$$

and any function of space and time as

$$F^n(i, j, k) = F(i\delta, j\delta, k\delta, n\Delta t) \quad (2.3.12)$$

where $\delta = \Delta x = \Delta y = \Delta z$ is the space increment, and Δt is the time increment.

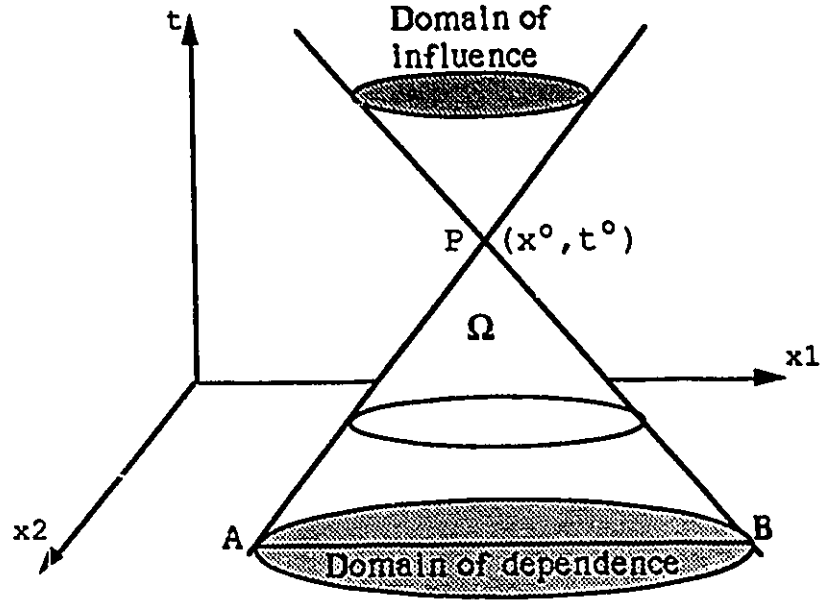


Fig. 2.3.2 Forward and backward characteristic cones with apex at P and domain of dependence of Maxwell's equations.

The function is evaluated at mesh position (i, j, k) for the n_{th} time step. Using the leap-frog scheme, the centered finite difference expressions for the space and time derivatives with second-order accuracy in δ and Δt are as follows:

$$\frac{\partial F^n(i, j, k)}{\partial x} = \frac{F^n(i + \frac{1}{2}, j, k) - F^n(i - \frac{1}{2}, j, k)}{\delta} + O(\delta^2) \quad (2.3.13)$$

$$\frac{\partial F^n(i, j, k)}{\partial t} = \frac{F^{n+\frac{1}{2}}(i, j, k) - F^{n-\frac{1}{2}}(i, j, k)}{\Delta t} + O(\Delta t^2), \quad (2.3.14)$$

where errors of (2.3.13) and (2.3.14) are accurate to the order $O(\delta^2)$ and $O(\Delta t^2)$ in the Taylor series expansion. Following Eq's (2.3.13) and (2.3.14), Maxwell's equations (2.3.5) are discretized as

$$\begin{aligned}
 H_x^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) &= H_x^{n-\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) + \frac{c\Delta t}{Z_o\Delta z\mu_r(i, j + \frac{1}{2}, k + \frac{1}{2})} \\
 &\quad [E_y^n(i, j + \frac{1}{2}, k + 1) - E_y^n(i, j + \frac{1}{2}, k)] - \frac{c\Delta t}{Z_o\Delta y\mu_r(i, j + \frac{1}{2}, k + \frac{1}{2})} \\
 &\quad [E_x^n(i, j + 1, k + \frac{1}{2}) - E_x^n(i, j, k + \frac{1}{2})]
 \end{aligned} \tag{2.3.15a}$$

$$\begin{aligned}
 E_x^{n+1}(i + \frac{1}{2}, j, k) &= E_x^n(i + \frac{1}{2}, j, k) + \frac{Z_o c \Delta t}{\Delta y \epsilon_r(i + \frac{1}{2}, j, k)} \\
 &\quad [H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j - \frac{1}{2}, k)] + \frac{Z_o c \Delta t}{\Delta z \epsilon_r(i + \frac{1}{2}, j, k)} \\
 &\quad [H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) - H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k - \frac{1}{2})]
 \end{aligned} \tag{2.3.15b}$$

where the H_x and E_x components are shown; the other components are discretized in a similar way. The stability inequality, (2.3.16), must be satisfied in the numerical procedure.

$$c \cdot \Delta t \leq \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-\frac{1}{2}} \tag{2.3.16}$$

If a uniform mesh ($\Delta x = \Delta y = \Delta z = \Delta \ell$) is used, the stability factor becomes

$$SF = \frac{c \cdot \Delta t}{\Delta \ell} \leq \frac{1}{\sqrt{n_d}} \tag{2.3.17}$$

where n_d is the number of dimensions involved. We use Yee's basic computational cell where the six field components are placed as shown in Fig. 2.3.3 for the uniform mesh.

Wilson [2-30] showed, using the theory of characteristics developed by Courant, Friedrichs, and Lewy [2-33] that the leap-frog scheme is stable if the condition (2.3.17)

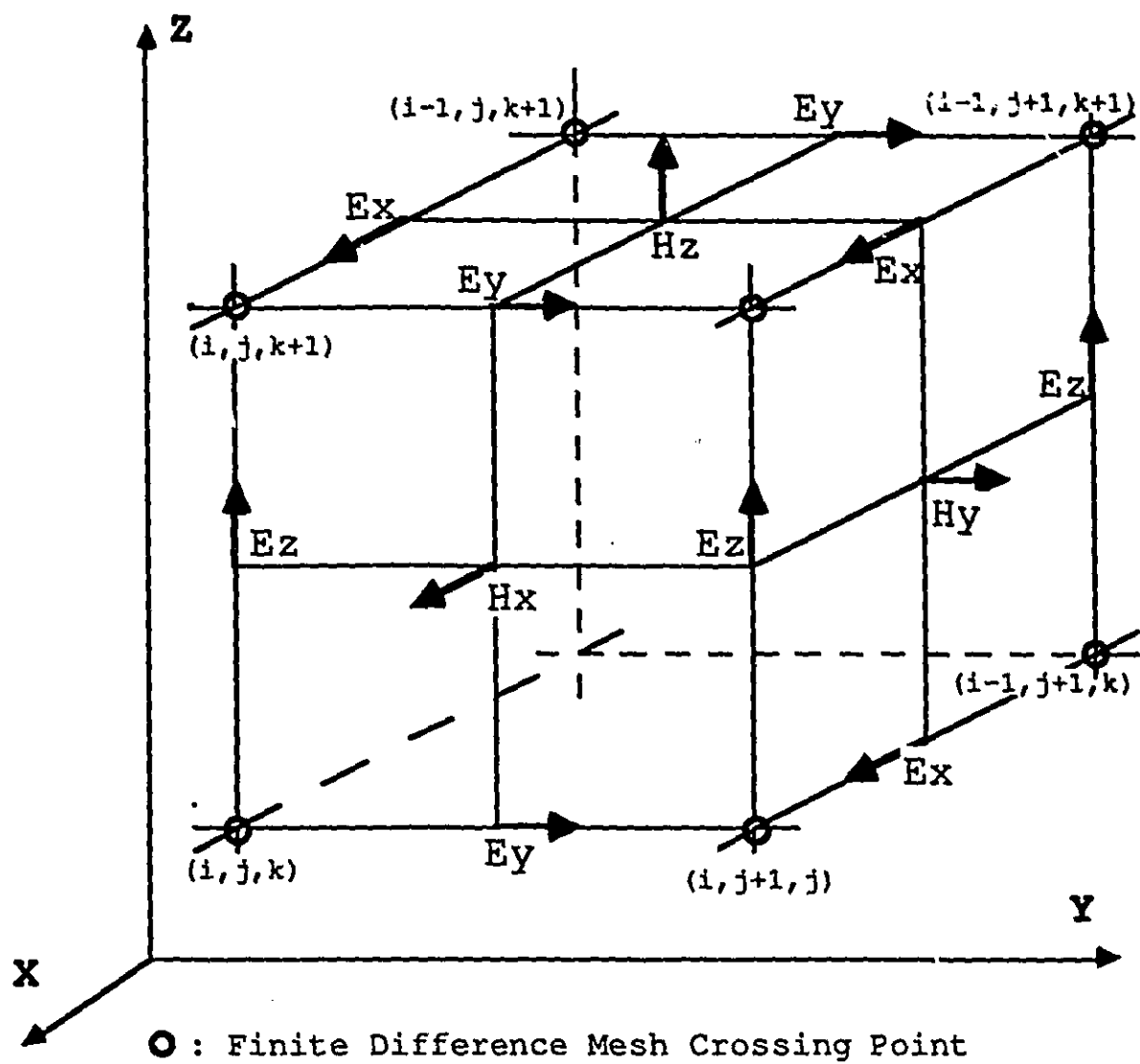


Fig. 2.3.3 Positions of the 6 field components about a unit cell of Yee's lattice.

(CFL stability condition) is met. According to Wilson, the leap-frog scheme is viewed as a two-step integration of the time dependent wave equation. This leap-frog scheme is introduced as a local wave propagation model rather than treating it as just a numerical approximation. There is a similarity between the characteristics of the continuous Maxwell's equations and the numerical wave propagation properties of the leap-frog scheme. This will be discussed in Chapter 3. The theory of the characteristics states that the numerical scheme is stable if and only if, the domain of dependence for the finite differenced equation includes that for the continuous equation.

Figure 2.3.4 shows the domain of dependence for the finite differenced equation in one space dimension. The point Q at time level t is calculated from the points A and B on time level $t - \frac{\Delta t}{2}$, which have in turn been calculated from C, D, and E on $t - \Delta t$, etc. Clearly the numerical domain of dependence of the point Q is limited by QAJ and QBN. The physical domain of dependence of Q is limited by the extreme characteristics J and N through Q. The extreme characteristics are determined by the upper limit value of the stability inequality. To obtain a convergent and thus stable calculation, it is necessary that any perturbation that can influence Q physically must also be able to do this numerically (the discretization may not cut off physically possible influences). This requires the physical domain of dependence to be contained completely in the numerical domain of dependence. The slope of the characteristics leads to the CFL condition which will also be described in the next chapter. The characteristics and the domain of dependence play an important role in wave propagation phenomena. The numerical wave propagation phenomena will be described with the characteristics in the next chapter.

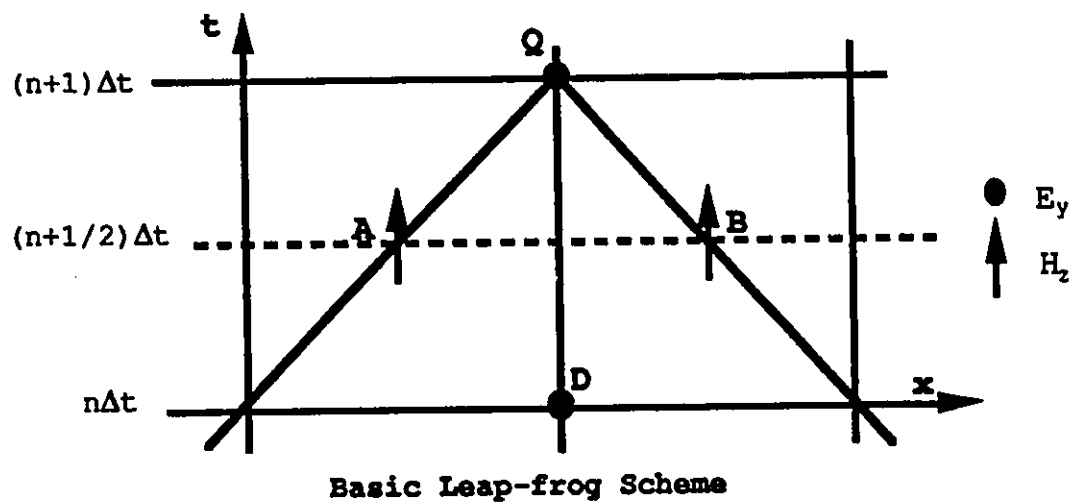
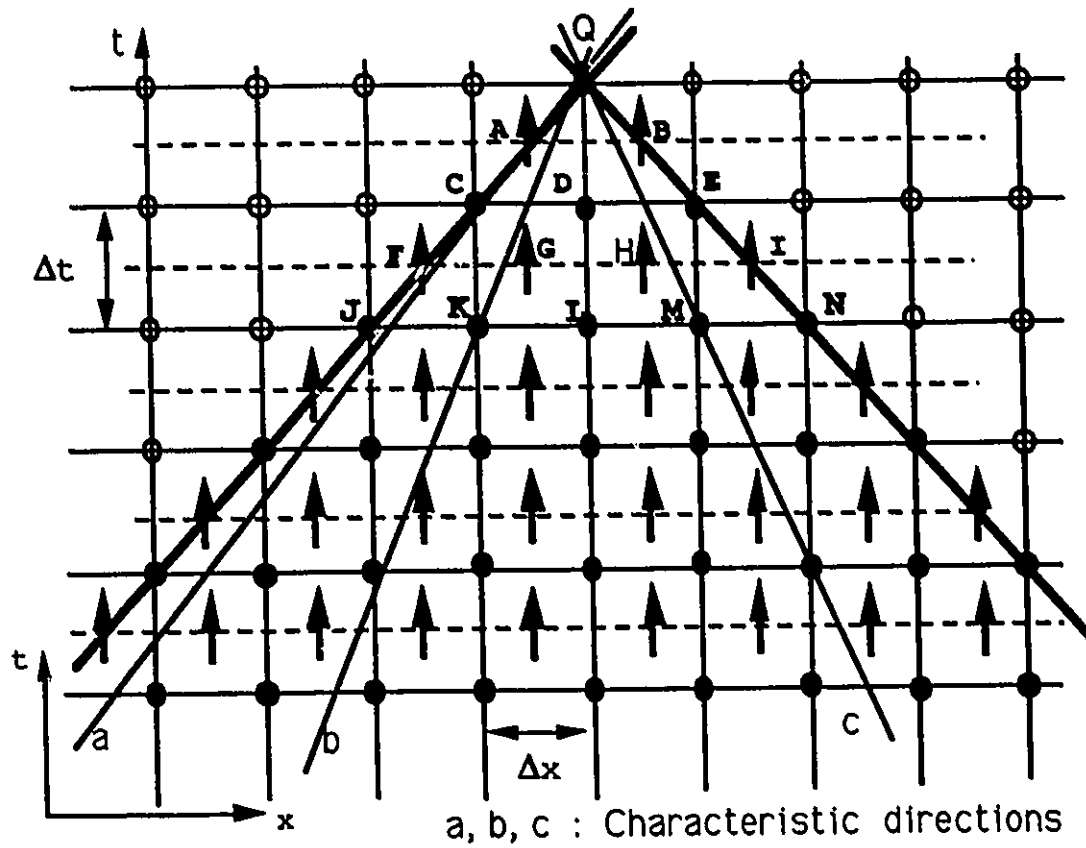


Fig. 2.3.4 Characteristics and domain of dependence on the time-space

grid structure.

2.4 Initial and boundary conditions Maxwell's equations are known as indefinite equations since they can apply to any macroscopic EM propagation problems, in general, but the equations per se do not define a specific problem. The EM propagation problem is defined only when a proper set of initial and/or boundary condition is given. For a given guiding structure, we need an auxiliary condition which includes initial and boundary conditions for the given physical problem. A matching boundary condition which truncates the computational domain is another essential condition in the method and will be described in more detail in Chapter 4.

The convergence process can roughly be divided into two parts. The first part corresponds to the elimination of the large initial errors and depends strongly on the initial conditions. But when the propagation is more or less settled, the convergence is determined by the dissipative effect of a numerical approximation and this dissipation must be remain very small to achieve good accuracy. This second part is characterized by an exponential decay of the error and depends on the scheme, but not on the initial conditions. The leap-frog approximation is supposed to be non-dissipative as shown in Appendix II.

For an initial excitation, a plane wave, or a linear sum of plane waves can be used in the CW case, and a Gaussian pulse excitation can be used for wideband applications. If an initial signal is monochromatic, the signal will not change form as it propagates. For sinusoidal excitation, the steady state must be reached before one can obtain any useful information from the responses of a discontinuity of a wave guiding structure. This usually requires huge computational effort and resources. However, the usefulness of computing in the time domain is that, in principle, a single simulation with a pulse excitation can provide the response of the discontinuity for a wide band of frequencies.

However, we cannot use any arbitrary pulse as an initial condition in practice since errors such as numerical noise or the Gibb's phenomenon introduced by the numerical discretization (numerical dispersion will be explained in the next chapter) affects the phase of the Fourier transformed output of the time domain response and results in a loss of accuracy.

The incident pulse must be smooth, and its derivative must be continuous since Maxwell's equations are differential equations. The influence of the initial condition has been evaluated numerically in terms of convergence to the physical properties of the uniform guiding structures for three different shapes of pulses: raised cosine, hyperbolic secant, and Gaussian pulses. We will use a Gaussian pulse exclusively as an initial condition for guiding structures because it yields the best convergence.

For the CW case, the implementation of a sinusoidal plane wave excitation composed of discrete time steps across a cross-sectional plane of the computational domain is trivial. However, for the wide band case a Gaussian pulse is used as an initial condition and is given by

$$g(z, t = 0) = e^{-z^2/W^2} \quad (2.4.1)$$

where $W=20 \Delta z$ has been used. If the pulse width W is expressed using time, then the spectrum of the Gaussian pulse is

$$G(f) = e^{-\pi^2 \cdot f^2 \cdot T^2} \quad (2.4.2)$$

The phase factor is not shown. As suggested in [2-22], the pulse width is defined to be the width between two points which are 5 % of the maximum value of the pulse.

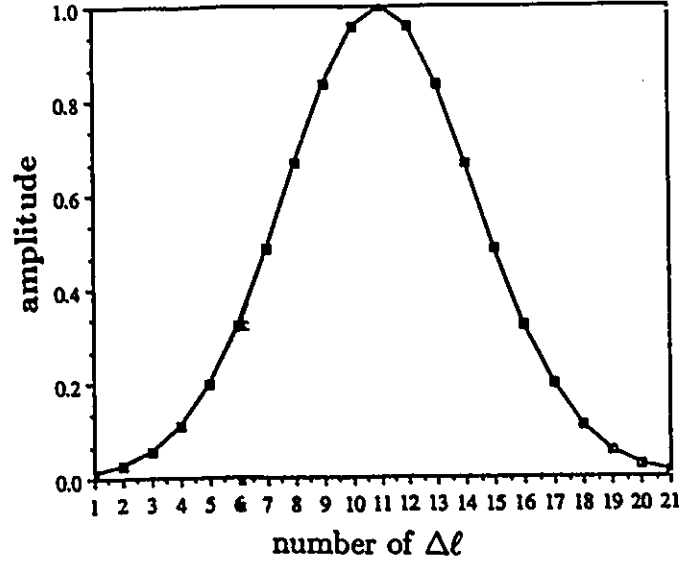


Fig. 2.4.1 Gaussian pulse as an initial condition

So, T is determined by

$$e^{-(z/2)^2/(cT)^2} = e^{(-3)} \simeq 5\%, \quad (2.4.3)$$

or

$$T = \frac{1}{\sqrt{3}} \cdot \frac{10\Delta z}{c}. \quad (2.4.4)$$

At $f = \frac{1}{2T}$, $G(f) \simeq 0.1$, thus the maximum frequency component of the Gaussian pulse is

$$f_{max} = \frac{1}{2T} = \frac{1}{2} \cdot \frac{\sqrt{3} \cdot c}{10 \cdot \Delta z} \quad (2.4.5)$$

In turn, the minimum wavelength in the spectrum of the pulse is

$$\lambda_{min} = 2 \cdot c \cdot T \quad (2.4.5a)$$

Note that we used an initial pulse excitation different from that in [2-22] where a train of discrete pulses was injected sequentially for around $50 \Delta t$ (for the first 50

iterations of a simulation). We have usually excited a complete $20 \Delta\ell$ -width-Gaussian pulse at a single time $t = 0$ by initializing the mesh according to its spatial distribution.

At the interior mesh points, Maxwell's equations are substituted by the leap-frog approximation. The substitution satisfies all conditions for local stability and convergence. At each computational step, information is transmitted from each point to its neighboring points via the computation of the leap-frog approximation of Maxwell's equations as shown in Fig. 3.2.2. In this way, the boundary mesh points influence their neighbors and transmit the effects of the boundary condition into the propagation field. For this to happen, the values of all physical quantities at boundary points must be known at each computational step. The electric and magnetic walls are the basic boundary conditions. They are implemented as follows: for the E_y component we have

$$\vec{E}_{\text{tangential}}^n(i, j + \frac{1}{2}, k) = 0.0 \quad \text{for electric wall} \quad (2.4.6a)$$

which represents a forcing condition, and for the H_z component we have

$$\vec{H}_{\text{tangential}}^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) = 0.0 \quad \text{for magnetic wall} \quad (2.4.6b)$$

which provides a symmetry condition. At an interface between two different media having different dielectric constants, the field components or their derivatives are continuous. Thus, [2-35] suggested that Maxwell's equations take this into account automatically. So, we do not need any special considerations on this matter.

2.5 Error sources and remedies The leap-frog approximation of Maxwell's equations, (2.3.15), are mathematical expressions different from the continuous

Maxwell's equations. This means that their solutions are different as well. Numerical methods have generally been developed to obtain as close an approximate solution as possible with respect to the analytical solution for given types of problems. In order to have an accurate TD-FD simulation result, the error sources must be understood before the numerical procedures are implemented. The approximate equation (2.3.15), and the numerical algorithm of the method both introduce errors which may be split into three types. The first is that of consistency error. This is the error which becomes vanishingly small when the sizes of $\Delta\ell$ and Δt are reduced. This will be described in Subsection 2.5.1. The second type of error is related to the stability problem which was expressed in (2.3.17) and explained in Subsection 2.5.2. If we have both a stable and consistent condition, we have a convergent condition in view of classical convergence theories [2-34]. As long as the numerical solution converges to the correct physical result when the size of the mesh is reduced, the solution is *consistent*. Ames and Richtmyer [1-15] and [1-16] mention that this convergence will normally take place provided that the difference model is *consistent* and *stable*. However, it is very difficult to obtain results from the approximate Maxwell's equations even though the above conditions are met. There are some more important types of errors in hyperbolic partial differential equations. The third type of error is called spurious error, which does not disappear when the mesh size tends to zero even though the stability inequality is satisfied. This type of error will be described in Section 2.5.3. The total errors in phase and amplitude which lead to numerical dispersion and dissipation, will be considered in the next chapter.

2.5.1 Consistency In most numerical methods, the truncation error is the dominant error. The truncation error in the TD-FD method is caused by the leap-frog approximation (truncation of Taylor series) of the continuous form of Maxwell's

equations. Such errors are dependent on the size of the mesh in time and space, Δt and Δl . The error involved in the leap-frog scheme shown in (2.3.13) and (2.3.14) has the order of (Δt^2) and (Δl^2) in terms of a Taylor series ($O(\Delta t^2)$, $O(\Delta l^2)$). The errors such as numerical dispersion and anisotropy belonging to this type will be explained in the next chapter.

Round-off error which is due to the accuracy with which a particular variable is described in the memory of the computer should be mentioned here. Real numbers are stored in terms of a mantissa and an exponent. Clearly if the calculation is performed with i decimal places, it will be less accurate than if it were solved with $i + 1$ decimal places. With modern computers (for example VAX), however, four bytes are used to represent numbers and so eight significant figures can be used. It is important to note that the computer arithmetic works with finite precision, but that the cumulative round-off error is not usually severe for TD-FD applications. As the mesh size Δt decreases the round-off error increases (since more calculation steps are required), but the truncation error decreases (the smaller Δt , the less truncation error). This relation is shown in Fig. 2.5.1.

Thus one cannot generally assert that decreasing the mesh size will always increase the accuracy. But, it is required, that in the limit of a small time step and small space step to zero, the difference system becomes identical with the differential system. This is the consistency property related with the truncation error. Formally the requirement of the consistency may be specified as:

$$\lim_{\Delta t \rightarrow 0} \lim_{\Delta l \rightarrow 0} \frac{(L_f(\Delta t, \Delta l) - I)\vec{U}}{\Delta t} = L\vec{U},$$

where L_f is the leap-frog difference operator, $\beta = \frac{\Delta l}{\Delta t}$ is finite, and L is the differential operator in (2.3.6). If this condition cannot be satisfied, the difference scheme can

not simulate the propagation problem of interest, thus it is clear this requirement is fundamental to a correct solution.

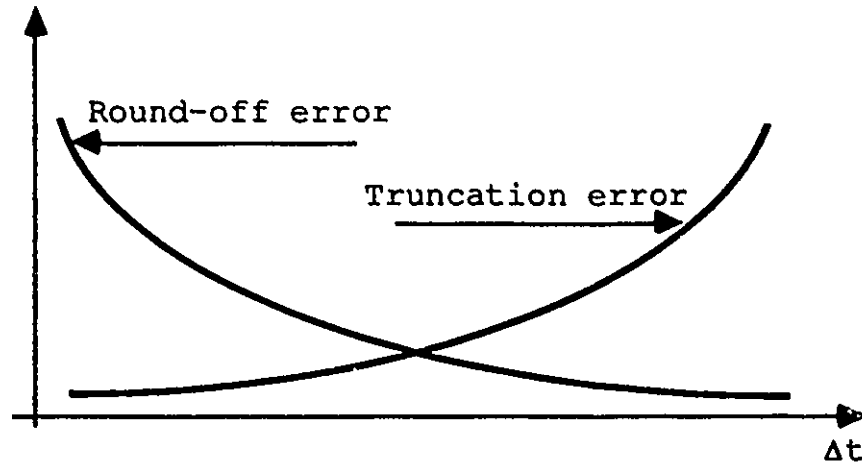


Fig. 2.5.1 A relationship between the truncation and round-off errors for a mesh size

2.5.2 Stability The stability condition in the method guarantees the continuous dependence of the discrete solution of the two equations in differential form. Courant [2-33] introduced the stability inequality (CFL stability condition) which ensures a convergence of the difference solutions for the basic type of linear hyperbolic partial differential equations. Von Neumann also obtained the same inequality from the study of error-growth with Fourier mode [2-34]. Meeting the inequality ensures that the numerical procedure is stable (the solution does not blow up). We do not consider contributions of reflections from an imperfect matching boundary. Reference [2-26] showed that accuracy in general is not very sensitive to variations in the stability factor. However, better

accuracy has been observed at $SF = \frac{1}{\sqrt{2}}$, than for lower values of the stability factor in the two space dimensional problems. For reasons of accuracy and economy [2-26] suggested a stability factor close to the upper limit of the inequality. It is believed that lower accuracy at lower values of the stability factor is due to the following reasons: firstly, the round-off error increases with the number of computational steps, secondly, more interference due to the *forerunner** can be expected at lower values of the stability factor, and thirdly, less numerical dispersion occurs as the value of the stability factor is increased, as shown in the next chapter.

When we derive the stability criteria shown in [2-35], the amplification factor for the leap-frog scheme should be unity. The amplitudes of all the eigenvalues (spectral radius) involved in the pulse excitation become unity as the computing time increases. This property provides an interesting characteristic called the *non - dissipativity* of the leap-frog scheme. Non-dissipativity offers convergence criteria for amplitude errors and numerical energy conservation. Phase error (dispersion) produced by the difference scheme can be checked by evaluating the propagation constant in a transmission line with uniform cross-section. These properties will be explained in Section 3.6.

2.5.3 Spurious errors Major sources of spurious error in the solution of the method using a uniform square mesh are:

- (a) discontinuous initial conditions [2-36], [2-37]
- (b) improper boundary conditions
- (c) insufficient number of iterations

* If a wave is created, then there are a main wave stream and a forefront part which is propagating faster than the main stream. The forefront part is called the forerunner.

Type (a) comes inherently from using a discontinuous initial condition, i.e., an abruptly changing input pulse excitation. A smoothly varying pulse is generally required for excitation to provide good results. The discrete Maxwell's equations are very sensitive to the shape of an input pulse. The optimum pulse shape for a given problem must be found with the criteria introduced in Section 2.6 before a specific simulation is tried.

Type (b) comes from an inaccurate symmetry boundary condition or accumulated reflections from a matching boundary condition. Since there is no perfect matching boundary condition, reflections from the imperfect boundary condition are accumulated as the number of iterations is increased. A good matching boundary condition is required to avoid this type of error. In this study, we have found a new local wideband matching boundary condition based on the transition operator concept. This will be described in detail in Chapter 4. Symmetry boundary conditions must be implemented carefully, since the electric and magnetic fields are not located on the same plane since they are actually a half-space apart. It is noted that an improper implementation of a symmetry boundary condition often creates dissipativity in a pulse simulation. Hence care must be taken when a symmetry boundary condition is implemented.

Type (c) is due to the finite duration of the calculation. It is directly related to Gibbs's phenomenon and is usually reduced by increasing the number of iterations. We cannot increase the number of iterations indefinitely, therefore we must find an optimum number of iterations for a given problem. The way to find the optimum number of iterations will be explained in Section 3.6.

2.6 Numerical solution procedure The TD-FD method employed an explicit scheme, which requires a stability criterion. The explicit scheme for iterations of

the differenced Maxwell's equations yields the solution everywhere in a computational domain from the solution known at a previous time. So the scheme functions as a "time-marching" procedure, in which the approximate Maxwell's equations are solved iteratively in a medium excited by CW or pulse.

Iterative methods involve the repeated application of the same procedure or algorithm, and they provide answers that gradually approach the true solution. The iterative procedure begins with an initial approximation to the solution to the desired accuracy. The speed of convergence for a given method depends strongly on the degree of accuracy of the initial approximation. Thus, intuitive engineering judgement can greatly influence the efficiency of the computational process. It is noted that the *block* iterative scheme* has been used in our study. In the next two subsections, TD-FD S-parameter extraction algorithms for the CW and pulse cases will be demonstrated for discontinuities in a guided wave transmission structure.

2.6.1 CW case Following the initial boundary value problem concept, an initial condition can be a transverse field distribution such as

$$\begin{aligned}\hat{e}_i(u_1, u_2, z) &= a_i \cdot \vec{E}^i(u_1, u_2) \cdot e^{\pm j\hat{\beta}_i z} \\ \hat{h}_i(u_1, u_2, z) &= b_i \cdot \vec{H}^i(u_1, u_2) \cdot e^{\pm j\hat{\beta}_i z}\end{aligned}\tag{2.6.1}$$

where a_i and b_i are the amplitude factor of the initial electric ($\vec{E}^i$) and magnetic ($\vec{H}^i$) field components, and $\hat{e}_i$, $\hat{h}_i$ and $\hat{\beta}_i$ are the transverse vector functions and propagation constant of the i_{th} mode. If the initial field function not known explicitly, it can be obtained with frequency domain numerical techniques such as finite difference [2-39]

* An algorithm is used to modify the approximate solution for a whole group of node values in the computational domain

and finite element [2-40] methods. By initializing the discrete Maxwell's equations (2.3.15) with a time dependent sinusoidal function, and enforcing the boundary condition wherever required, a steady state condition of the field distribution is gradually reached. Once a steady state condition is satisfied, $\vec{E}_{max}^n(i, j, k_1) - \vec{E}_{max}^n(i, j, k_2) \leq \epsilon$ for two peak points along the propagation direction, where ϵ is a very small number proportional to the amplitude of the initial incident wave, and the S-parameters can be extracted from the field distribution as follows;

$$S_{11}(\omega) = \frac{E_{ref}(\omega)}{E_{inc}(\omega)} \quad (2.6.2)$$

with a matching boundary condition on port 2, and

$$S_{21}(\omega) = \frac{E_{trans}(\omega)}{E_{inc}(\omega)} \quad (2.6.3)$$

with no incident field from port 2,

or

$$S_{11}(\omega) = |S_{11}| \angle \Theta_{11}, \quad (2.6.4)$$

where

$$|S_{11}| = \frac{\left| \frac{E_{max}}{E_{min}} \right| - 1}{\left| \frac{E_{max}}{E_{min}} \right| + 1}$$

$$\Theta_{11} = 2kz - \pi$$

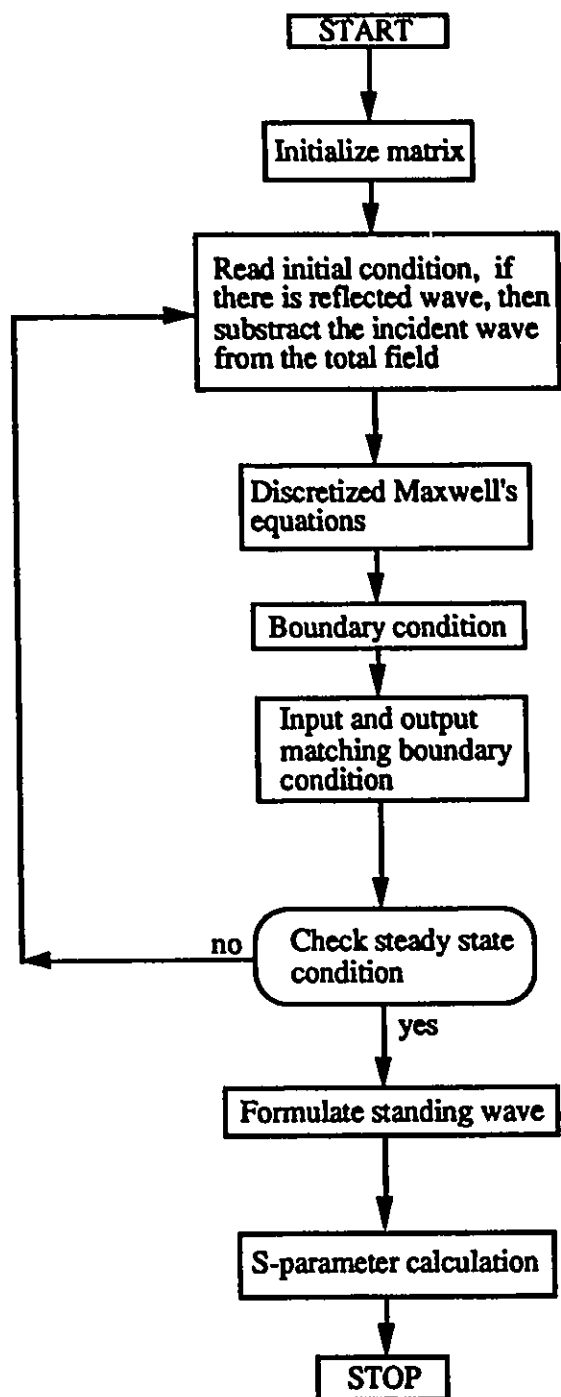


Fig. 2.6.1 Flow chart for CW case.

The unitary property must also be satisfied for lossless case:

$$|S_{21}| = [1 - |S_{11}|^2]^{\frac{1}{2}} \quad (2.6.5a)$$

$$\Theta_{21} = \Theta_{11} \pm \frac{\pi}{2} \quad (2.6.5b)$$

where the “-” sign in (2.6.5.b) designates inductive behaviour. The computational steps for the CW case are shown in the flow chart in Fig. 2.6.1.

2.6.2 Pulse case The wideband frequency response for a given problem can be obtained by using a pulse excitation at $t = 0$, and a Fourier transform after the *steady state condition** has been reached. In contrast to the CW case, the pulse case requires two computer runs for an S-parameter extraction. During the first run, we calculate the incident field distribution in a structure in which the discontinuity under study is replaced by a wideband absorbing wall, and during the second run we calculate the field distributions with the discontinuity in place. Therefore, we need two computational domains as shown in Fig. 2.6.2. The incident field, $E_{inc}(\omega)$, is sampled in the domain (a), while the total field is sampled in the computational domain (b). A reflected field

* The steady state condition for a pulse excitation has been defined in [2-41] as follows:

In the most general terms, the steady state solution of a differential equation is the one that is asymptotically approached as the effect of the initial condition dies out. This condition is also used to determine the iteration number of a given application.

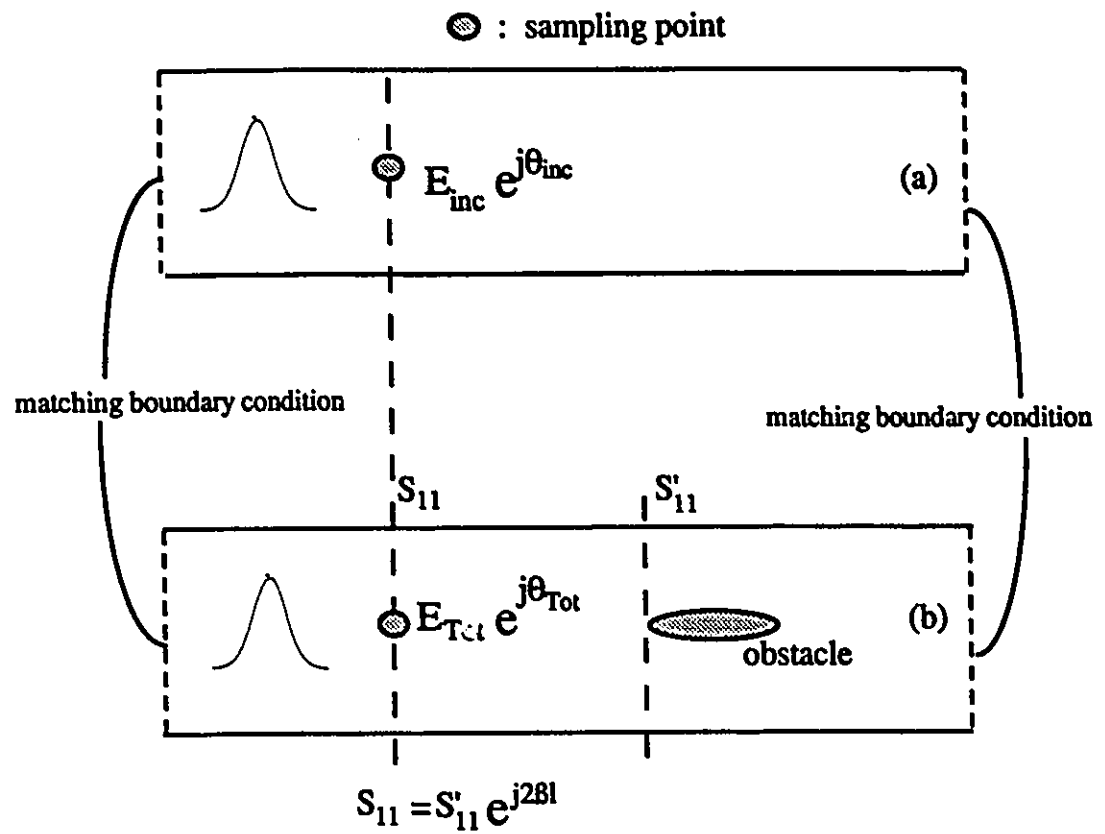


Fig. 2.6.2 Two computational domains for computing (a) incident and (b) total field distributions.

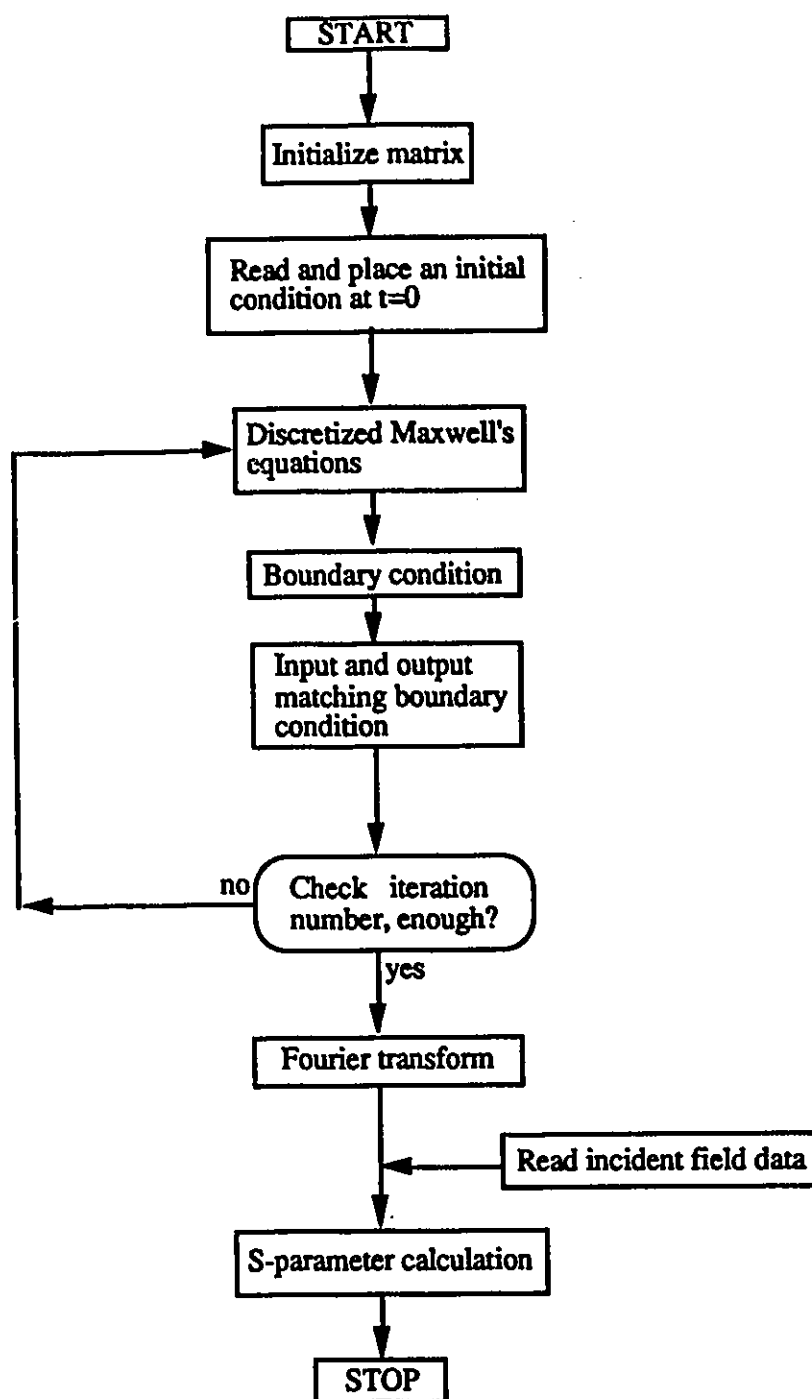


Fig. 2.6.3 Flow chart for pulse case.

quantity, S_{11} , for example, is obtained as follows;

$$S_{11}(\omega) = \frac{E_{ref}}{E_{inc}} \angle(\theta_{ref} - \theta_{inc}) \quad (2.6.6)$$

where subscripts *inc* and *ref* indicate the incident and reflected field quantities respectively. The steps in the calculation procedure for the pulse case is shown in the flow chart Fig. 2.6.3.

2.7 Summary After a brief review of the historical development of the TD-FD method, the discussion in this chapter has focussed on the formulation of the numerical EM propagation algorithm as an initial boundary value problem. Errors involved in the numerical approximation of Maxwell's equations have been described, and remedies have also been briefly introduced. The numerical algorithm for S-parameter extraction from simulations with both CW and pulse excitation has been illustrated. This chapter thus serves as an introduction to the principal themes of this thesis. The next chapter will introduce the local wave propagation characteristics of the numerical TD-FD process.

CHAPTER 3

Numerical Wave Propagation Characteristics

3.1 Introduction In the previous chapter, we have described the TD-FD method mathematically as an initial boundary value problem. Physical relationships between continuous and discrete models for EM wave propagation will be introduced in this chapter in order to better understand the numerical method. This means that we do not consider the numerical approach blindly as mere number crunching. The numerical wave motion in a discrete mode is interpreted in analogy to the continuous wave propagation phenomenon. We have already observed that the behaviour of the leap-frog approximation resembles that of the characteristics and the domain of dependence of the continuous model shown in Fig. 2.3.2 for the one dimensional case. The leap-frog approximation will be treated as a local propagation model in a discrete computational domain in the next section.

In Section 3.3, we will study the geometrical meaning of the stability factor to better understand numerical wave propagation phenomena in two space dimensions. (Three space dimensions cannot be shown on the two space plane. We also omit the

one-dimensional case.) Dispersion characteristics and group velocity analysis for the numerical model will be included, the relationship between the velocity (phase and group velocity) errors and the stability factor will be introduced, and we propose to use a value close to the upper limit of the stability inequality in Sections 3.4 and 3.5. In Section 3.6, the global error (phase and amplitude) checking algorithm for general guiding structures is introduced and related to the non-dissipativity of the leap-frog scheme in Section 3.6.

3.2 Leap-frog scheme as a propagation model In a source free case, the

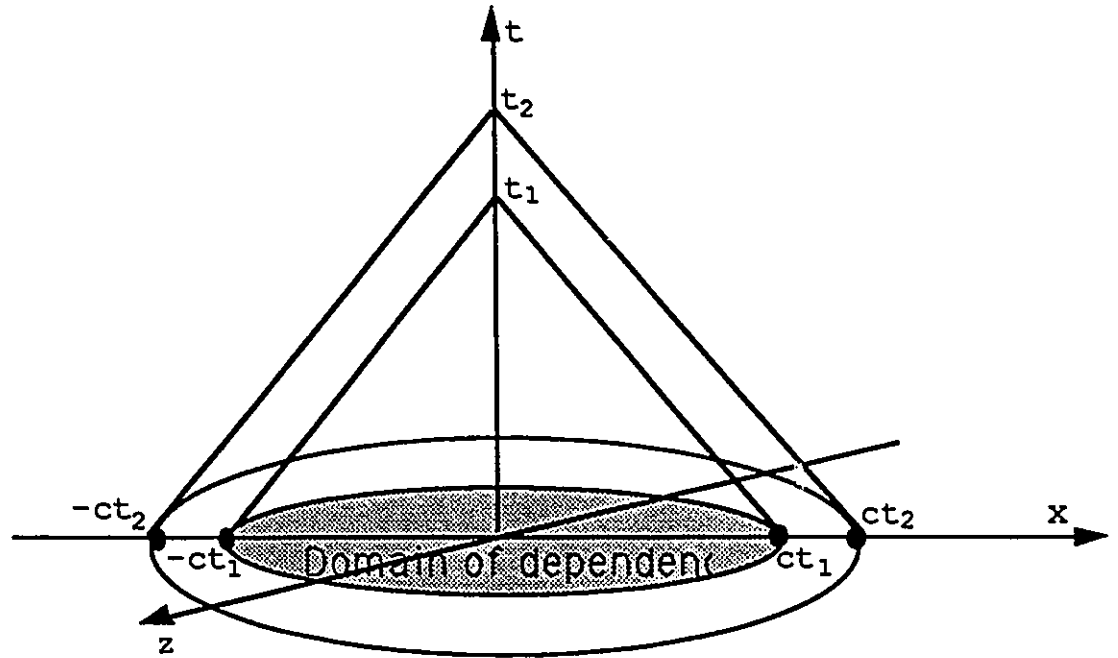


Fig. 3.2.1 Characteristic cones and domains of dependence for the two space dimensions at the time steps t_1 and t_2 .

characteristic cones of the continuous model in two space dimensions are shown at two specific times (t_1 and t_2) in Fig. 3.2.1. For the leap-frog approximation, we illustrate a

local wave motion based on TE mode propagation in the discrete domain. This is shown in Fig. 3.2.2 with the time-space mesh structure. The leap-frog scheme in Fig. 3.2.2 shows that the $\vec{H}$ field values at the points F, G, I, and K at a time step $(n + \frac{1}{2})\Delta t$ are dependent upon the $\vec{E}$ field values at A, B, C, and D at a time $n\Delta t$ and $\vec{H}$ field at the same position F, G, I, and K at a time step $(n - \frac{1}{2})\Delta t$. And the $\vec{E}$ field value at the point P_1 at a time $(n + 1)\Delta t$ is updated by using the $\vec{H}$ field values at the points K, F, G, and I at a time $(n + \frac{1}{2})\Delta t$ and the $\vec{E}$ field value at the point P from the previous time step $n\Delta t$.

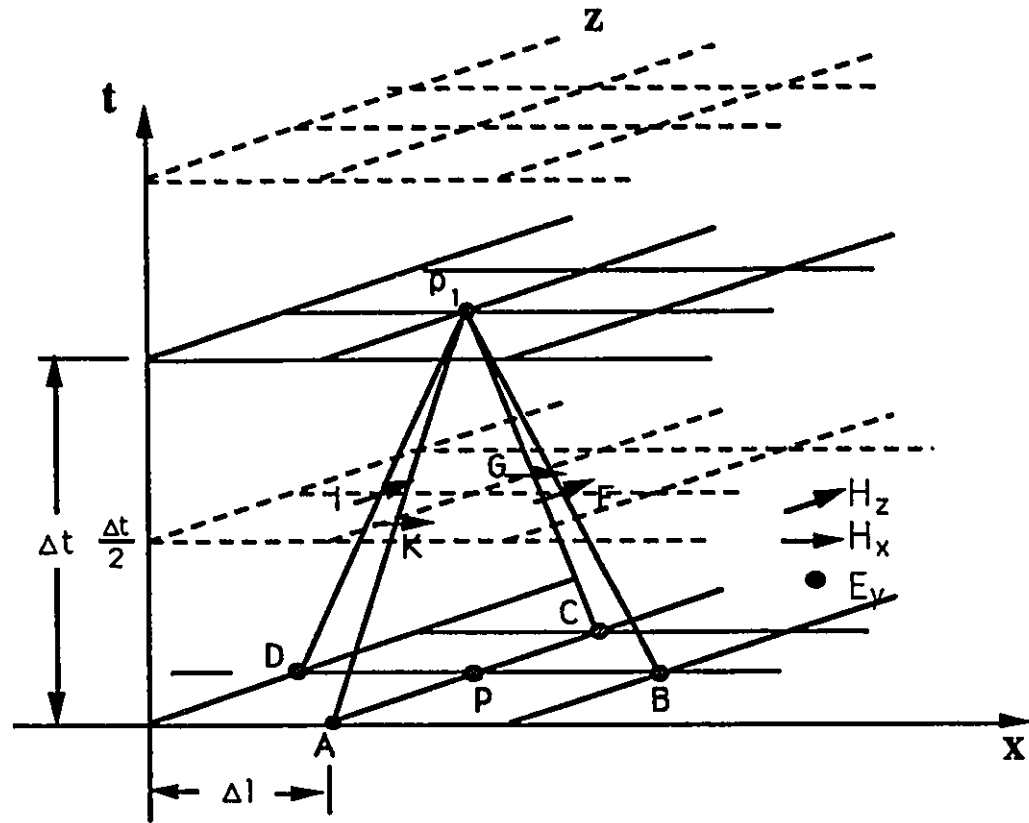


Fig. 3.2.2 Three-dimensional (x, z, t) diagram showing the discrete characteristic of the leap-frog approximation for TE mode propagation.

The $\vec{E}$ field components are placed at the points A, B, C, and D. The $\vec{H}$ field components are placed at the points K, F, G, and I, which are on the characteristic lines ($\bar{A}P_1$, $\bar{B}P_1$, $\bar{C}P_1$, and $\bar{D}P_1$) at the half time steps on the half space intervals. The discrete characteristics of the leap-frog approximation for a time step form a square with the four points A, B, C, and D for the $\vec{E}$ fields and K, F, G, and I for the $\vec{H}$ fields since a uniform mesh size is employed. Otherwise a rhombus is generally formed. This square behaves like the domain of dependence in the continuous case [2-33]. It is obvious that in the three-dimensional (x, z, t) mesh structure the characteristics of the differential equations are circular cones, whereas those of the differenced (leap-frogged) equations are four-sided pyramids.

3.3 Geometrical meaning of the stability factor Projections of characteristics (the domain of dependence) for continuous propagation are shown on the discretized computational domain as projections of the discrete characteristic lines on the two space plane in Fig. 3.3.1. The squares are domains of dependence for the leap-frog approximation. The CFL (Courant-Fredriechs-Lewy) stability condition for the differenced equations, Reference [2-33], states that in order to be convergent for all smooth initial data, the square of dependence of the difference equations must contain completely the circle of dependence of the differential equations. There is no loss of generality if we consider the grid point O to lie on the t-axis at $x = x_0$ and $z = z_0$. If $T = n\Delta t$, then the domain of dependence for the differential equation is given by

$$x_n^2 + z_n^2 \leq n^2 \Delta t^2 \quad (3.3.1)$$

and so in Fig. 3.3.1, $OQ = n\Delta t$ where n is 1.

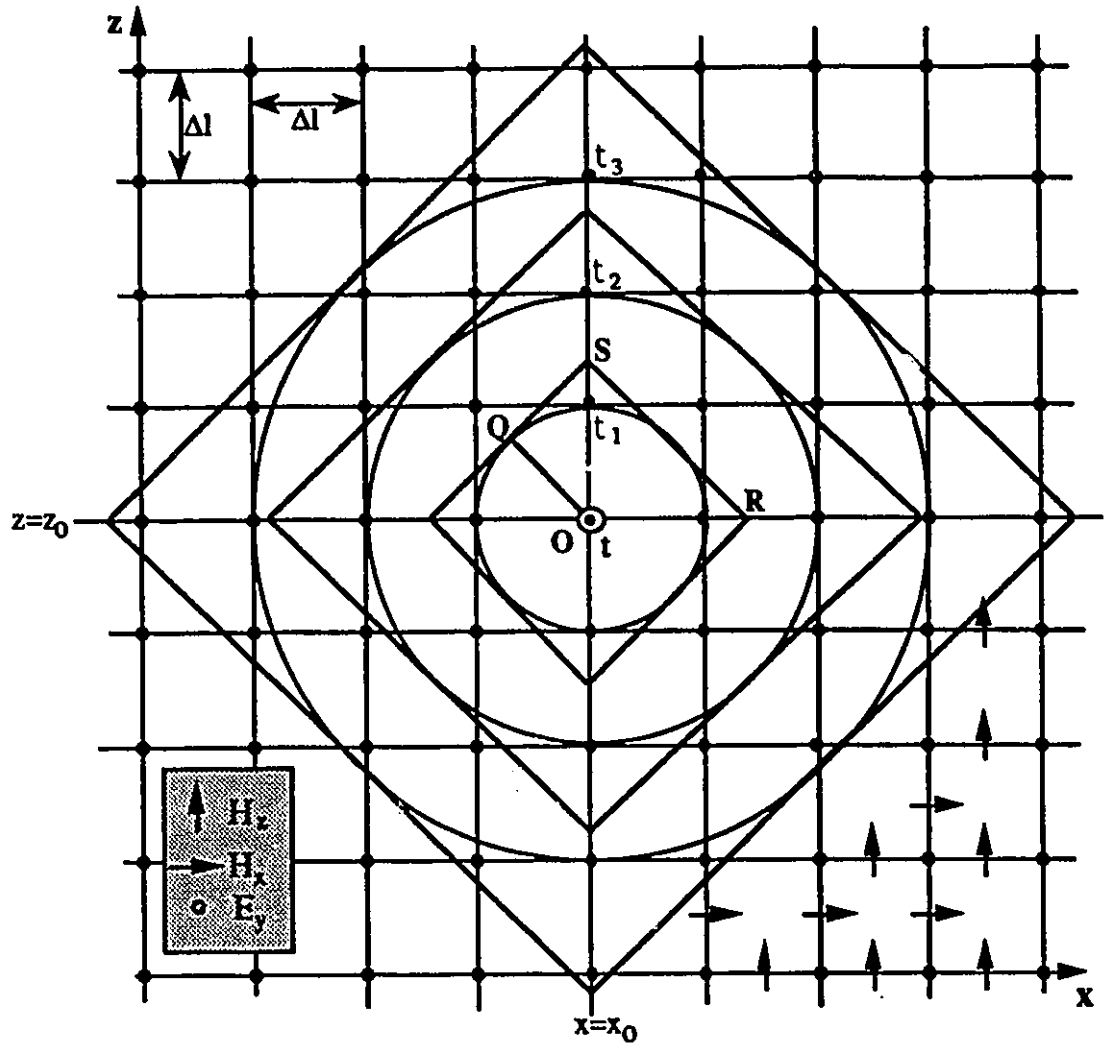


Fig. 3.3.1 Projections of the characteristic circles and squares (propagation behaviour) in the space plane (x,z) at time steps t_1 , t_2 , and t_3 .

Now the square of dependence for the difference equation, shown in Fig. 3.3.1, has

$OR = OS = n\Delta l$ where n is 1, and so the CFL condition is satisfied provided the square includes the circle, and this is the case [2-34] if

$$n \cdot \Delta t \leq \frac{1}{\sqrt{2}} \cdot n \cdot \Delta \ell, \quad (3.3.2a)$$

or

$$\frac{\Delta t}{\Delta \ell} \leq \frac{1}{\sqrt{2}} \quad (3.3.2b)$$

where the speed of light is normalized ($c = 1$). This confirms the stability inequality given by Courant [2-33] and Von Neumann [2-34] and is also shown in Appendix II.

While the circles are interpreted as wave fronts at given instants in the continuous case, the squares are wavefronts in the discrete case. Since a wavefront is normal to the propagation direction, a numerical propagation direction at 45° in a uniform mesh naturally meets that of the continuous model as shown in Fig. 3.3.1. As the angle of propagation direction changes, i.e., from the direction of OQ to the axial direction, the difference between the two cases increases. The numerical wave propagation behaviour shown in Fig. 6 is independent of the choice of the stability factor.

The stability factor can be considered as a proportionality coefficient which controls the propagated distance in the discrete computational domain since the stability factor determines the value of the normalized distance vector on the grid structure. So, the propagated distance is maximum for the maximum value of the stability factor (which provides the maximum Δt). We can predict how the numerical wave propagates in a uniformly meshed domain with the formula

$$c \cdot n \cdot \Delta t = SF \cdot k \cdot \Delta \ell, \quad (3.3.3)$$

where SF is the stability factor and k is the number of the node in the direction of numerical wave propagation. If SF is zero, then the numerical wave is stationary, i.e., does not propagate at all. Some value close to zero requires a large number of iterations.

This effect of the stability factor must be included in the Fourier transform as follows:

$$s(f) = \sum_{n=1}^N S_n(i_o, j_o, k_o) e^{-j2\pi \cdot n \cdot f \cdot SF} \quad (3.3.4)$$

where s is the spectrum, S is the time domain sample, n is the iteration number, (i_o, j_o, k_o) is the sampling position in the computational domain, N is the total number of time intervals for which the simulation (calculation) is made, and $f = \frac{\Delta \ell}{\lambda}$ is the frequency measured in cycles per sampling interval.

3.4 Numerical dispersion relation and anisotropy The standard way of analyzing the distortion of a propagating wave is to study its dispersion relation. The numerical discretization of Maxwell's equations produces a numerical dispersive phenomenon, that is different from the physical dispersion phenomena. As its name indicates, this numerical artifact causes the phase velocity to become a function of the mesh size. A wave propagating in a discrete mesh become progressively dispersed with increasing travel

time. Hence, numerical dispersion is a significant problems in the method and thus its effect must be reduced as much as possible. To see the dispersion effects of the numerical approximation, we will analyze dispersion characteristics in a region away from any boundary in order to avoid boundary effects. The velocity is also a function of the stability factor. The numerical dispersion characteristic has been studied in [3-1]. The dispersion relation for the 3-D leap-frog approximation, (2.3.15), is given by

$$\sin^2\left(\frac{\omega\Delta t}{2}\right) = SF^2\left[\sin^2\left(\frac{\beta_x\Delta x}{2}\right) + \sin^2\left(\frac{\beta_y\Delta y}{2}\right) + \sin^2\left(\frac{\beta_z\Delta z}{2}\right)\right] \quad (3.4.1)$$

where β_x , β_y , and β_z are x -, y -, and z - components of the wave number, and $SF = \frac{v_{ph} \cdot \Delta t}{\Delta \ell} \leq \sqrt{\frac{\epsilon_r \mu_r}{n}}$. We know that the continuous dispersion relation in free space (no dispersion) is

$$\beta_o^2 = \frac{\omega^2}{c^2} = \beta_x^2 + \beta_y^2 + \beta_z^2. \quad (3.4.2)$$

As Δx , Δy , Δz , and Δt go to zero, (3.4.1) reduces to (3.4.2). This means that the dispersion increases, as the mesh size $\Delta \ell$ becomes larger. For TE mode propagation in the two dimensions, (3.4.1) reduces to

$$\sin^2\left(\frac{\omega\Delta t}{2}\right) = SF^2\left[\sin^2\left(\frac{\beta \cdot \cos \theta \cdot \Delta x}{2}\right) + \sin^2\left(\frac{\beta \cdot \sin \theta \cdot \Delta z}{2}\right)\right] \quad (3.4.3)$$

where θ is the propagation angle with respect to positive x -axis. Equation (3.4.3) is further reduced for the normalized phase velocity by using a uniform mesh as

$$\frac{v_{ph}}{c} = \frac{\lambda_o}{SF \cdot \pi \cdot \Delta \ell} \sin^{-1} [SF \sqrt{\sin^2(\frac{\pi \cdot \Delta \ell \cdot \cos \theta}{\lambda_o}) + \sin^2(\frac{\pi \cdot \Delta \ell \cdot \sin \theta}{\lambda_o})}] \quad (3.4.4)$$

The normalized phase velocity, (3.4.4), is plotted as a function of the propagation angle for four different mesh sizes at $SF = \frac{1}{\sqrt{2}}$. This is shown in Fig. 3.4.1 where the unity of the normalized phase velocity indicates no dispersion at all. Fig. 3.4.2 demonstrates the same characteristic at $SF=0.5$ as shown in [3-1]. By comparing the two figures, Figs. 3.4.1 and 3.4.2, the smaller numerical dispersion error is shown at $SF = \frac{1}{\sqrt{2}}$ rather than at $SF=0.5$ for the two-dimensional case. For the mesh size, $\frac{\lambda_o}{\Delta \ell} = 10$, and any propagation angle in the mesh the maximum dispersion error predicted for $SF = \frac{1}{\sqrt{2}}$ is 0.837%, whereas for $SF=0.5$ the minimum dispersion is 1.24 %.

Fig. 3.4.3 illustrates the effect of the stability factor on the numerical dispersion error if the mesh size is $\frac{\lambda_o}{\Delta \ell} = 10$. A comparison of the dispersion property at four different values of the stability factor (0.1, 0.3, 0.5, and $\frac{1}{\sqrt{2}}$) means that the upper limit of the stability inequality would yield the least error due to numerical dispersion for a given mesh size.

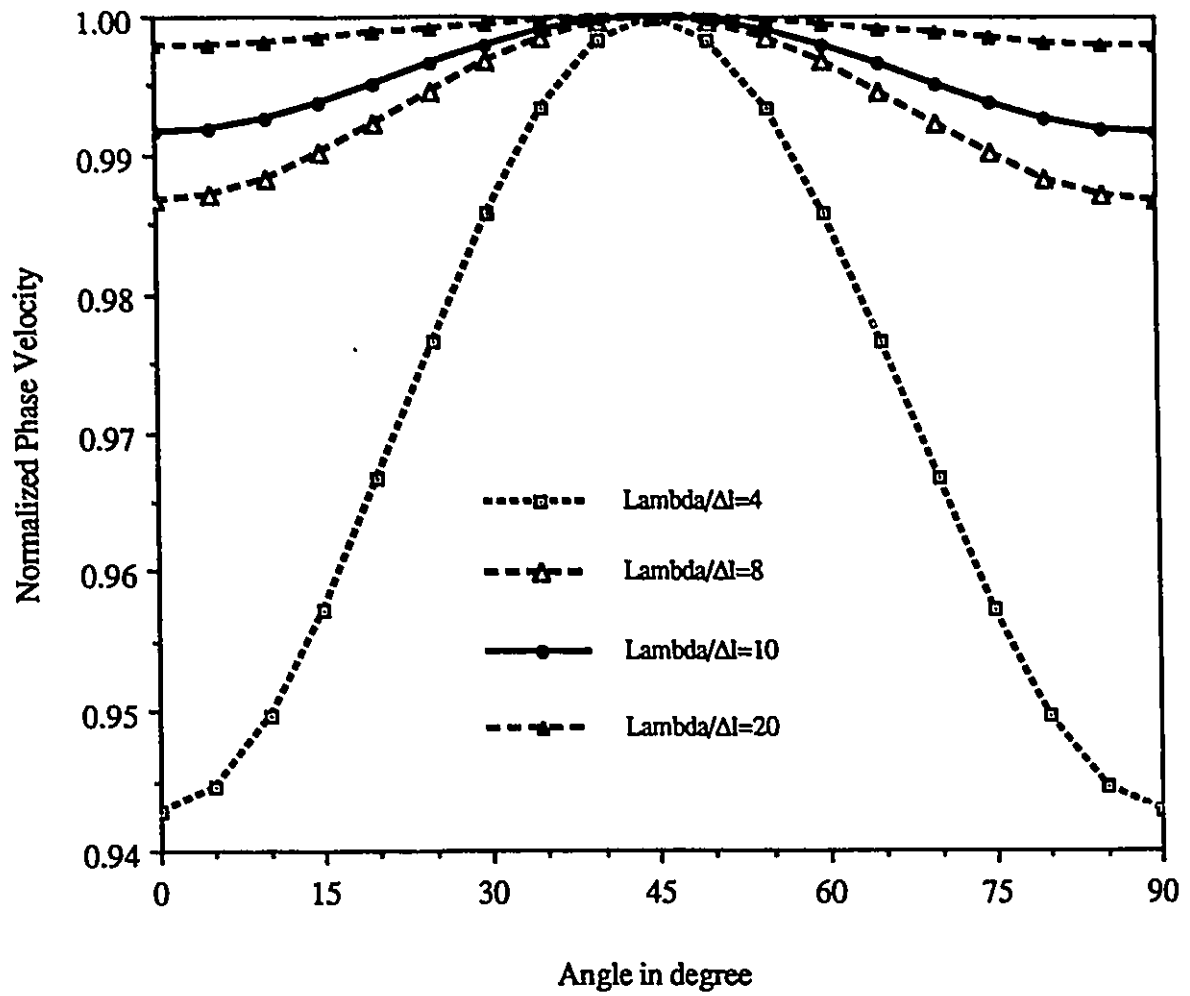


Fig. 3.4.1 Numerical dispersion characteristics for various mesh sizes at a stability factor $SF = \frac{1}{\sqrt{2}}$.

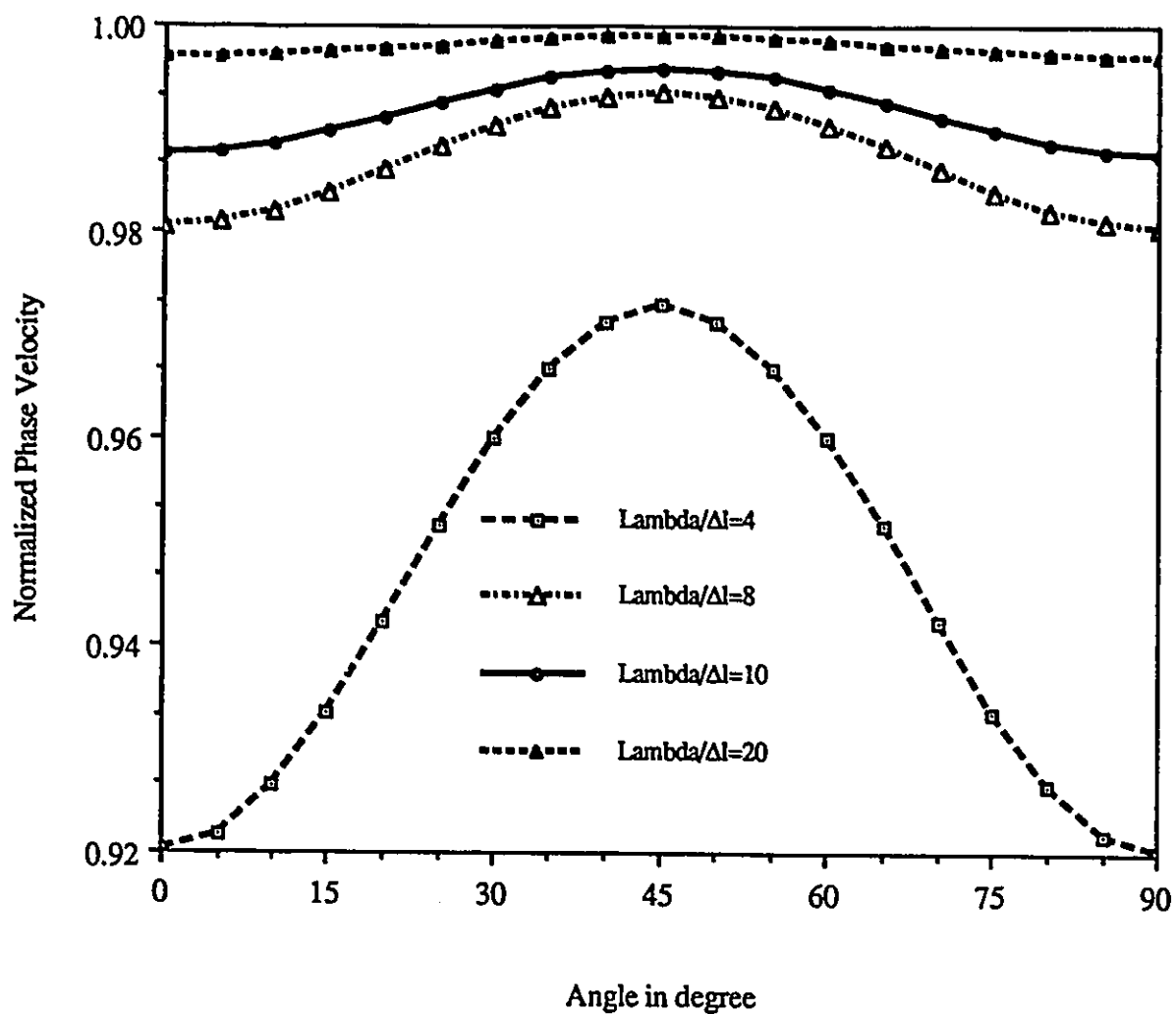


Fig. 3.4.2 Numerical dispersion characteristics for various mesh sizes at $SF = 0.5$.

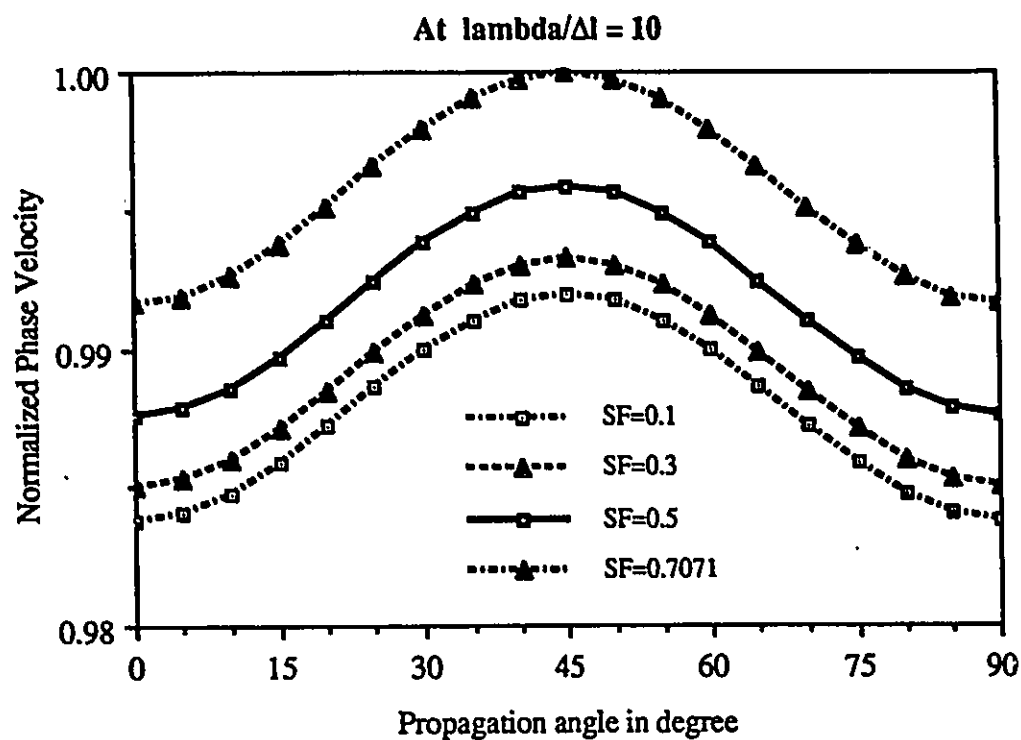


Fig. 3.4.3 Numerical dispersion characteristics for various values of the stability factor.

From Figs. 3.4.1, 3.4.2, and 3.4.3, it is observed that the numerical phase velocity is maximum at a propagation angle of 45° and minimum at angles of 0° and 90° for any mesh size. We can see from Fig. 3.3.1 that only at 45° the discrete propagation characteristic meets that of the continuous propagation. This agrees with the above dispersion analysis. The numerical dispersion also causes the higher frequency components to be delayed relative to the lower frequency components and thus substantial *tailing* of the signal arises. In order to keep the dispersion error less than 0.5 % in the 2-D case, $SF = \frac{1}{\sqrt{2}}$ and a minimum mesh parameter of $\frac{\lambda}{13}$ must be used in the program formulation. Fig. 3.4.3 suggests that the upper limit of the stability inequality [3-2] will ensure lowest dispersion error and the smallest number of iterations.

In addition to being dependent upon frequency, the propagation velocity of the numerical solutions is also dependent upon direction. This property is called the numerical anisotropy resulting from the space discretization, not from the time discretization. This occurs in the numerical approximation of hyperbolic equations in two space dimensions, but not in one-dimensional cases. This error depends also on the number of $\Delta\ell$ per wavelength, and is minimized by increasing the number of mesh elements per shortest wavelength ($\frac{\lambda}{\Delta\ell} \geq 12$ for less than 0.5%) in the simulation. The derivation for TE modes is included in Appendix I. For a uniform mesh and the leap-frog approximation, the numerical phase velocity associated with the space discretization can be obtained with

$$\frac{c^*}{c} = \{\sin^2(\beta\Delta\ell \cos \theta) \cos^2(\beta\Delta\ell \sin \theta) + \sin^2(\beta\Delta\ell \sin \theta) \cos^2(\beta\Delta\ell \cos \theta)\}^{\frac{1}{2}} \quad (3.4.5)$$

where θ is the propagation direction with respect to the x axis. The derivation of (3.4.5) is shown in Appendix I. Note that if $\beta\Delta\ell \rightarrow 0$, $c^* \rightarrow c$. A polar diagram representing

the normalized phase velocity $\frac{c}{c}$ as a function of $\beta\Delta\ell$ and propagation direction θ is shown in Fig. 3.4.4. It is interesting to note that the anisotropy error can be neglected if a wavelength is resolved by more than $8\Delta\ell$.

3.5 Group velocity As we noted in the last section, errors due to numerical dispersion are introduced by the leap-frog approximation of Maxwell's equations. Thus the numerical group velocity involved in the initial (Gaussian) pulse must be considered. The group velocity indicates the speed and direction of the propagation of the energy contained in the spectral component of a wave packet or wave group. *Energy* is used here in the general sense of a quantity proportional to the amplitude of the variable squared. For dispersive waves, the group velocity differs from the phase velocity and is perhaps a more important quantity to examine in an error evaluation than the phase velocity. The CFL stability condition also governs the numerical group velocity. As in the numerical phase velocity case, the numerical group velocity error is minimum at the upper limit of the stability inequality as will be shown later in this section.

The group velocity, $v_g = \frac{d\omega}{d\beta}$, is derived from the dispersion relation (3.4.1) [2-42] and is

$$v_g = \frac{SF \sqrt{\sin^2(\beta\Delta\ell \cdot \cos \alpha_x) + \sin^2(\beta\Delta\ell \cdot \cos \alpha_y) + \sin^2(\beta\Delta\ell \cdot \cos \alpha_z)}}{\sin(\omega\Delta t)}, \quad (3.5.1)$$

where SF is the stability factor and α_x , α_y , and α_z are the wave propagation angles with respect to the coordinates x , y , and z respectively.

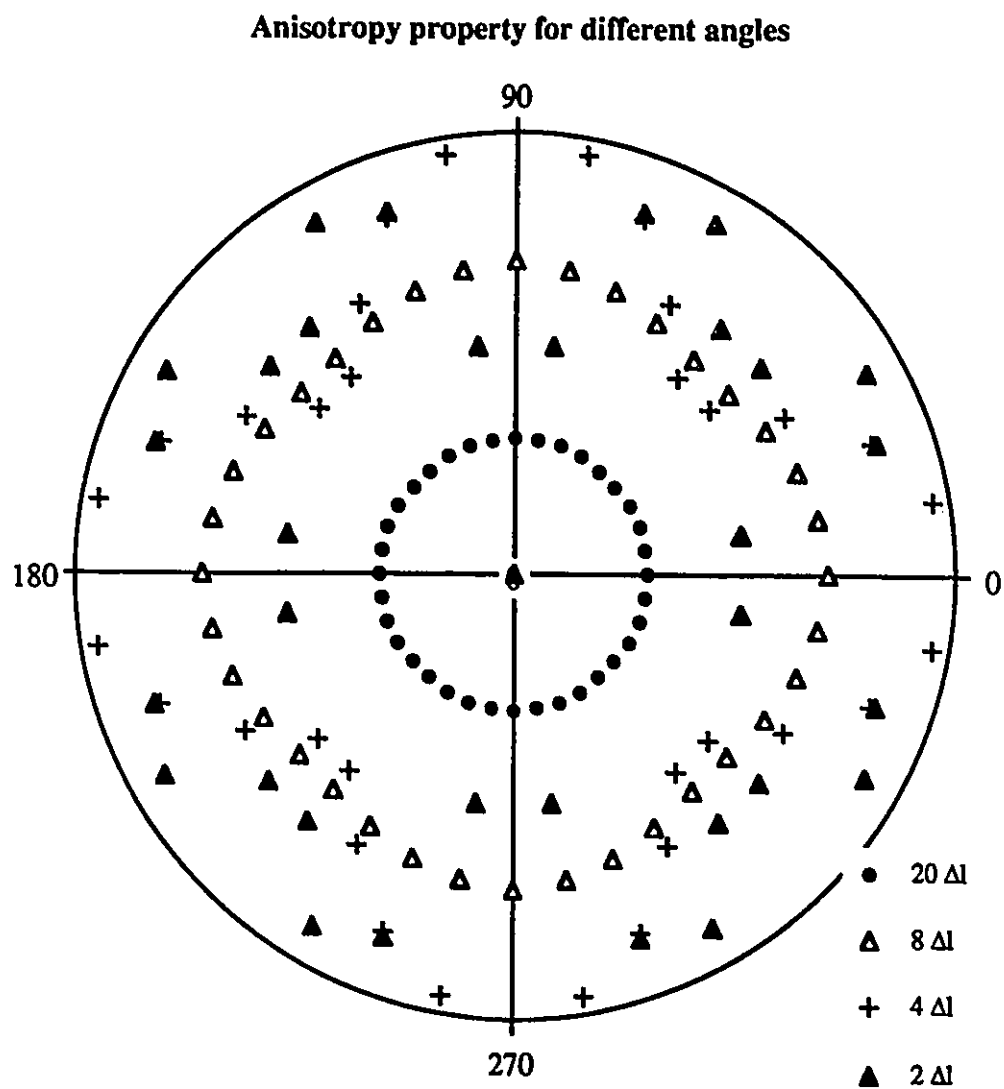


Fig. 3.4.4 The anisotropy is represented in a polar diagram for four different mesh sizes. Note that amplitudes are not related to each other.

In Fig. 3.5.1, the numerical group velocity characteristic at propagation angles 0° or 90° (along the mesh) versus $\beta\Delta\ell$ (radian) is shown for different values of the stability factor. This characteristic again suggests the use of a value close to the upper limit of the stability inequality. Another point is that the group velocity will be zero at $\beta\Delta\ell = \pi$ which corresponds to a wavelength $2\Delta\ell$ in an axial direction. This is directly related to the Nyquist sampling criterion for the minimum case.

In Fig. 3.5.2, the group velocity characteristic at a propagation angle of 45° , (diagonal in the mesh) as a function of $\beta\Delta\ell$ (radian) is illustrated for four different values of the stability factor. This figure shows that the group velocity is faster for a propagation angle of 45° than that at 0° or 90° .

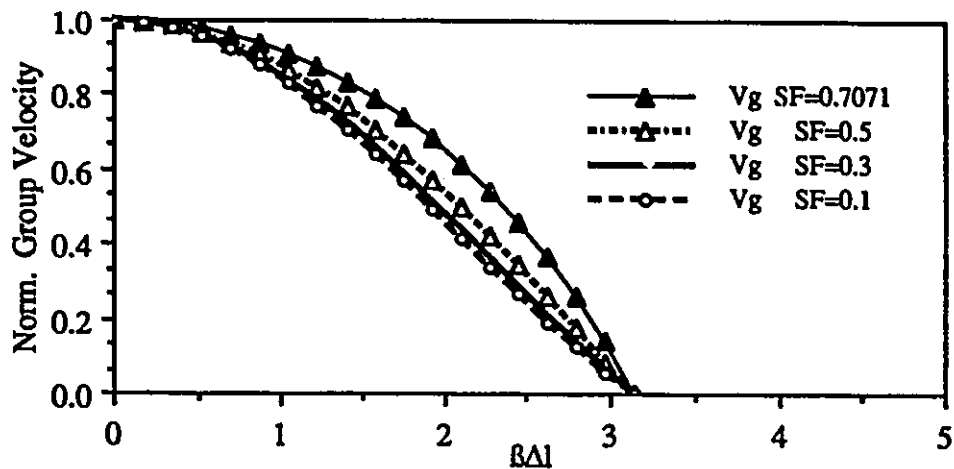


Fig. 3.5.1 Comparison of the group velocity error at the propagation angle (0° or 90°) for different values of the stability factor.

In particular, no group velocity error occurs at the upper limit of the stability inequality. This again confirms that the local TD-FD wave propagates in the discretized computational domain as the continuous case at the propagation direction 45° as mentioned in the previous section in this chapter.

In Fig. 3.5.3, a comparison between the group and the phase velocity characteristics at a propagation angle of 45° (diagonal), with respect to $\beta\Delta\ell$ is illustrated for three different values of the stability factor.

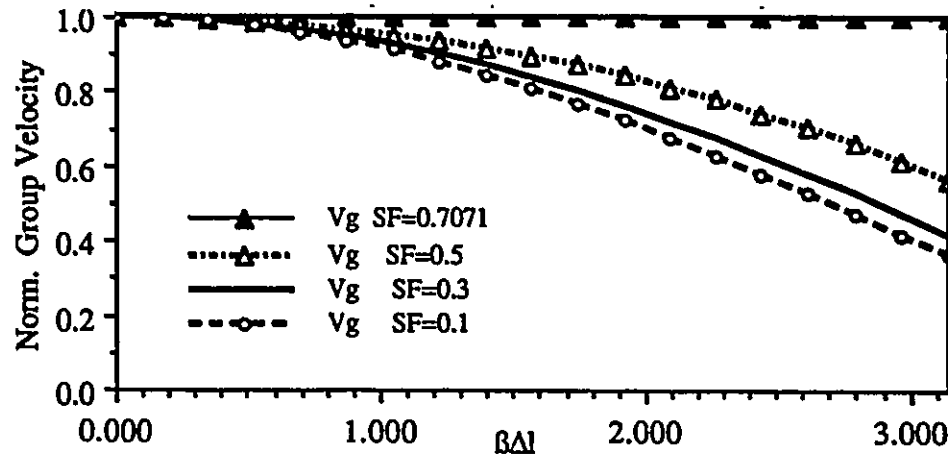


Fig. 3.5.2 Comparison of the group velocity error at the propagation angle (45°) for different values of the stability factor.

It shows that no velocity error (for both the group and the phase velocity) occurs at

the upper limit of the stability inequality. This comparison also illustrates that the group velocity is always slower than the phase velocity. As a result, both velocity errors decrease as the value of the stability factor decreases.

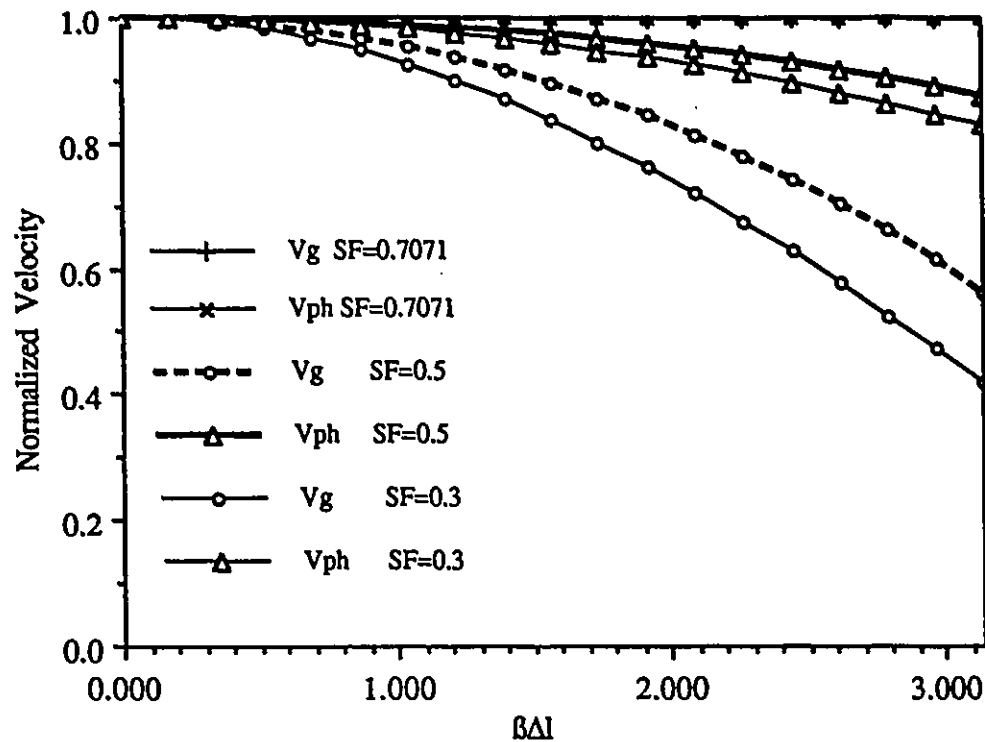


Fig. 3.5.3 Comparison of the phase and the group velocity errors at the propagation angle (45°) for different values of the stability factor.

3.6 Global error checking algorithm Any simulation must be checked for convergence to a correct physical result. But the method requires a huge amount of memory to analyze a practical guided wave transmission structure. A breadboard model has therefore been introduced to help illustrate the ability of the method to simulate guided wave propagation. It is straightforward to discuss the accuracy of the method in a waveguide with uniform cross-section in terms of its amplitude and phase errors. We have introduced the relevant physical properties to check the convergence of CW and pulse excitation cases for any guided wave transmission structure. These are the magnitude of a standing wave in the uniform waveguide without obstacles for the CW case, or the phase linearity (constant phase difference between any two points separated by the same distance along a guide) and non-dissipativity of the leap-frog scheme for the pulse case. The non-dissipativity property ensures constant amplitude characteristics at a single frequency along the uniform waveguide. The global error checking criteria will be introduced in the next two subsections for TE_{10} mode propagation with a standard homogeneous waveguide used as a breadboard model. Before complex guiding structures can be analyzed, results from uniform guides without obstacles should be tested for proper convergence. Studies of waveguides with uniform cross-section may provide useful indications of behaviour in more complex structures containing some discontinuities.

The computational domain is shown in Fig. 3.6.1 with the field positions on the fundamental mesh block.

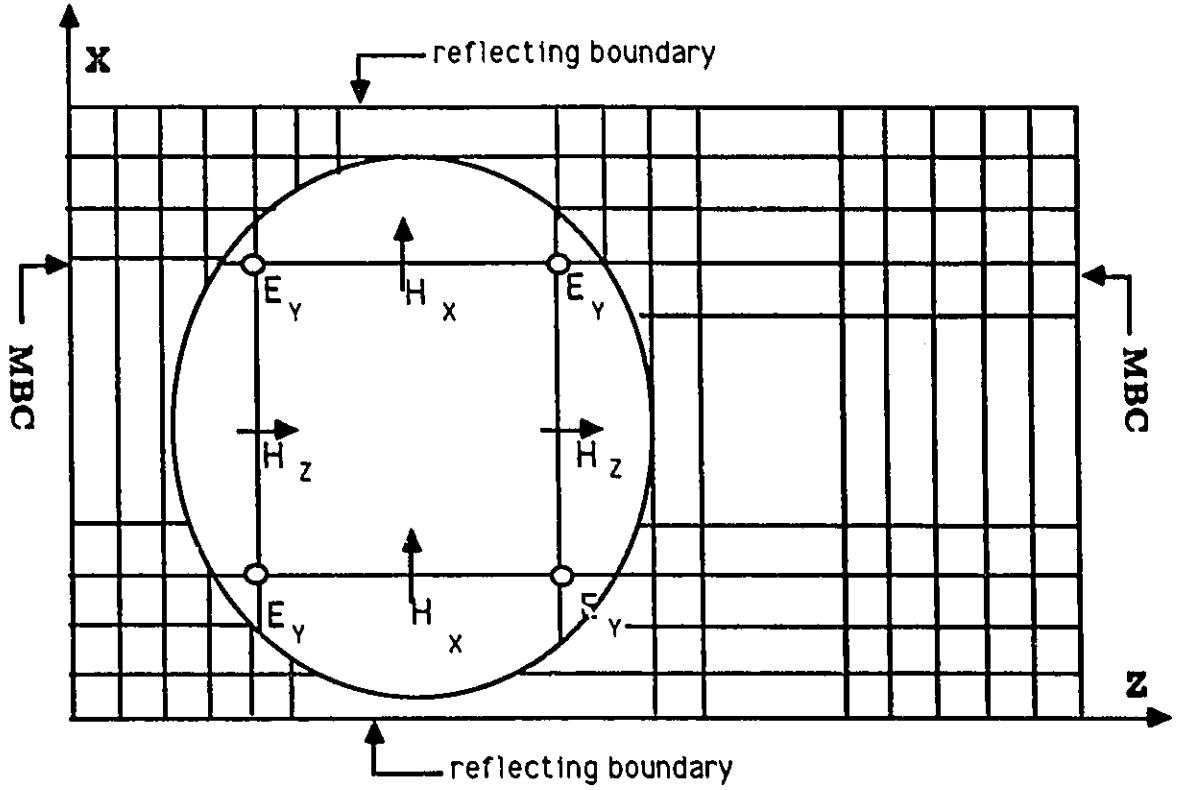


Fig. 3.6.1 TD-FD cell based on Ampere's law for TE mode propagation in the computational domain.

3.6.1 CW case A numerical standing wave envelope is formulated in a waveguide with uniform cross-section without any discontinuities as follows:

$$E_y(z, t) = \text{Re}\{E_{y0}e^{j\beta z}(1 + \Gamma_o e^{-j2\beta z})e^{j\omega t}\}, \quad (3.6.1)$$

$$|E_y(z, t)|_{\max} = |E_{y0}|(1 + |\Gamma_o|), \quad (3.6.2a)$$

$$|E_y(z, t)|_{\min} = |E_{y0}|(1 - |\Gamma_o|), \quad (3.6.2b)$$

where E_{y0} is the incident wave and $E_y(z, t)$ is the resultant standing wave. We have the maximum and minimum standing wave ratios, $S_{\max}$ and $S_{\min}$ as follows;

$$S_{\max} = \frac{|E_y(z, t)|_{\max}}{|E_{y0}|} = 1 + |\Gamma_o| \quad (3.6.3a)$$

$$S_{\min} = \frac{|E_y(z, t)|_{\min}}{|E_{y0}|} = 1 - |\Gamma_o| \quad (3.6.3b)$$

When the matching boundary condition is perfect ($\Gamma_o = 0$),

$$S_{\max} = S_{\min} = 1. \quad (3.6.4)$$

This condition serves as the convergence checking criterion for the CW case.

3.6.2 Pulse case Assuming a wave propagating in the + z direction, the excitation field E_y (Gaussian pulse) was initially applied along the z direction at $t = 0$ with a half-sinusoidal distribution in the x direction as

$$E_{yi}(x, z, t = 0) = E_{yio}(x) \cdot e^{-\frac{z^2}{W^2}}, \quad (3.6.5)$$

where W is the pulse width. The Gaussian pulse may be expressed as a sum of many plane waves as

$$E_{yi}(x, z) = \int_{\omega_1}^{\omega_2} A(\beta_z) \cdot e^{-j(\beta_x z + \beta_z z)} \cdot d\beta_z = \sum_{i=\omega_1}^{\omega_2} A_i \cdot e^{-j\beta_i z}, \quad (3.6.6)$$

where $\beta_z = \sqrt{\beta_o^2 - \beta_x^2}$. The quantity $A(\beta_z)$ can be thought of as the amplitude of that component of the plane wave whose wave number in the z direction is β_z . $A(\beta_z) = \frac{W}{2\sqrt{\pi}} E_{yio}(x) \cdot e^{-\frac{W^2 \beta_z^2}{4}} = \frac{W}{2\sqrt{\pi}} \sin(\beta_x x) \cdot e^{-\frac{W^2 \beta_z^2}{4}}$. Then by virtue of the linearity of the problem, the properties of the solution may be assessed from the propagation of a single Fourier mode $e^{-j\beta z}$ (when using the Fourier transform, β is allowed to range over

all real numbers). The amplitude and phase of the Gaussian pulse at an arbitrary plane z can be obtained as follows:

$$E_{yo}(x, z) = E_{yoo}(x, z) \cdot e^{-j\theta_o(x, z)}, \quad (3.6.7)$$

where the amplitude is

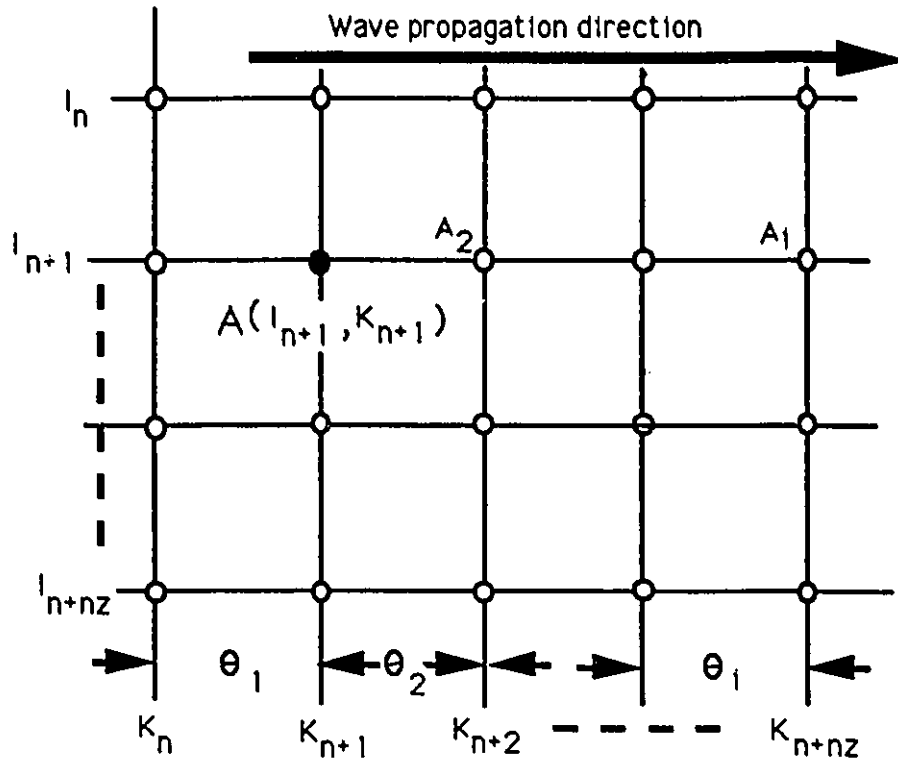
$$E_{yoo}(x, z) = \frac{\sqrt{\frac{\beta_o}{2}} W E_{yio}(x, z)}{(1 + x^2)^{\frac{1}{4}}} \cdot e^{-\frac{2\beta_o z^2 \sqrt{1+x^2}}{\beta_o^2 W^2 + 4x^2}}$$

and the phase is

$$\theta_o(x, z) = -(1 + \frac{z}{2x})\beta_o z + \frac{\pi}{8} = \beta \cdot z.$$

The propagation constant along the transmission line is β .

A convergence criterion can be defined as follows: the complex phasor obtained from the Fourier transform is characterized by its amplitude and its phase. It has the following two properties: firstly, for any frequency component, the amplitude of the Fourier transform must be constant along a waveguide of uniform cross-section. (This is directly related to the non-dissipative nature of the leap-frog scheme.). Secondly, each cross-sectional plane is a locus of constant phase or propagation constant. For each frequency, the phase factor βz must decrease uniformly along the propagation direction. Thus, as shown in Fig. 3.6.2, the phase difference between any two points having the same distance must be constant along the guide. From this property, the eigenvalues of the transmission line can be calculated.



A and N are amplitudes of field values on various node points, and θ is the phase difference between two adjacent K 's.

Fig. 3.6.2 A section of a discretized guiding structure.

As a result, we can summarize the criteria at one frequency as follows:

$$\theta_{oi+1}(I, K_{n+1}) - \theta_{oi}(I, K_n) = \text{constant}, \quad (3.6.8)$$

and

$$A_i(I_{\text{const}}, K) = \text{constant}. \quad (3.6.9)$$

The non-dissipativity property directly related to the numerical energy conservation is mathematically shown in Appendix II for TE propagation.

3.7 Summary In this chapter, we have introduced the numerical wave propagation characteristics of the TD-FD method in an attempt to better understand the method. The discrete wave propagation properties of the method have been based on the characteristic phenomena in the continuous case. Waves distorted by the numerical approximation have been analyzed with the TD-FD dispersion relation which includes the stability factor. So, as the value of the stability factor is decreased, the dispersion error (velocity error) is increased as mentioned in Sections 3.4 and 3.5. Therefore, we propose to use a value close to the upper limit of the stability inequality for an accurate TD-FD simulation as in [3-3] and [3-2]. It is important to note that the stability factor must also be included in the discrete Fourier transform since the stability factor functions as a proportionality coefficient for the propagation distance on the mesh as mentioned earlier in this chapter.

Finally, we have introduced a global error (phase and amplitude) estimation scheme [3-4] for a wave guiding structure. This scheme uses relevant physical properties which must be consistent with any uniform transmission structures for both CW and pulse propagation to produce guidelines for determining the optimum number of iterations (the steady state condition must also be considered) involved in a simulation and developing a good excitation pulse shape. Both properties confirm the fact that Maxwell's two curl equations can be separated into transverse and longitudinal parts in any guide of uniform cross-section. It also allows us to use a small computational domain

in the form of the computational breadboard model and enables us to check that the code works properly.

CHAPTER 4

Matching Boundary Condition

4.1 Introduction For the analysis of guided wave transmission structures, the matched condition of the reflection coefficient, $\Gamma = 0$, is required. This condition is usually obtained in an infinitely long wave guiding structure where the domain of the computed field is not deteriorated by some reflected waves. No computer can store an unlimited amount of data, and so the field computation zone must be limited. Therefore, it is necessary to introduce artificial boundaries to obtain a matched condition at the edge of a finite computational region.

The artificial boundaries that have been developed do not provide perfect matching and thus produce reflections which obscure the simulated propagation phenomena. The mismatch becomes very apparent when simulating scattering from discontinuity in a wave guiding structure. To obtain the best accuracy when computing the field, the matching boundary condition (MBC) must produce only very small reflections when a wave (CW or pulse excitation) is incident upon it. Otherwise, the

waves reflected into a computational domain will degrade the simulation results and possibly cause instabilities in the computation.

A considerable amount of research [4-1]-[4-13] has been done to develop and improve boundary conditions which minimize reflections. These absorbing boundaries can be grouped into two broad classes: global and local boundaries. Most research effort has been devoted to local boundaries. The class of global boundaries is one that obtains an absorbing property from the calculation of a whole computational domain [4-13]. The local class is characterized by its local spatial and temporal nature, and is based on physical or mathematical approximations. The term *local* implies that the conditions involve only spatial and temporal points in the neighborhood of the boundary point under consideration at the time of evaluation.

This study is concerned only with the local boundary class. Two techniques for the local boundary condition were reviewed in [4-2]: (1) the far field approximation technique and (2) the one-way wave equation approximation technique. Three other different approaches that have been devised are i) the short and open circuit approach proposed by Smith [4-3], ii) the super absorbing boundary condition by Fang and Mei[4-11], and iii) the correction of velocity error near the boundary using the dispersion relation [4-14].

With the short and open circuit approach, the simulation is done twice for each absorbing boundary: once with an open circuit condition, and once with a short circuit condition. Since these two boundary conditions produce reflections that are opposite in sign, the sum of the two cases will cause a cancellation of the reflected fields. The main shortcoming of this approach is that the entire set of computations must be repeated many times.

The super absorbing boundary approach sounds excellent from its title, but there have been no test results published and no details of the approach exposed. The last approach works fine, but only for a narrow frequency range (around 8 % of the whole standard waveguide operating frequency band for return loss better than 30 dB).

The far field approximation technique is based on the far field expansion of outward radiating solutions (the Sommerfeld radiation condition [4-5]). For pulse applications, the radiating solution of the scalar wave equation (i.e., solutions propagating in directions which are outward from the origin of a spherical coordinate system) has been expanded in a convergent series in [4-6] and [2-22]. In this approach one must translate the coordinate system if Cartesian coordinates are used.

The one-way wave equation approximation technique will be reviewed briefly in this chapter. A number of researchers have been involved in this approach. It was introduced to the applied mathematical community by Engquist and Majda [4-7] in 1977, and by Mur [4-8] to the EM engineering community in 1981. Some recent theoretical advances have been made by Trefethen and Halpern [4-9] and Higdon [4-10], and a review paper describing the approach was published by Blaschak and Kriegsmann [4-1] in 1988.

In [4-1], it is noted that the approach using lower orders of Pade approximations has created problems (reflections) in pulse applications, even in 2-D cases, and that higher orders of Pade approximations have also been used, however, the same problem (instability) persisted.

I am introducing a new approach for wide band applications, which seems promising for future research, and is based on the transition operator (matrix) concept discussed in Section 4.3. The reflection property obtained with this new approach will be illustrated in Section 4.4. We will also suggest to use an absorbing termination

approach which includes the conductivity terms in Maxwell's equations for a dissipative terminations and this will be described in Section 4.5. At the end of this chapter there is a summary and discussion of this new method.

4.2 One-way wave equation approximation Maxwell's equations cannot be used to formulate the matching boundary conditions directly since the equations require a coupled form of boundary. We thus use the wave equation. The wave equation shown in (4.2.1) describes a wave propagating in all directions.

$$\frac{1}{c^2} \vec{U}_{tt} = \vec{U}_{xx} + \vec{U}_{yy} + \vec{U}_{zz} \quad (4.2.1)$$

where $\vec{U} = [E_x, E_y, E_z, H_x, H_y, H_z]^T$ and the double subscripts indicate the second order partial differential operators such as $\vec{U}_{tt} = \frac{\partial^2}{\partial t^2} \vec{U}$.

The equation, which describes a wave propagating in only one direction, (in the positive or negative direction of z for example), is called the one-way wave equation. For the one space dimensional case, it is easily obtained by using the following formal factorization of the differential operator for the wave equation,

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial z^2} \right) \vec{U} = \left(\frac{1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial z} \right) \cdot \left(\frac{1}{c} \frac{\partial}{\partial t} - \frac{\partial}{\partial z} \right) \vec{U} = L_+ L_- \vec{U} = 0, \quad (4.2.2)$$

and the general solutions of which are $f(t \mp \frac{z}{c})$. The constant c is the velocity of propagation. The operator $L_+ = \frac{1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial z}$ dictates the forward moving part of wave, the other operator $L_- = \frac{1}{c} \frac{\partial}{\partial t} - \frac{\partial}{\partial z}$ dictates the backward moving part of the wave. To obtain a non-reflecting condition we set

$$L_{\pm} = 0. \quad (4.2.3)$$

The solution of (4.2.2) is given by

$$\vec{U} = e^{j(\omega t - \beta z)} + \Gamma e^{j(\omega t + \beta z)}. \quad (4.2.4)$$

Substituting (4.2.4) into the boundary condition (4.2.3) and solving for Γ , we obtain

$$\Gamma = 0. \quad (4.2.5)$$

More generally, the wave front of interest in our model can be represented by a sum of plane waves so that a wave travelling backward can be represented by

$$\vec{U}(z, t) = \sum_{i=1}^{\infty} A_i e^{j(\omega_i t + \beta_i z)}, \quad (4.2.6a)$$

and a wave traveling forward can be represented by

$$\vec{U}(z, t) = \sum_{i=1}^{\infty} A_i e^{j(\omega_i t - \beta_i z)}, \quad (4.2.6b)$$

where $\omega_i = \beta_i c$ and $i=1, 2, \dots$. These two conditions also yield the condition $\Gamma = 0$, if we substitute them into (4.2.2).

Here we will digress a bit to explain the function of the electric wall boundary condition used in the method as

$$\vec{U}_{\text{tangential}}(a, t) = 0. \quad (4.2.7)$$

Substituting (4.2.4) into (4.2.7) and solving for Γ , we find that

$$|\Gamma| = 1. \quad (4.2.8)$$

Equation (4.2.8) implies that all the waves incident on the boundary will be reflected with the same amplitude, whereas (4.2.5) implies that no reflected wave will be created by the boundary condition (4.2.3).

The one-dimensional case is trivial, and works well, but the 2-D and 3-D cases are not easy to implement. We will review the 2-D case (see [4-12] for details). The matched condition can be written by using (4.2.1):

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \nabla\right) \cdot \left(\frac{1}{c} \frac{\partial}{\partial t} - \nabla\right) \vec{U} = 0. \quad (4.2.9)$$

The general solution of (4.2.9) is of the form

$$\vec{U} = f_1(\vec{R} - ct) + f_2(\vec{R} + ct),$$

which is the expression shown in Chapter 2. The total field including reflections for an electric field can be expressed by

$$\vec{E}(x, z, t) = e^{j(\omega t \pm \beta x \sin \theta - \beta z \cos \theta)} + \Gamma e^{j(\omega t \pm \beta x \sin \theta + \beta z \cos \theta)} \quad (4.2.10)$$

Through the factorization (4.2.2), a MacLaurin Series expansion, and algebraic manipulation, we obtain

$$\left| \frac{\partial}{\partial z} \frac{1}{c} \frac{\partial}{\partial t} \pm \partial_{zz} + \frac{1}{2} (\partial_{zz}) \right| \vec{U} = 0, \quad (4.2.11)$$

where '+' is for forward moving wave components and '-' for backward moving wave components. Substituting (4.2.10) into (4.2.11), we obtain

$$|\Gamma| = \left| \frac{\cos \theta - 1}{\cos \theta + 1} \right|. \quad (4.2.12)$$

This reflection property is shown in Fig. 4.2.1 (see the no modification case) as a function of the angle of incidence angle θ . The reflection property is not good except at around

0° incident angle. However, if the coefficient $\frac{1}{2}$ in the numerator of (4.2.11) is modified to $\frac{SF}{1+SF}$ and $SF = \frac{1}{\sqrt{2}}$, then we obtain better reflection properties, which are also shown in Fig. 4.2.1 (see the modified case). Equation (4.2.11) is modified to read

$$\frac{1}{c} \frac{\partial^2}{\partial z \partial t} + \frac{\partial^2}{\partial z^2} + \frac{SF}{1+SF} \left(\frac{\partial^2}{\partial x^2} \right) = 0, \quad (4.2.13a)$$

$$\frac{1}{c} \frac{\partial^2}{\partial z \partial t} - \frac{\partial^2}{\partial z^2} - \frac{SF}{1+SF} \left(\frac{\partial^2}{\partial x^2} \right) = 0, \quad (4.2.13b)$$

Rearrange (4.2.13b) and multiply by $(1 + SF)$,

$$\frac{SF}{c^2} \frac{\partial^2}{\partial t^2} + \frac{(1 + SF)}{c} \frac{\partial^2}{\partial z \partial t} + \partial^2 \partial z^2 = 0, \quad (4.2.14)$$

or

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial z} \right) \left(\frac{SF}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial z} \right) = 0 \quad (4.2.15)$$

Similarly, a matching boundary condition for the backward moving wave is

$$\left(\frac{1}{c} \frac{\partial}{\partial t} - \frac{\partial}{\partial z} \right) \left(\frac{SF}{c} \frac{\partial}{\partial t} - \frac{\partial}{\partial z} \right) = 0. \quad (4.2.16)$$

The explicit finite-difference approximation of a E field component at $z = a$ becomes

$$\begin{aligned} E^{n+1}(i, a) = & E^n(i, a) + E^n(i, a - 1) - E^{n-1}(i, a - 1) \\ & - SF[E^n(i, a) - E^n(i, a - 1) - \{E^{n-1}(i, a - 1) - E^{n-1}(i, a - 2)\}] \end{aligned} \quad (4.2.17)$$

where a is an integer.

From the modified case of Fig. 4.2.1, we can see that the reflections for an incident angle greater than 50° are getting bigger, and that at 90° there will be total reflection. But it is noted that at the incident angle of 45°, we obtain zero reflection from the modified version. Remember that in the last chapter, the phase velocity error at the propagation angle 45° and at $SF = \frac{1}{\sqrt{2}}$ is minimum.

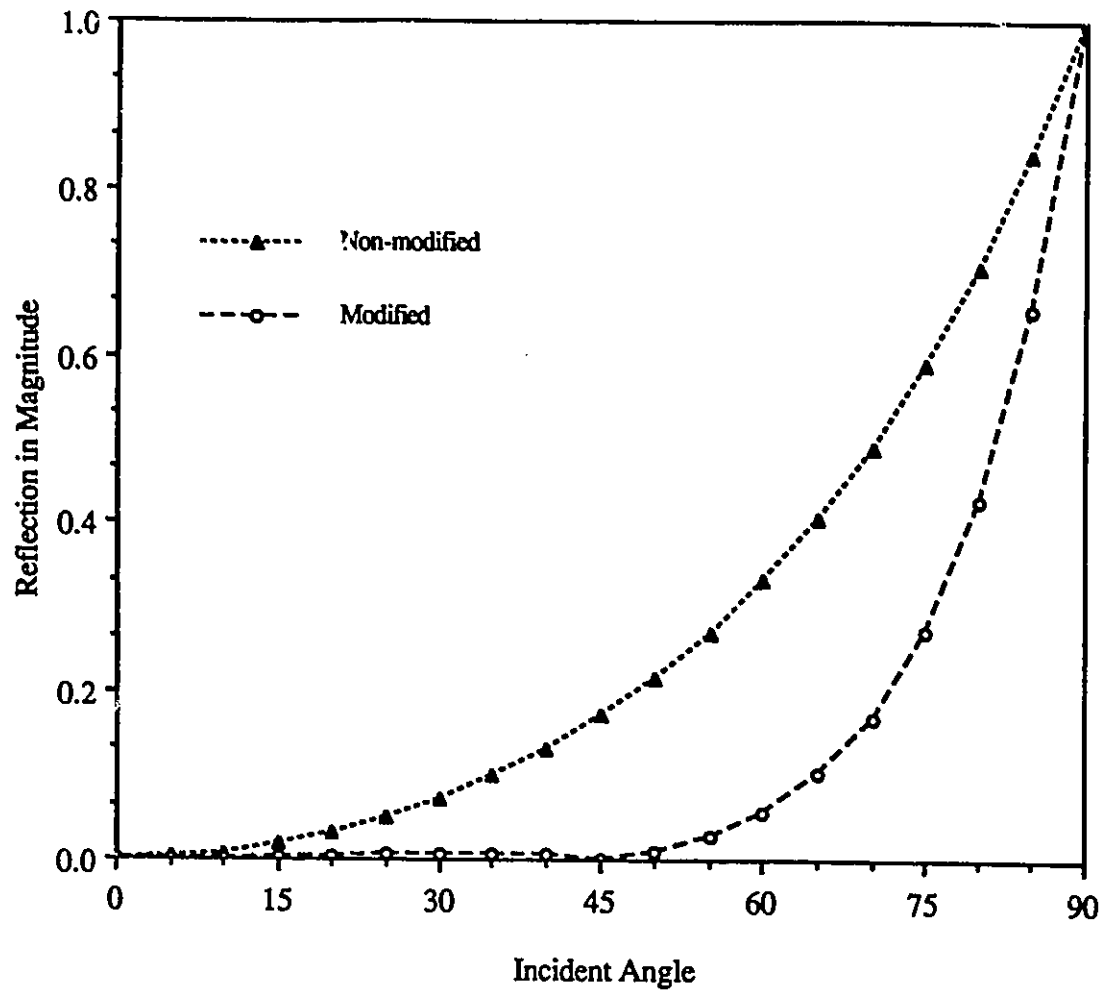


Fig. 4.2.1 Comparison of reflection property for modified and non-modified approximation of the one-way wave equation.

We have tested this boundary condition when we used it as the standard waveguide matching boundary condition for CW application. The reflection property of a MBC can be checked with a numerical SWR measurement in front of a MBC suggested in the last chapter. An empty waveguide is excited with a TE_{10} mode as an initial condition for this numerical experiment. Two MBC's for backward and forward moving waves are placed at each end of the computational domain of the standard rectangular waveguide. The numerical standing wave envelope is computed to sample S_{max} and S_{min} as the main stream of the numerical wave is propagating along the guided path. The standing wave envelope must satisfy the unity condition for the matched condition shown in Section 3.6. The value of S_{max} and S_{min} at the simulation output are checked with the unity condition for the upper limit of the stability inequality. The result obtained with the above procedure for different numbers of $\Delta\ell$ in the waveguide width are compared with the unity condition and compiled in Table 4.2.1. They represent the worst cases obtained over the operating bandwidth of the dominant mode of the waveguide at a constant propagation velocity (the number of iterations required increases as $\Delta\ell$ decreases). The numbers indicating the percentage in the max. and min. columns of SWR are giving the deviation from the matching criterion *unity*, i.e., the positive numbers indicate an error greater than unity in percent, and the negative numbers the errors less than unity in percentage. Also, we can observe numerical wave propagation phenomena through the boundary as computing time increases as shown in Fig. 4.2.2. Fig. 4.2.2a illustrates the E_y component of the TE_{10} mode propagating in an empty waveguide, and Fig. 4.2.2b the same field component with a metallic discontinuity in the same waveguide. MBC's were placed at the left and the right ends of the waveguide, for both cases, and the incident wave was launched at the right end of the waveguide. The waveforms were sampled after 2000 iterations. No significant reflections can be noticed as already shown from the

numerical SWR measurement of Table 4.2.1. Note that a small metallic discontinuity is shown in a circle of Fig. 4.2.2b.

The approximation procedure for the one-way wave equation can be considered as a para-axial approximation as follows;

The dispersion relation of the 2-D wave equation is

$$\omega = c(\beta_x^2 + \beta_z^2)^{\frac{1}{2}}, \quad (4.2.23)$$

where ω is a real function of the spatial wave numbers, β_x and β_z . If we consider spatial extrapolation of the 2-D wave equation (say, in the z-direction), the appropriate form of the dispersion relation is

$$\beta_z = \pm \left(\frac{\omega}{c} \right) \left[1 - \frac{c^2 \beta_x^2}{\omega^2} \right]^{\frac{1}{2}}. \quad (4.2.24)$$

Size of Waveguide	width	7 Δl	14 Δl	21 Δl	28 Δl
	Length	110 Δl	220 Δl	330 Δl	440 Δl
Iteration No.		220	440	660	880
SWR	max.	5.66%	5.21%	4.52%	3.95%
	min.	1.21	-0.39	-0.81	-1.77

Table 4.2.1 The numerical SWR experiment showing the reflection property of the MBC.

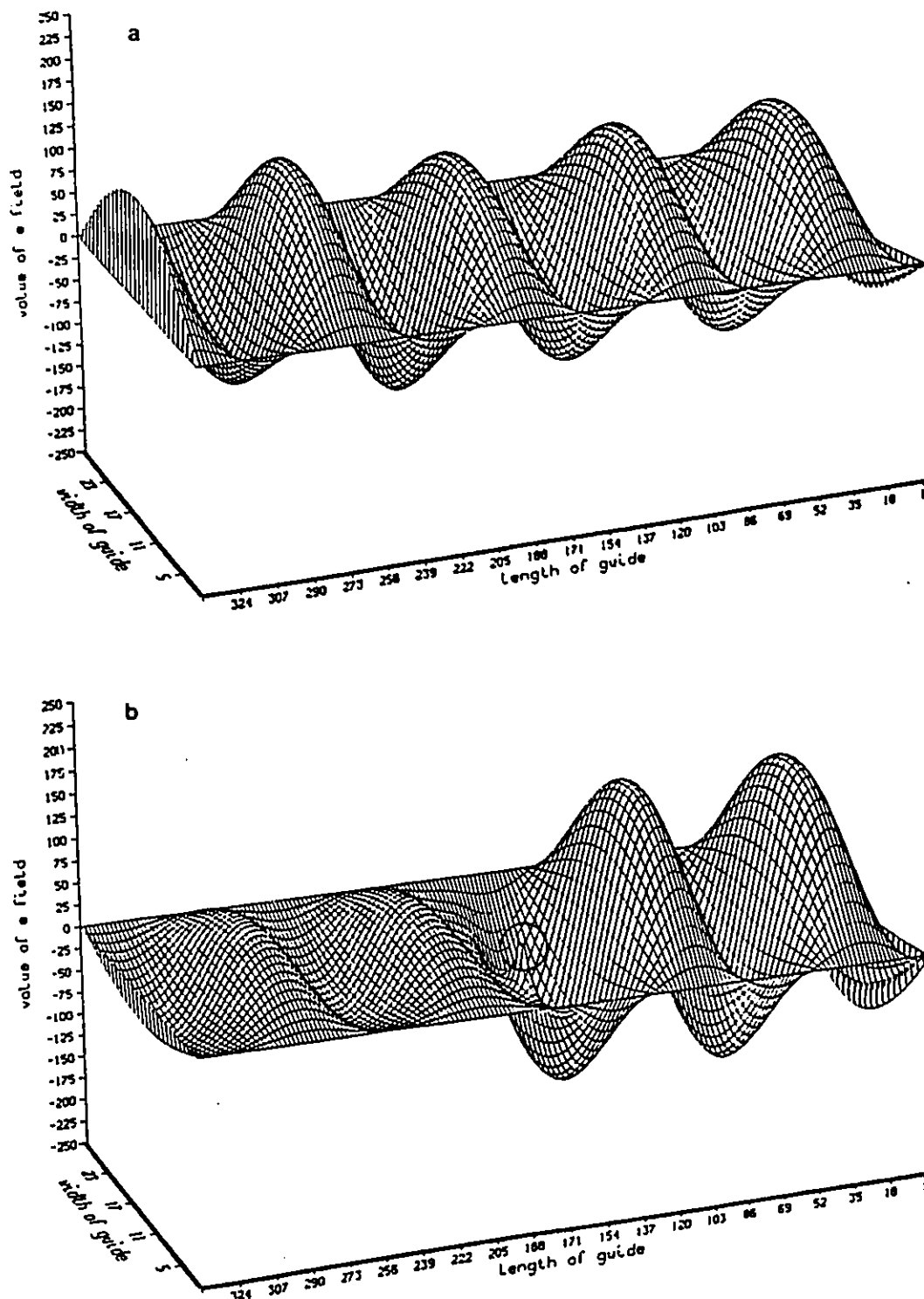


Fig. 4.2.2 Numerical wave propagation simulation in standard waveguide showing the MBC's reflection property (a) empty waveguide, (b) with discontinuity.

Clearly, there is a stability problem when $|\frac{c\beta_z}{\omega}| > 1$ (evanescent waves), since β_z becomes imaginary. It is therefore necessary to modify the wave equation in such a way as to eliminate the evanescent components of the solution. A relatively simple way of accomplishing this is to restrict the range of solutions to those waves that are traveling within a cone of the z-axis (para-axial waves). Note that the $\pm$ sign in (4.2.24) is to describe wave fields moving in opposite directions in z .

4.3 Transition operator matching boundary condition The idea behind this concept for a matching condition in the time domain is as follows: if a wave (a series of points discretized in time) is passing a certain location in an infinite guiding structure, the transition state of the wave function as a function of time can be obtained at a specific location or point. The transition state of the time domain wave function can be treated as a matching condition at the point where waves are passing through. The advantage of this MBC, is that it will be independent of the incident angle, unlike the one-way wave equation approximation approach and thus will have a wide band characteristic. The reflection property, however, is dependent on whether the MBC is simulated as an infinitely long wave guide or with an absorbing material as a waveguide termination (dummy load).

The transition operator, $\vec{T}$, is defined with an open loop system [4-15] as shown in Fig. 4.3.1. The transition operator associated with any linear system presented Fig. 4.3.1 is defined by

$$\vec{T}(t, \tau) \triangleq \vec{U}_1(t) \vec{U}^{-1}(t_o) \quad (4.3.1)$$

where $\tau = t - t_o$, $\vec{U}(t_o)$ is an input signal, and $\vec{U}_1(t)$ an output signal.

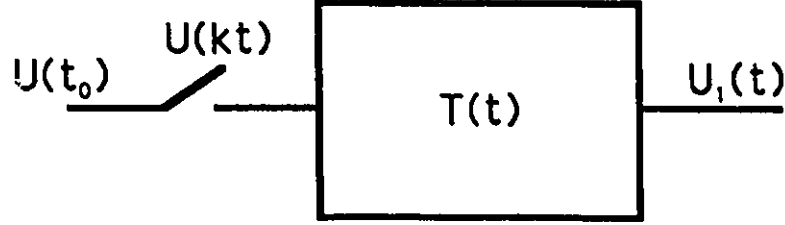


Fig. 4.3.1 Open-loop sampled system.

For the MBC in the discrete domain, the transition operator for only one of the three electric and magnetic field components is needed. So, the transition operator for an E-field wave passing a certain location is

$$\vec{T}^n(I, k1) = \frac{\vec{E}^{n+1}(I, k1 - 1)}{\vec{E}^n(I, k1)}$$

where the E field time distribution is as shown in Fig. 4.3.2 and the transition is considered over one Δt . In the three-dimensional case, assuming the waves are propagating in the k direction (z direction), the transition operator becomes

$$\vec{T}^n(i, j, k) = \frac{\vec{U}^{n+1}(i, j, k + 1)}{\vec{U}^n(i, j, k)}, \quad (4.3.2)$$

where $\vec{U} = [E_x, E_y, E_z, H_x, H_y, H_z]^T$.

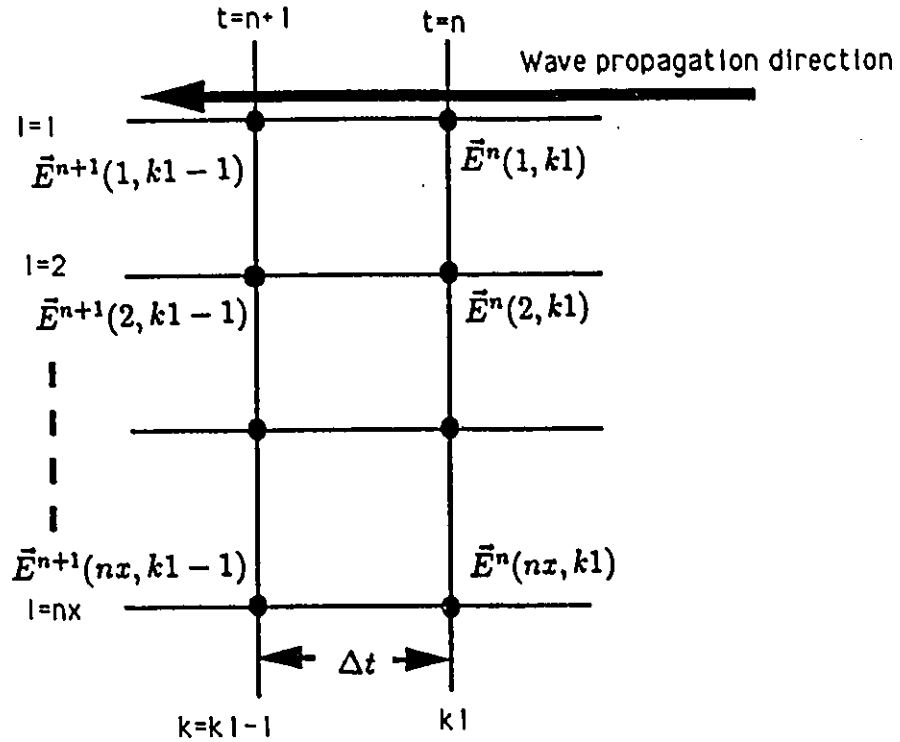


Fig. 4.3.2 A description of the procedure for obtaining the transition operator for a Δt difference in two dimensional space.

As we explained above, a time domain matching condition for the continuous time case may generally be obtained at a specific location by recording the time history of a wave function passing the specific location. The transition operator, $\vec{T}$, the electric field $\vec{E}$, and a source quantity $\vec{K}$ (if it exists) are introduced to use a state transition equation as in modern control theory. If we assume that EM waves are propagating in

+z direction, then the general inhomogeneous equation for the updated field quantities at the specific location, $z = z + dz$, may be expressed as

$$\begin{aligned}\vec{E}(x, y, z + dz, t) = & \vec{T}(x, y, z, t, t_0) \cdot \vec{E}(x, y, z, t_0) \\ & + \int_{t_0}^t \vec{T}(x, y, z, t, \tau) \cdot \vec{K}(x, y, z, \tau) d\tau\end{aligned}\quad (4.3.3)$$

where t and t_0 are the updated time and previous (initial) time $t > t_0$, respectively. For a homogeneous case, the transition operator, $\vec{T}$, of a backward or a forward propagating wave at a specific location is the only parameter required to solve (4.3.3) because $\vec{K}$ is zero in this case.

In the TD-FD formulation, the transition operator is obtained in a preprocessing procedure from the computational domain of a long waveguide at positions $k = k_\mu$, $k = k_{\mu-1}$, $k = k_m$, and $k = k_{m+1}$ and at time steps $t = n$ and $t = n+1$ respectively, to obtain the time domain matching condition, as shown in Fig. 4.3.3. If there is a discontinuity in the computational domain (an inhomogeneous case), then the source quantity $\vec{K}$ must be obtained by comparing the homogeneous case and a condition different from the homogeneous case at k_μ and k_m . Assuming the same propagating direction as in the case of continuous time described above, then an updated $\vec{E}$ field value in discrete form on the boundary $k = k_{m+1}$ can be obtained from the following expression

$$\vec{E}^{n+1}(i, j, k_{m+1}) = \vec{T}^n(i, j, k_m) \cdot \vec{E}^n(i, j, k_m) + \vec{T}^n(i, j, k_m) \cdot \vec{K}^n(i, j, k_m) \quad (4.3.4)$$

for one transition Δt step. The boundary at $k = k_{\mu-1}$ for the other propagation direction can be obtained in a similar manner. Therefore, the solution of (4.3.4) will provide the desired future state of the boundary condition.

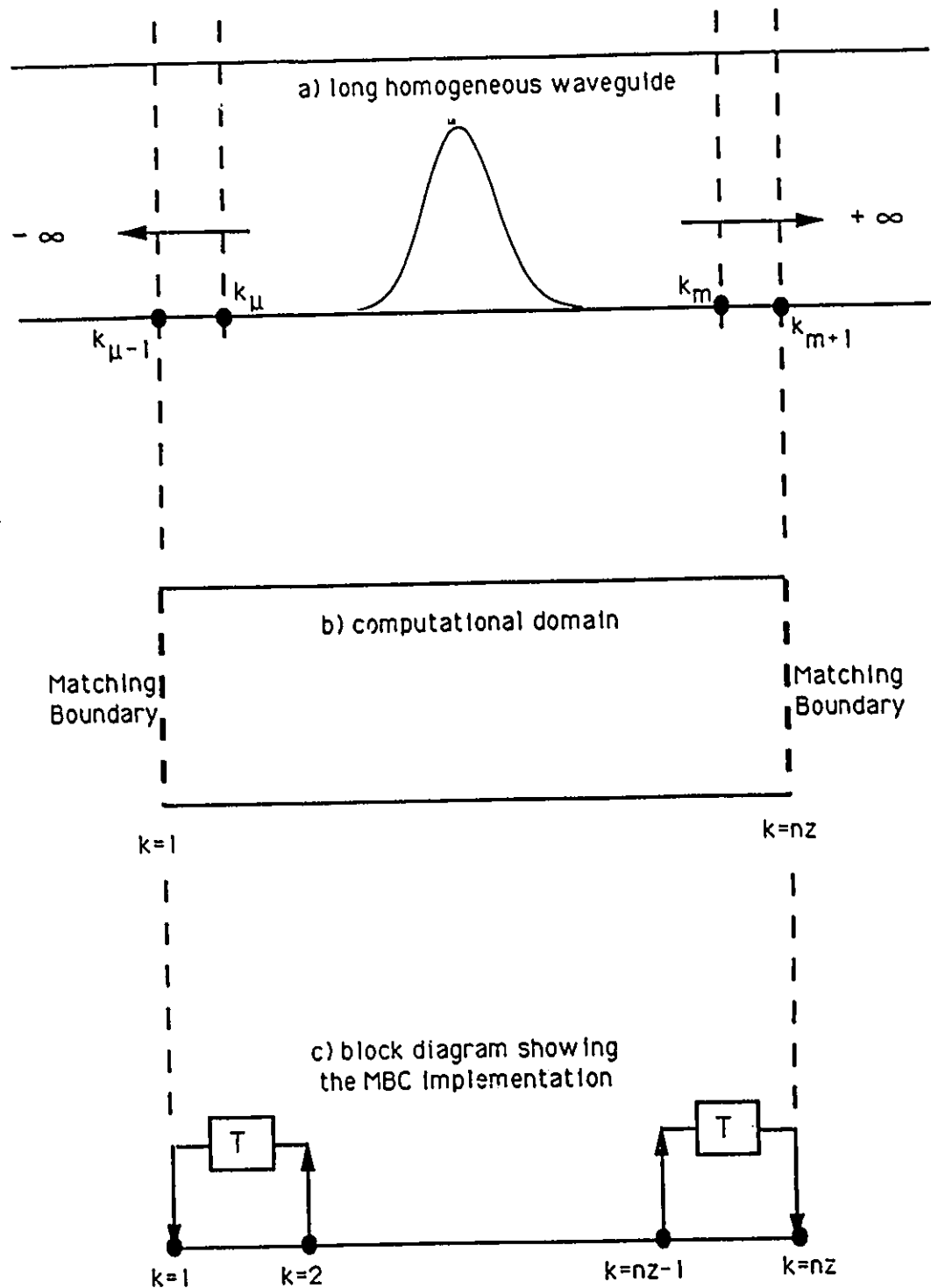


Fig. 4.3.3 A pictorial view of the steps involved in implementing the MBC based on the transition operator concept.

Once $\bar{T}$ is obtained, any discontinuity in the same domain can be analyzed. If a different mesh size is employed, then the transition operator, $\bar{T}$, must be calculated for the different mesh size.

4.4 Test of reflection property To test the reflection property of the MBC described in the last section, the standard homogeneous rectangular waveguide has again been chosen as the computational domain. The matching boundaries are placed at the left and the right ends of the domain. Two guides, $14 \Delta\ell$ and $21 \Delta\ell$ wide, both of length $47 \Delta\ell$, are shown in Fig. 4.3.3b. A Gaussian pulse was excited at the center of the guide, and allowed to propagate in both directions. It was then sampled at points located along the longitudinal direction, and the Fourier transform was performed to obtain the frequency response. The transformed data at every frequency must satisfy the matched condition in a long homogeneous waveguide. Then, the return losses for the above two domains with the MBC were calculated and compared with the return losses for the long waveguide cases (sampled before the reflections come back), as illustrated in Fig. 4.4.1. The observations made for width = $21\Delta\ell$, showed a matching behaviour closer to that of the long homogeneous waveguide, which was used as the convergence criterion for the TD-FD method. We have also tested the MBC when there is a discontinuity in the guide. S-parameters have been calculated for the discontinuity of an E-plane metallic object (the discontinuity dimension is shown in Fig. 4.4.2) that was centered in the rectangular waveguide (width = $21\Delta\ell$). The results were compared with the mode matching results, and are shown in Fig. 4.4.2. Note that between the results obtained with the two methods are different in the higher frequency range (above 38 GHz).

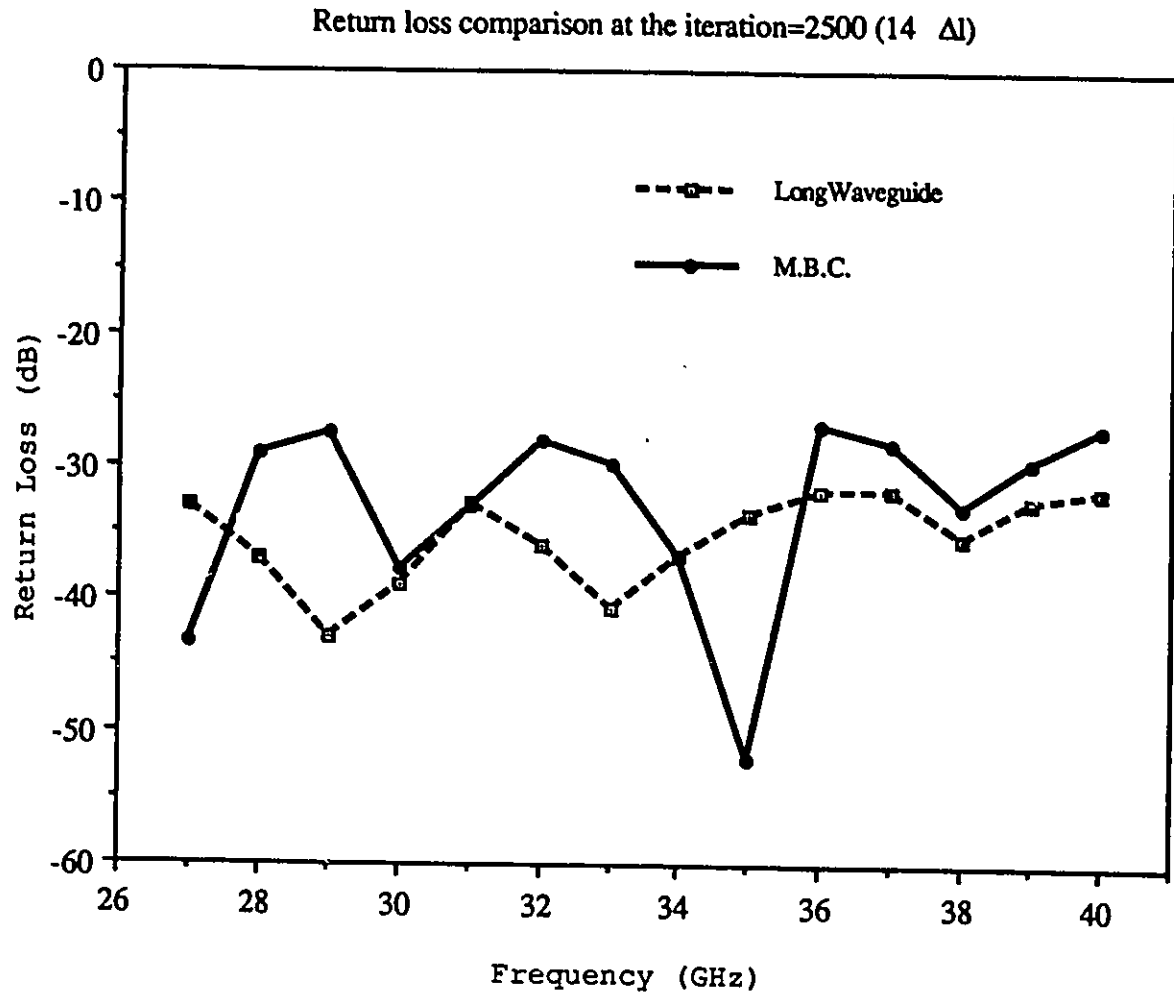


Fig. 4.4.1a Comparison of the return loss of a long homogeneous waveguide with that of a MBC over the standard waveguide band for a width of $14 \Delta \ell$. The domain has a length of $47 \Delta \ell$ in the longitudinal direction.

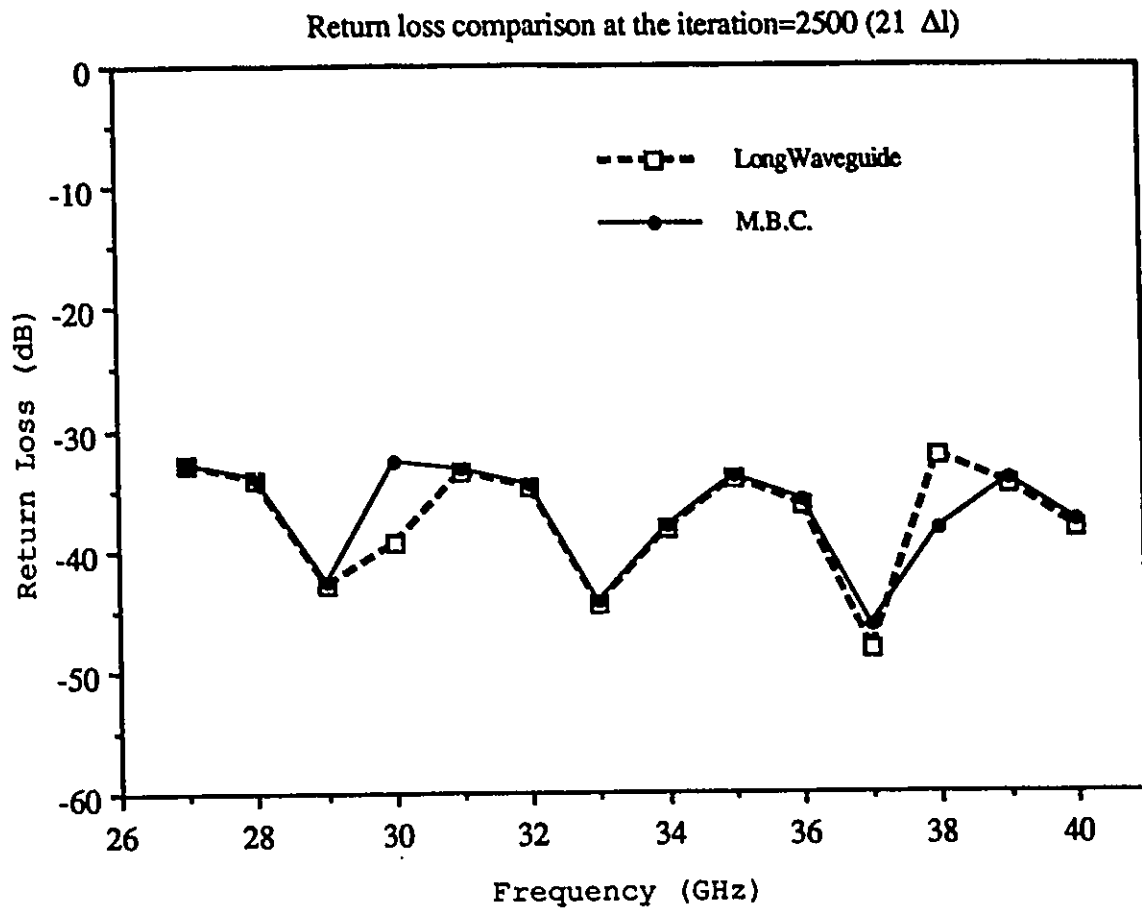


Fig. 4.4.1b Comparison of the return loss of a long homogeneous waveguide with that of a MBC over the standard waveguide band for a width of $21 \Delta \ell$. The domain has a length of $47 \Delta \ell$ in the longitudinal direction.

This is due to the fact that $21 \Delta \ell$ is not a fine enough discretization across the waveguide width to calculate S-parameters. A much finer mesh is required to analyze S-parameter problems in the guide. It was shown in Fig. 4.4.1 that the MBC produced very little reflection, but more study is required to improve the reflection property in cases where the problem is not homogeneous. A return loss of better than 40 dB is required to calculate the S-parameters accurately.

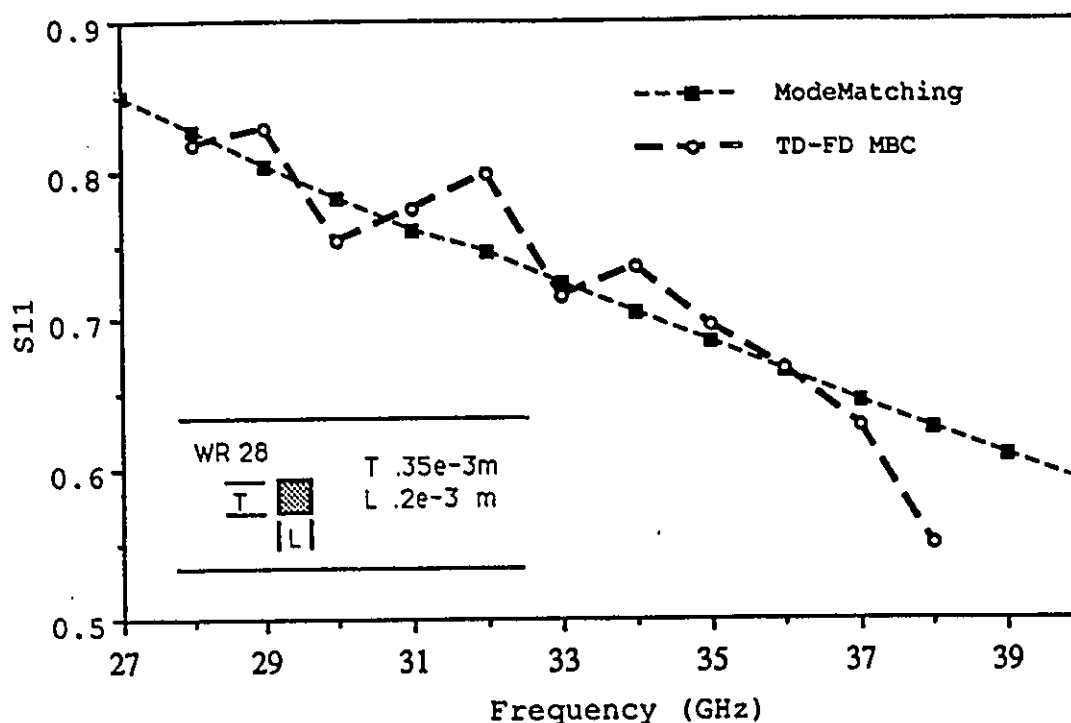


Fig. 4.4.2 Comparison of S_{11} for the E-plane discontinuity shown to test the reflection property of the MBC for an inhomogeneous case.

4.5 Absorbing termination approach The dissipativity property can be obtained by including the electric and magnetic conductivity, σ_E and σ_H in Maxwell's equations,

as

$$\epsilon \frac{\partial \vec{E}}{\partial t} = -\sigma_E \vec{E} + \nabla \times \vec{H} \quad (4.5.1a)$$

$$\mu \frac{\partial \vec{H}}{\partial t} = -\sigma_H \vec{H} - \nabla \times \vec{E}. \quad (4.5.1b)$$

The waveguide matching termination can be simulated with a length of around $200 \Delta \ell$ or more in the wave propagation direction for a return loss of better than 40 dB. The dissipative profile of the matching termination is calculated as

$$\sigma(z) = a \cdot e^{b \cdot z}, \quad (4.5.2)$$

and a and b can be tuned with the criteria introduced in Section 3.6. A slight improvement in the return loss could be obtained with this termination over that obtained with the transition operator matching boundary condition described in the previous section. However, the phase is deteriorated slightly compared to long waveguide case. We can use this absorbing material termination in formulating the transition operator boundary condition. Then, we can have the same return loss characteristics in both cases. But, the phase deteriorated will provide worse S-parameter results.

4.6 Discussion After pointing out the importance of the absorbing boundary condition used in the TD-FD method and presenting a brief historical development, we have reviewed the 3-D MBC approximating the one-way wave equation for CW applications, which has been originally developed for the 2-D case by Reynold [4-12]. For pulse excitation, the transition operator concept used in modern control theory was introduced to obtain a matching boundary condition. The MBC works well but has

certain limitations; i) the location through which the waves are passing must not be far from the source position. ii) The distance of the matching boundary from the source position is an inverse function of the number of iterations. Thus the number of iterations is reduced, as the location of the MBC can be placed farther away from the source. The reason for this limitation is not yet understood and will be studied further.

CHAPTER 5

Local Mesh Refinement Algorithm

5.1 Introduction It is rather straightforward to model a region with smoothly varying field by using a uniform grid system of large mesh size. However, when the computational domain contains sharp discontinuities or localized objects, the fields become highly non-uniform in the vicinity of the discontinuities, and a mesh of very small mesh size must be employed. This requires considerable computational effort and resources.

There are two ways to take into account the strong non-uniformity around a local discontinuity. The first is to use a mesh with gradually changing mesh size as it is currently employed in the TLM method. Such a procedure was introduced in the TD-FD method by Choi and Hoefer [5-1]. The problem with this method is that for a constant stability factor throughout the mesh, the time step Δt must always be varied in accordance with the local mesh size $\Delta \ell$.

In this chapter, we propose an alternative approach which is a local regridding procedure for the leap-frog approximation of Maxwell's two curl equations, referred

to as a *mesh refinement scheme*. This approach was mathematically analyzed by [5-2]. Berger and Oliger [5-3] have presented a computational algorithm in more general form for simple general hyperbolic partial differential equations in 1984. I have applied this approach specifically to Maxwell's two curl equations. In this approach we embed a locally uniform mesh of higher density into the larger mesh adaptively. The local uniformity of the mesh is important for keeping the same stability criterion, in both the fine and coarse mesh regions during a simulation. This means that in the different subparts of the mesh, the ratio of Δt and $\Delta \ell$ is kept the same. This has the advantage that in all subareas of the mesh exactly the same TD-FD algorithm can be employed.

On the other hand, Holland and Simpson [5-4] introduced the thin-strut formalism to include arbitrary fine wires in their TD-FD code, THREDE, in 1981. Kunz and Simpson [5-5] also introduced an expansion approach to resolve locally fine objects. They first computed the field with a coarse mesh, thus obtaining the values of the tangential electric field at interfaces with a subsequently refined mesh area, which was analyzed in a second run.

In my approach, the coarse and the fine mesh regions are solved simultaneously, and the boundary conditions between the two regions are enforced to ensure a smooth transition of highly non-uniform field quantities. Furthermore, this scheme is recursive, that is, it can provide a finer and finer resolution if necessary.

The algorithm for this local mesh refinement scheme is presented in detail in Section 5.2. To demonstrate the accuracy and the efficiency of our algorithm, we have modeled a thin metallic discontinuity in a standard rectangular waveguide, and have compared results with those obtained with a uniform mesh. This is done in Section 5.3. Finally, we will discuss some limitations and further study of the approach in the last section.

5.2 Mesh refinement algorithm For ease of understanding, we introduce the mesh refinement algorithm for the two space dimensional case and assume TE mode propagation. In this case, the discretized Maxwell's equations are:

$$H_x^{n+\frac{1}{2}}(i, k + \frac{1}{2}) = H_x^{n-\frac{1}{2}}(i, k + \frac{1}{2}) + \frac{c\Delta t}{Z_o\Delta z}[E_y^n(i, k+1) - E_y^n(i, k)] \quad (5.2.1a)$$

$$H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, k) = H_z^{n-\frac{1}{2}}(i + \frac{1}{2}, k) - \frac{c\Delta t}{Z_o\Delta x}[E_y^n(i+1, k) - E_y^n(i, k)] \quad (5.2.1b)$$

$$\begin{aligned} E_y^{n+1}(i, k) = E_y^n(i, k) + \frac{Z_o c \Delta t}{\Delta z} [H_x^{n+\frac{1}{2}}(i, k + \frac{1}{2}) - H_x^{n+\frac{1}{2}}(i, k - \frac{1}{2})] \\ - \frac{Z_o c \Delta t}{\Delta x} [H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, k) - H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, k)] \end{aligned} \quad (5.2.1c)$$

where indices (i, k) correspond to the Cartesian coordinates (x, z) in the discrete domain, and the superscript n indicates the time step.

The computational cell for the TE mode and the definition of the field vector components in a cell are shown in Fig. 5.2.1. The fine mesh is denser than the coarse mesh by a factor of four. Fig. 5.2.2 illustrates the leap-frog scheme which all previous researchers using the TD-FD method have exclusively used, in three dimension (x, z, t) , and shows the characteristic lines for the discretized Maxwell's equations (dotted lines). The characteristic lines from the apexes P_1 and P_2 shown in Fig. 5.2.2 imply that the numerical wave is propagating from the coarse (P_1) to the fine (P_2) mesh. The propagation of the waves corresponding to the TD-FD solution should point in the direction of these lines of determination. The slope of the line of determination in the three dimension must be consistent (identical and continuous) in the coarse mesh, the fine mesh, and in the transition regions.

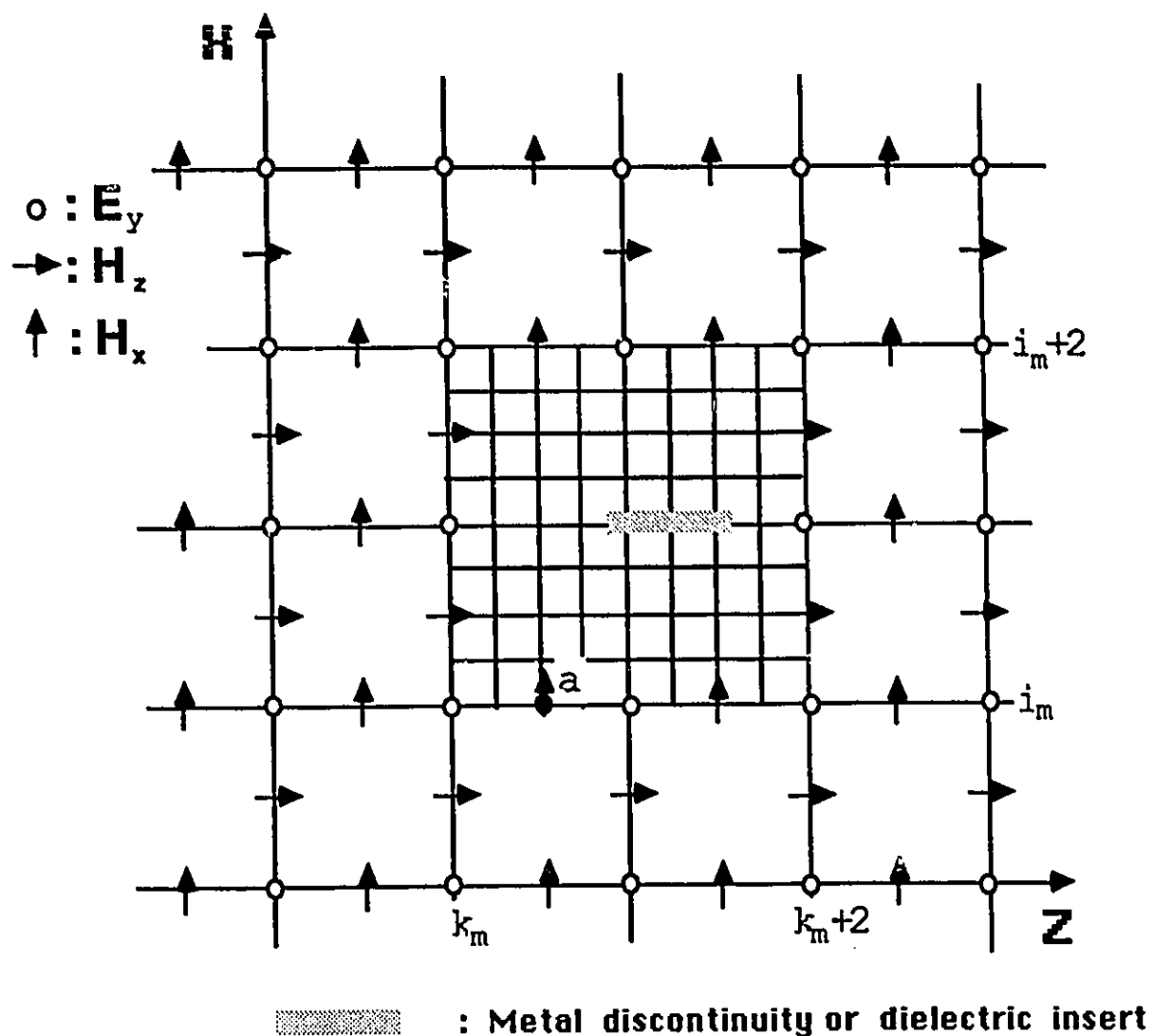


Fig. 5.2.1 The 1:4 local mesh refinement scheme in two space dimensions, and the field components allocated on the cell by Ampere's law.

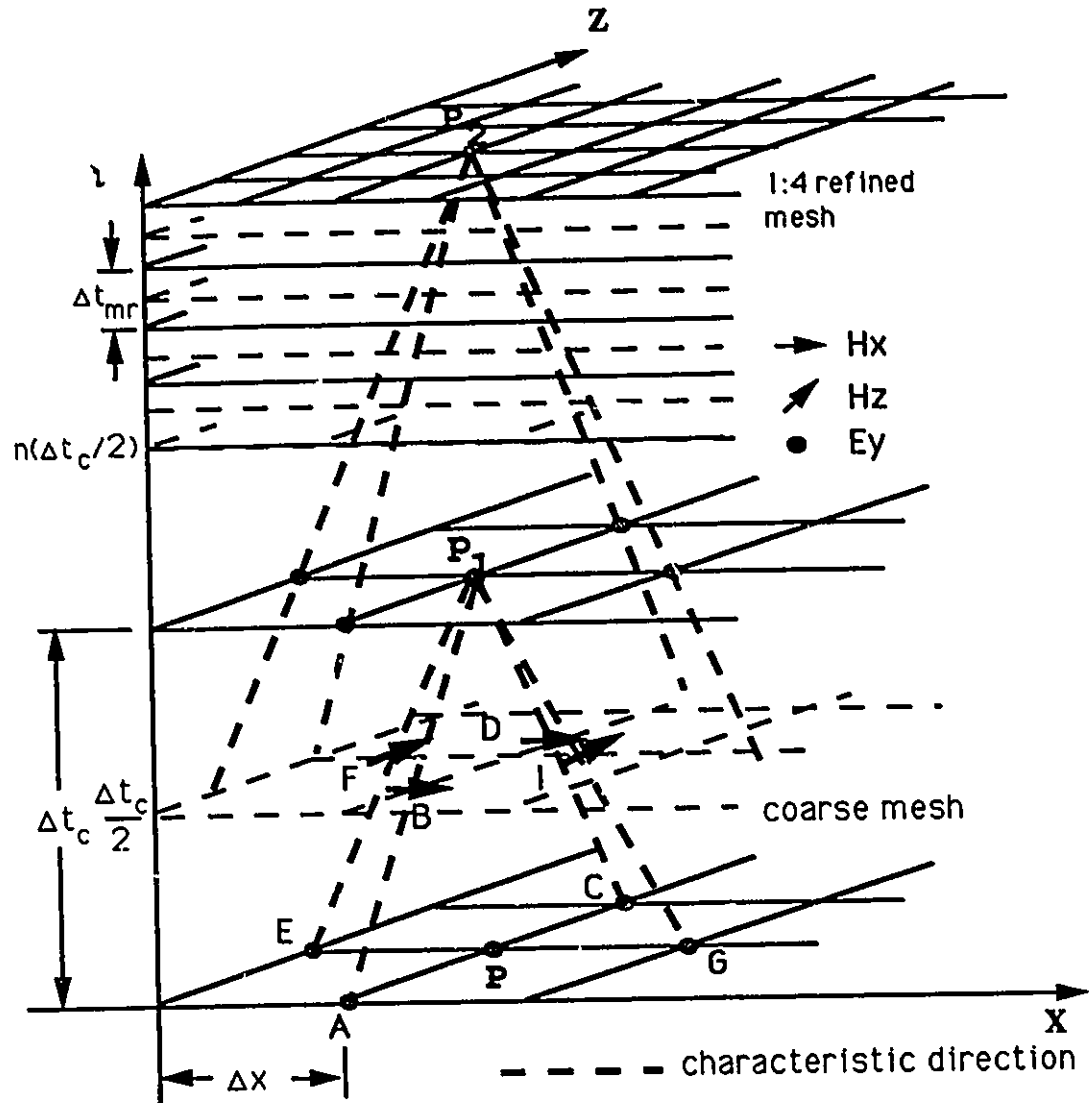


Fig. 5.2.2 Three-dimensional (x,z,t) diagram showing the leap-frog scheme following the lines of determination of Maxwell's two curl equations. The E fields are calculated at the points A, E, C, G, and P, and the H fields at the points B, F, D, and I for TE mode propagation.

As a first principle, these characteristic lines should be continuous even in the region with discontinuous mesh size. Secondly, field values calculated in the coarse and in the fine mesh regions must satisfy the interface conditions at the boundaries between the two.

It is also recommended that the stability criteria remain the same in the coarse and in the fine mesh. In the case of a one-to-four mesh ratio, this means that the time increment in the fine mesh must be one fourth of the time increment in the coarse mesh, as shown in Fig. 5.2.3. Note, however, that any integer mesh ratio may be chosen.

Here, we first summarize the main task in this approach and then present the details of the main task scheme for computer coding. One important task in the mesh refinement algorithm is to ensure continuity of fields across the interfaces between coarse and fine meshes. In the following we summarize the three steps which are schematically indicated in Fig. 5.2.3 along the time axis:

1. Initialize the field values at the coarse-fine mesh boundary by setting $E_c^n = E_{mr}^0$, $E_c^{n+1} = E_{mr}^4$. The superscript designates the time step, and the subscripts mr and c designate the refined and coarse mesh, respectively. Hence, the boundary values in the fine mesh are calculated by initializing and interpolating values in the coarse mesh. For example, for $1 \leq k \leq m-1$, E_{mr}^k is obtained by linear interpolation in time between E_c^n and E_c^{n+1} , or, equivalently, E_{mr}^0 and E_{mr}^4 on the time-space interface.
2. Obtain $\tilde{H}_c^{n+\frac{1}{2}} = \tilde{H}_{mr}^{\frac{4}{2}}$, and $\tilde{E}_c^{n+\frac{1}{2}}$ by time and space averaging of $\tilde{H}_{mr}^{\frac{5}{2}}$ and $\tilde{H}_{mr}^{\frac{3}{2}}$ and time averaging of $\tilde{E}_c^n$ and $\tilde{E}_c^{n+1}$, respectively. Since the field values of $\tilde{H}_c^{n+\frac{1}{2}} = \tilde{H}_{mr}^{\frac{4}{2}}$ and $\tilde{E}_c^{n+\frac{1}{2}} = \tilde{E}_{mr}^2$ are required to follow the characteristic lines of Maxwell's curl equations. Note that there are no $\tilde{H}_{mr}^{\frac{4}{2}}$ and $\tilde{E}_c^{n+\frac{1}{2}}$ on the boundaries of the space-time grid structure in the 1 : 4 ratio scheme at first.

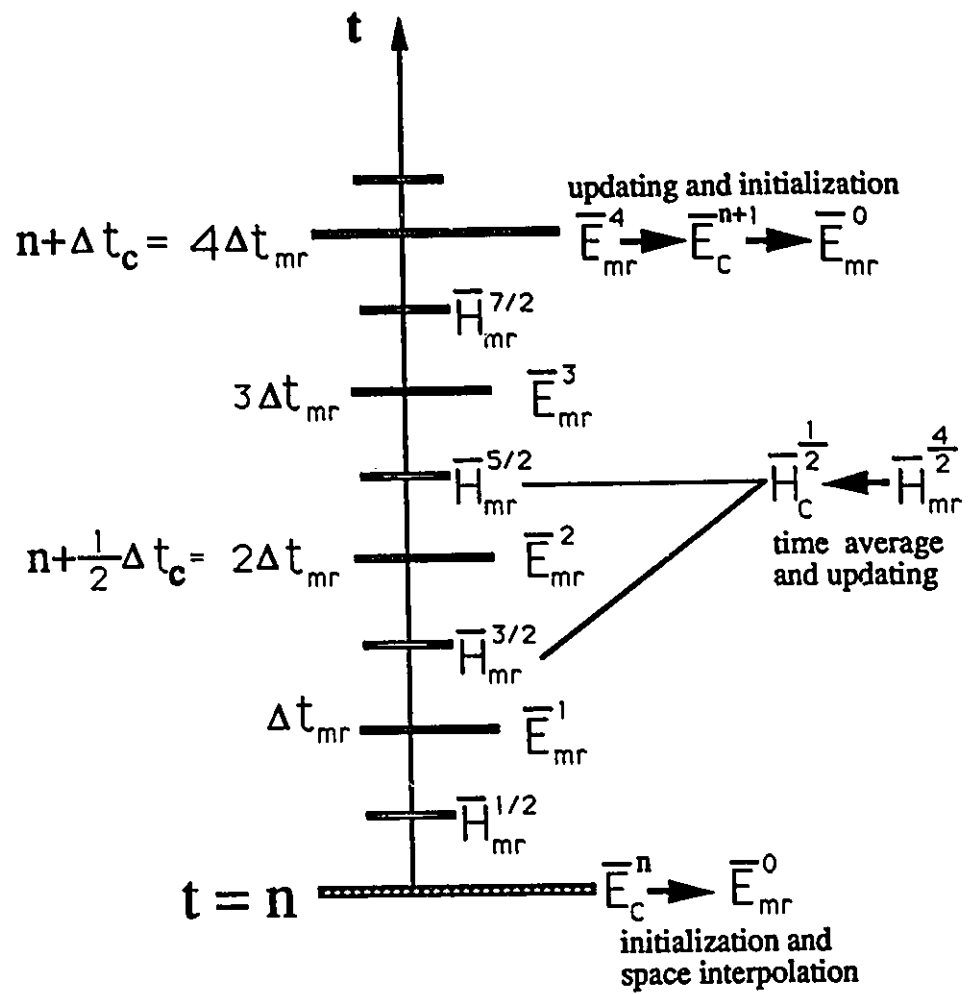


Fig. 5.2.3 The 1:4 mesh refinement scheme sequence along the time axis.

3. Update field values by injecting the fine mesh solution values into the coarse mesh.

Since a finer mesh is nested in a coarse mesh, the field values on the boundaries (interfaces) are updated every Δt_c , i.e., every 4 Δt_{mr} . The strong non-uniform field behaviour in the fine mesh region is transferred into the coarse mesh region by this step.

These three steps are performed at every coarse time step as shown in Fig. 5.2.3. The details of the above three steps are presented for computer coding, with the assumption of TE mode propagation.

- a. If a forerunner of a numerical wave has marched to the end of the refined mesh region, for example, $k_m + 2$ as shown in Fig. 5.2.1, determine $E_{y_{mr}}$ on the four boundaries, (top, bottom, left, and right interfaces between the coarse and fine meshes) and the overlapped node point as shown in Fig. 5.2.1 at the time steps t_c^n and t_c^{n+1} by using linear space interpolations.
- b. Find the time average values of $E_{y_{mr}}$ on the four boundaries by using linear time interpolation with $E_{y_{mr}}$ at t_c^n and t_c^{n+1} . For example,

$$E_{y_{mr}}^1(i, k) = E_{y_{mr}}^0(i, k) + [E_{y_{mr}}^4(i, k) - E_{y_{mr}}^0(i, k)]/4$$

since

$$E_{y_{mr}}^0(i, k) \Leftarrow E_{y_c}^n(i, k)$$

- c. At every refined time step, let the numerical wave propagate through the discretized Maxwell's equations (5.2.1), i.e., determine H field values in the refined mesh region at every refined time step.
- d. Impose boundary conditions if necessary in the refined mesh region

- e. Find six time average values of $H_{x_{mr}}$ and $H_{z_{mr}}$ on the interfaces at the time step $2\Delta t_{mr}$. Then update H_{x_c} and H_{z_c} from the field values $H_{x_{mr}}$ and $H_{z_{mr}}$, i.e., $\bar{H}_c^{\frac{1}{2}} \Leftarrow \bar{H}_{mr}^{\frac{1}{2}}$. For example, at the location 'a' shown in Fig. 5.2.1,

$$H_{x_{mr}}^4(a) = [H_{x_{mr}}^4(i_{mr} = 1, k_{mr} = 2) + H_{x_{mr}}^4(1, 4)]/2$$

$$H_{x_{mr}}^0(a) = [H_{x_{mr}}^0(1, 2) + H_{x_{mr}}^0(1, 4)]/2$$

$$H_{x_c}^{n+\frac{1}{2}}(a) = [H_{x_{mr}}^0(a) + H_{x_{mr}}^4(a)]/2$$

- f. Update all the $\bar{H}$ field values for the next iteration in the refined mesh region.
- g. Update $\bar{E}$ field values on the interfaces between the refined mesh region and the coarse region. For example,

$$E_{y_c}^{n+1} \Leftarrow E_{y_{mr}}^4$$

The steps c to f above are iterated in a ratio equal to that of the mesh refinement scheme. For our study, four iterations in a refined mesh region have been performed for every coarse mesh iteration time step.

5.3 Example As an example, we have considered a local scattering problem in a standard rectangular waveguide (WR-28). A centered thin metal insert located in the E-plane of the waveguide was considered. The object had 5 mil thickness and 5 mil length. To characterize the small object with a locally refined mesh, we inject a sinusoidal signal and process it according to (5.2.1a) - (5.2.1c). Three different computations of the structure have been performed, each with a different discretization scheme, namely a uniformly fine, a uniformly coarse, and a composite mesh with a 1:4 gridding ratio. The magnitude of S_{11} and the guided wavelength in the structure were computed in

the three simulations. The accuracy of the latter has been verified by comparison with theoretical results for the guided wavelength. These values are shown in Table 5.3.1. The CPU times for the three cases are also listed in Table 5.3.1. The mesh refinement scheme yielded very good results 70 times faster than the uniformly fine mesh, and represented a considerable improvement over the uniformly coarse mesh. In Fig. 5.3.1, $|S_{11}|$ obtained for the whole operating frequency range of WR 28 waveguide is compared with the mode matching technique result for the same discontinuity above.

scheme	CPU sec	$ S_{11} $	Wavelength(m)	computational mesh size
uniform fine mesh	38998.74	0.856	0.01778	57 * 681
local refined mesh	537.68	0.834	0.01827	15 * 171 + 9 * 9
uniform coarse mesh	322.72	0.237	0.01524	15 * 171
	72.5 times faster		0.01777 theoretical result	

Table 5.3.1 Comparison of accuracy of $|S_{11}|$ and CPU time for the three different mesh schemes to analyze a 5 mil thick and 5 mil long metal insert discontinuity in WR-28 waveguide at 27 GHz on VAX-11/750.

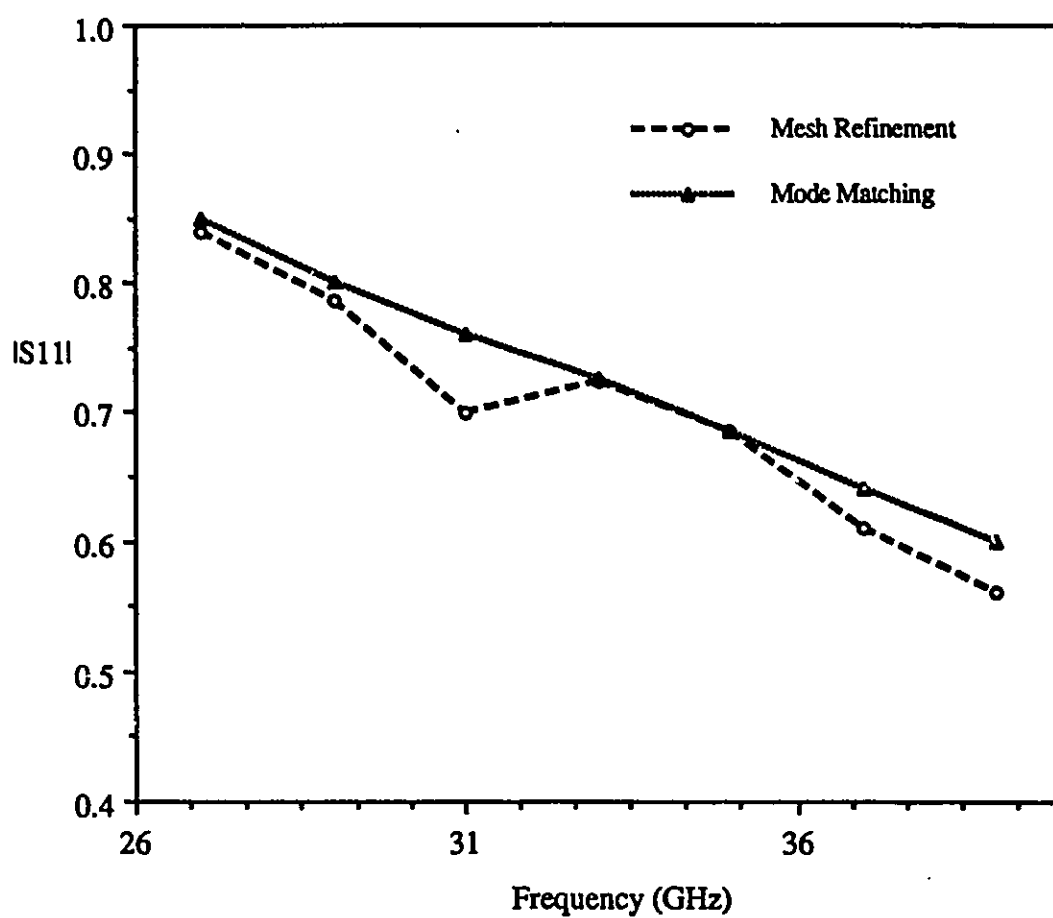


Fig. 5.3.1 $|S_{11}|$ comparison with the mode matching technique for the whole operating frequency range of the WR-28 standard waveguide.

5.4 Discussion In this chapter we have considered an efficient local mesh refinement algorithm subdividing a computational domain to resolve fine dimensions in the TD-FD space-time grid structure. At a discontinuous coarse-fine mesh interface, the boundary conditions for the tangential and normal field components have been enforced for a smooth transition of highly non-uniform field quantities. The results are promising. However, there are two problems one should be cautious about when implementing the local mesh refinement algorithm [5-2]. Firstly, the abrupt change of the mesh size invariably causes spurious reflections. They can be reduced by using a proper interpolating scheme conformal with the behaviour of the solution. Secondly, any wave which is poorly resolved in a coarse mesh, will change phase velocity when passing into a fine mesh. If this wave later passes from the fine mesh back into coarse mesh, a serious interaction can result with that part of the wave which remained in the coarse mesh. To minimize this velocity error, care must be taken to ensure that the coarse mesh size is still much smaller than the shortest wavelength under study. In the future, we will analyze reflection properties of an abrupt change of mesh size in a TD-FD computational domain, by using the dispersion relation shown in the last chapter.

CHAPTER 6

Results of Numerical Analyses

6.1 Introduction The TD-FD simulation technique is based on the discrete characteristic of the leap-frog approximation of Maxwell's equations. The initial and boundary conditions define the problem physically, whereas the numerical EM wave propagation properties are determined by the convergence criteria and the effects of the stability factor. These elements of the method have been presented in Chapters 2 through 5 and have been used to model discontinuity problems in guided wave transmission structures by simulating the field quantities for use in S-parameter extraction.

Before starting the analysis of specific discontinuity problems, it will be helpful to show that the numerical procedure converges to the correct solution, and how the numerical wave propagates for CW and pulse excitation cases. A series of numerical experiments have been done using the standard rectangular waveguide with uniform cross-section as a computational domain. The results presented in this chapter have been produced using computer codes implemented on Digital Electronic Corporation (DEC) VAX 3500 and DEC RISC computers. The results of these experiments are shown in

Section 6.2. In Section 6.3, 2-D and 3-D rectangular waveguide discontinuity problems, such as inductive irises, an inductive metal strip, two metal insert E-plane filters, and capacitive irises will be analyzed. The results of inductive irises will be compared with results obtained with the mode matching technique and with theoretical results. The results of capacitive irises will be compared with the Marcuvitz's results.

6.2 Qualitative observations In this section, a qualitative view of how a numerical wave propagates in a standard rectangular waveguide is presented. TE_{10} mode propagation has been simulated for both CW and pulse cases. Four different simulations of numerical wave propagation have been examined: i) without discontinuity, ii) with discontinuity, iii) below cutoff frequency (these three use CW excitation), and iv) pulse excitation without any discontinuity. For all four cases, a matched boundary condition was placed at the left and right ends of the rectangular waveguide, and an electric wall boundary condition was placed at the top and bottom of the domain.

E_y components were sampled and plotted in a 3-D graphical mode for each case. In the CW case which will be illustrated first, the excitation was of the form

$$E_y(i, n \cdot \Delta t) = \cos(\omega \cdot n \cdot \Delta t) \sin \frac{\pi(i-1)}{NX}, \quad (6.2.1)$$

where NX and i are the number of segments $\Delta\ell$, and node points across the width of the waveguide, respectively. The size of the computational domain was $28\Delta\ell$ in the x direction and $340\Delta\ell$ in the z direction. The input signal was applied at $z = 10$ for each CW case.

The numerical wave propagation in a homogeneous rectangular waveguide was observed at 6 different iteration numbers: 100, 200, 400, 500, 800, and 1700. The snapshots at those iteration numbers are shown in Figs. 6.2.1(a)-(f). We can see that the wave propagates from the right to the left hand side. The forerunners to the wavefront of the propagating wave have much smaller amplitudes than the wavefront as can be seen in Figs. 6.2.1(a), (b), (c), and (d). In Fig. 6.2.1(f), we can see that a steady state condition has been reached.

A numerical wave propagating below cutoff can be observed in the snapshots of the E field plotted in Figs. 6.2.2(a)-(j). The WR-28 waveguide was excited with a signal of frequency 16 GHz. Observations were made for the iteration numbers (for one period in time): 1886, 1891, 1896, 1901, 1906, 1911, 1916, 1921, 1926, and 1931. The figures clearly show that no propagation exists below cutoff. The same cutoff phenomena have been observed as shown in Figs. 6.2.2(a)-(j) during the first 1885 iterations. However, there was a very small amount of the numerical wave propagated. We believe that the high frequency components which propagate are due to errors introduced by the discrete excitation.

We also simulated wave propagation phenomena in the presence of a discontinuity. A thin inductive metal strip was placed at the center of the waveguide (WR-28). The field distribution was observed at the iterations 100, 500, 800, 1000, 1200, and 1900. The results are shown in Figs. 6.2.3(a)-(f). The reflections from the discontinuity increase the time it takes for the field to reach a steady state condition. Figures 6.2.3(c)-(f) illustrate the transmitted field distribution on the left hand side of the discontinuity (the discontinuity is inside the circles), and the total field distribution (the incident and reflected fields) on the right hand side of the discontinuity. Note that the SWR and S-parameters can be easily calculated from these field distributions.

We can also observe pulse propagation phenomena in a standard rectangular waveguide. A Gaussian pulse,

$$E_y(i, k) = e^{-k^2/W^2} \sin\left(\frac{\pi(i-1)}{NX}\right), \quad (6.2.2)$$

is applied at the middle of the waveguide at time $t = 0$, where W is the pulse width as shown in Fig. 6.2.4(a). As described in Chapter 2, we can see from Figure 6.2.4(b) that the incident pulse immediately splits into two pulses. Figs. 6.2.4(c)-(g), show the propagation of the two pulses in two opposite directions. This observation confirms that Maxwell's equations describe two solutions propagating in two opposite directions. Note that the pulse width broadens as the wave propagates, since the waveguide is dispersive. Figures 6.2.4(h) and (i) use a different scale, since almost all the energy has been absorbed by the matching boundaries at the right and left ends of the waveguide. As was mentioned in Chapter 3, both the higher and lower frequency components below cutoff remain in the computational domain, especially in Fig. 6.2.4(h) at iteration number of 500, where we used an amplitude scale one fourth that in Fig. 6.2.4(a). At iteration number 2500, (Fig. 6.2.4(i)), all lower frequency components have disappeared since the higher frequency components propagate slower than the lower frequency components (dispersive nature). Only the lower frequency components below cutoff remain stationary since they are not propagating. For this case, 2500 iterations were sufficient to obtain an accurate frequency domain response through Fourier transform. If a smaller number of iterations were used, we would observe Gibb's phenomenon.

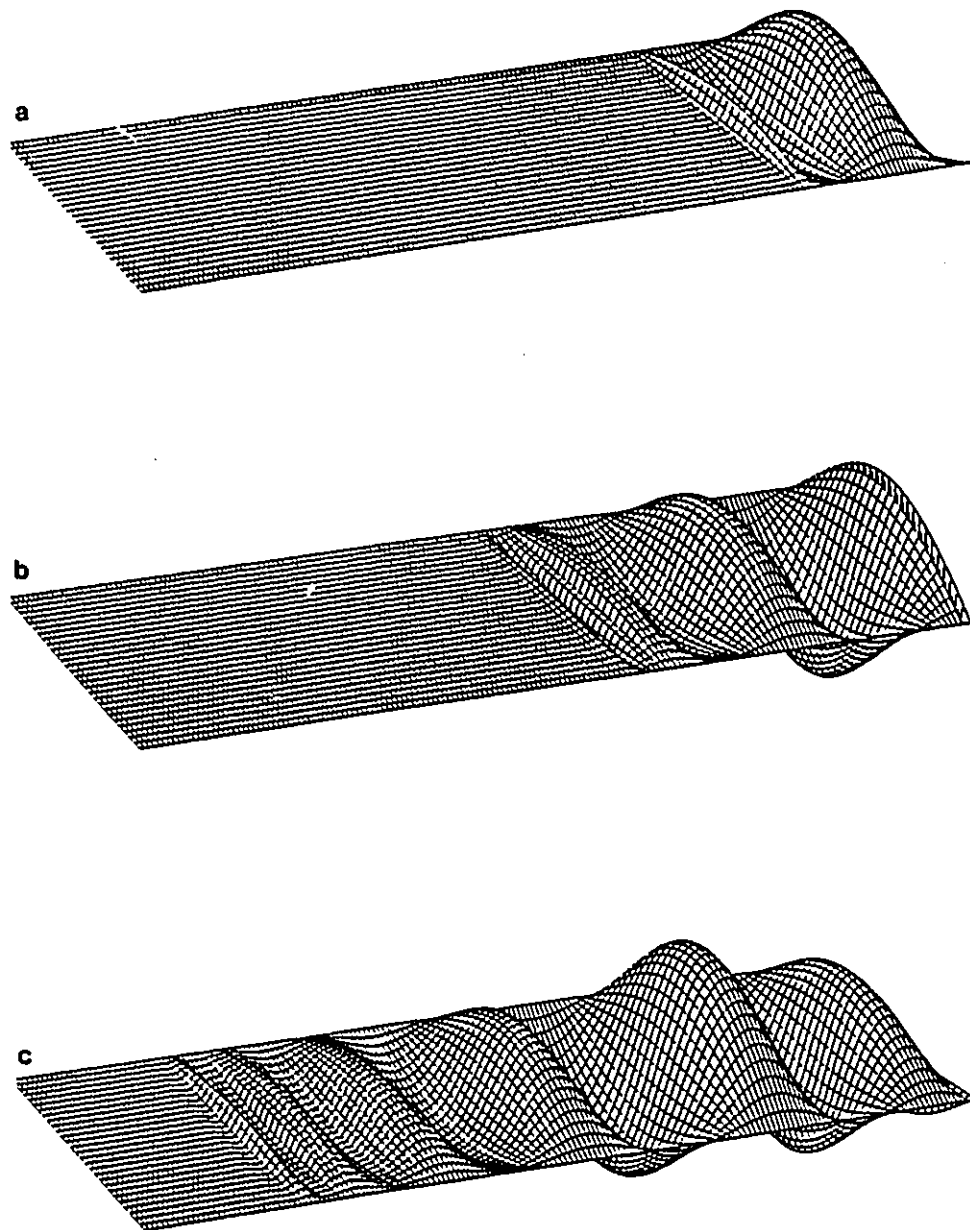


Fig. 6.2.1 Numerical wave propagation in a standard homogeneous rectangular waveguide at iterations (a) 100, (b) 200, and (c) 400. Excitation : CW.

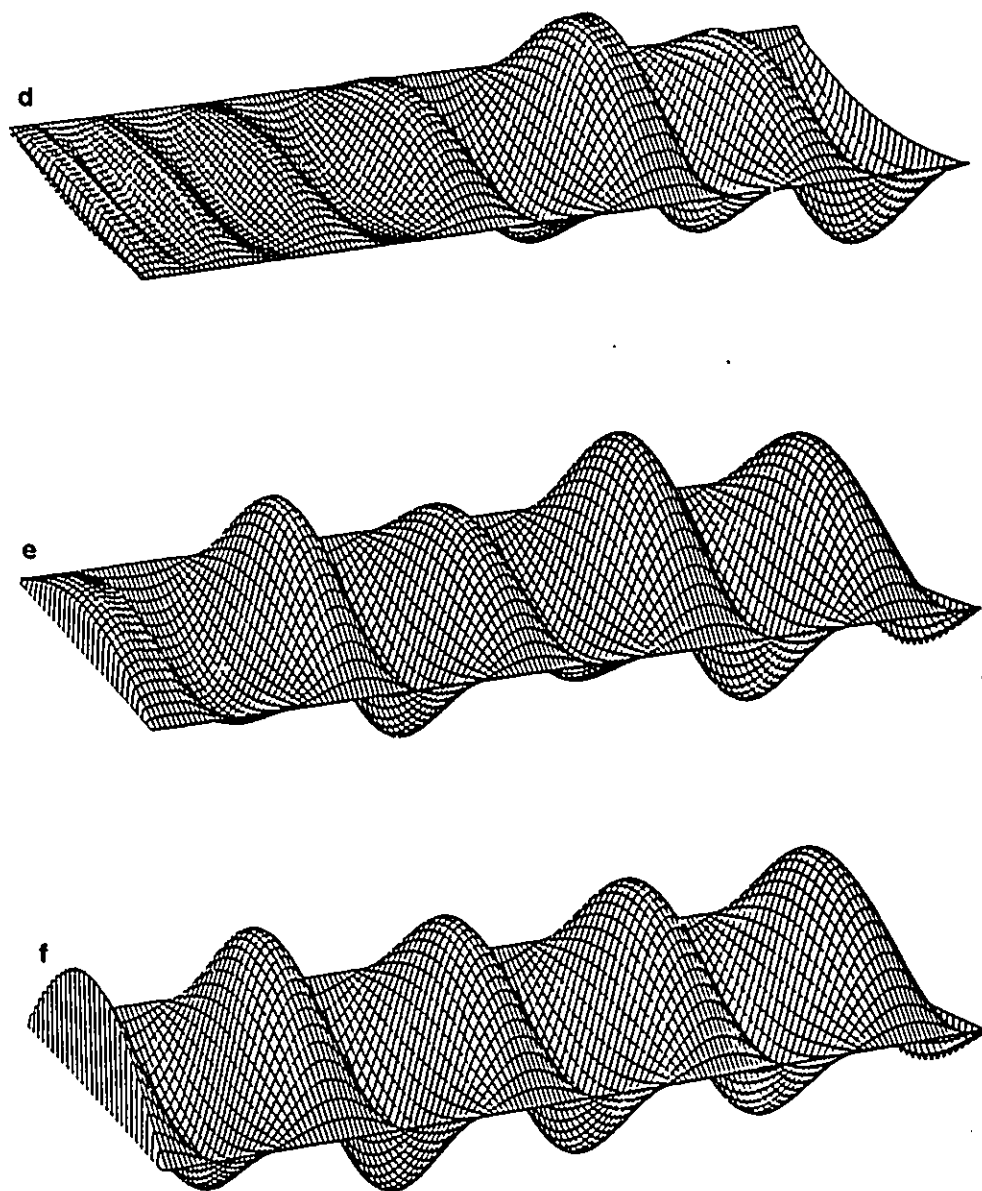


Fig. 6.2.1 Numerical wave propagation in a standard homogeneous rectangular waveguide at iterations (d) 500, (e) 800, and (f) 1700. Excitation : CW.

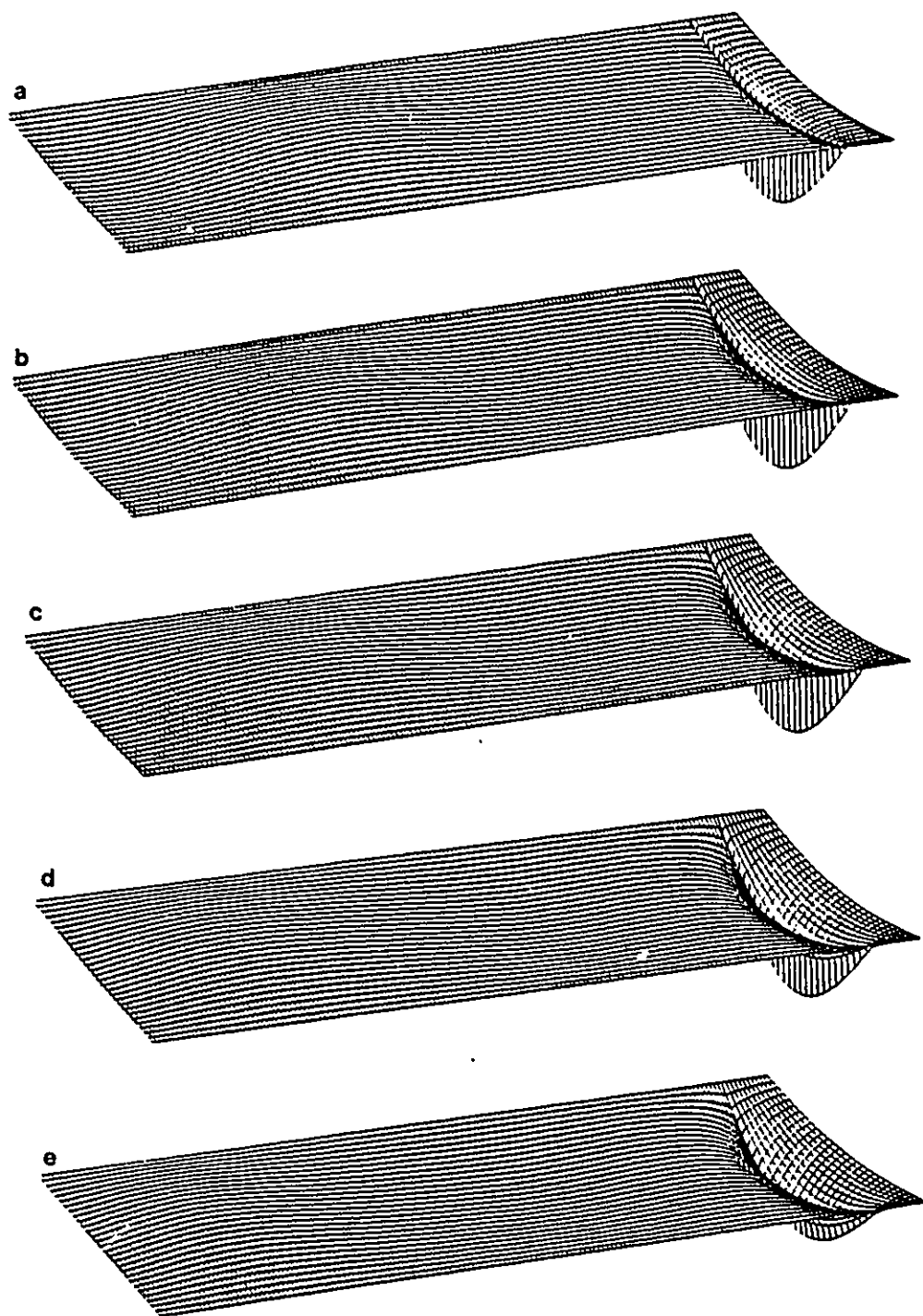


Fig. 6.2.2 Numerical wave propagation below cutoff in a standard homogeneous rectangular waveguide at iterations (a) 1886, (b) 1891, (c) 1896, (d) 1901, and (e) 1906. Excitation : CW.

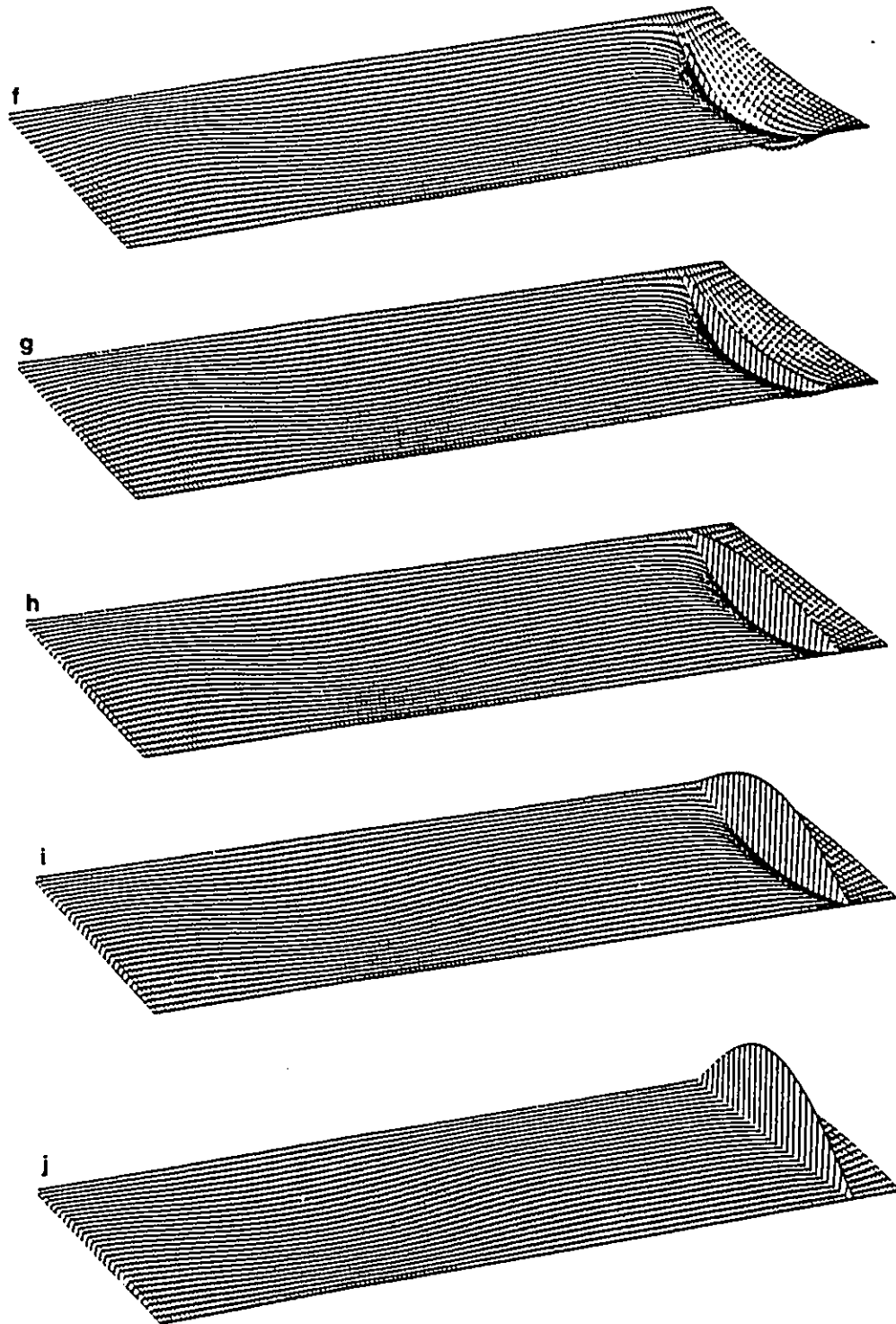


Fig. 6.2.2 Numerical wave propagation below cutoff in a standard homogeneous rectangular waveguide at iterations (f) 1911, (g) 1916, (h) 1921, (i) 1926, and (j) 1931. Excitation : CW.

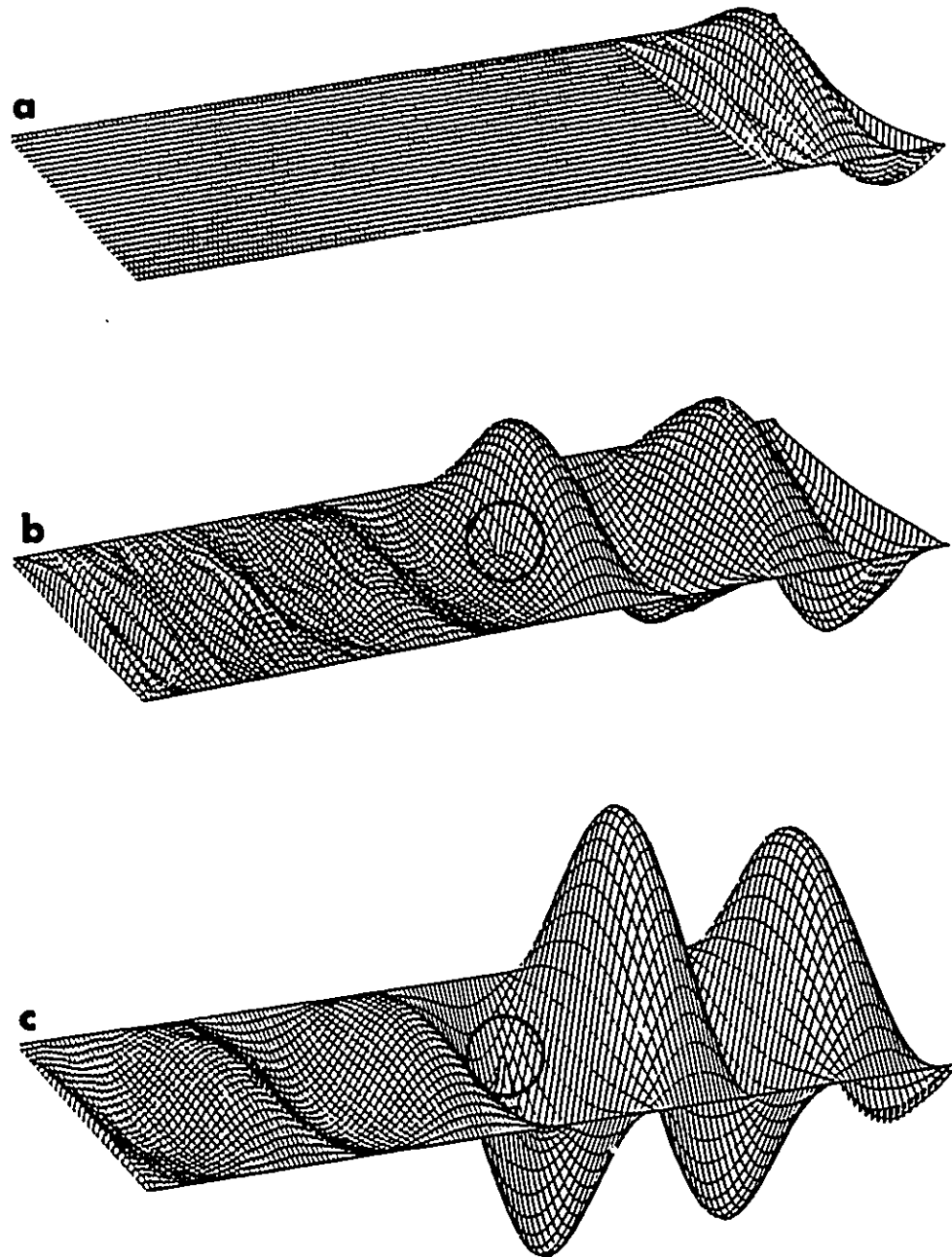


Fig. 6.2.3 Numerical wave propagation in a standard homogeneous rectangular waveguide with an inductive metal strip at iterations (a) 100, (b) 500, and (c) 800. Excitation : CW.

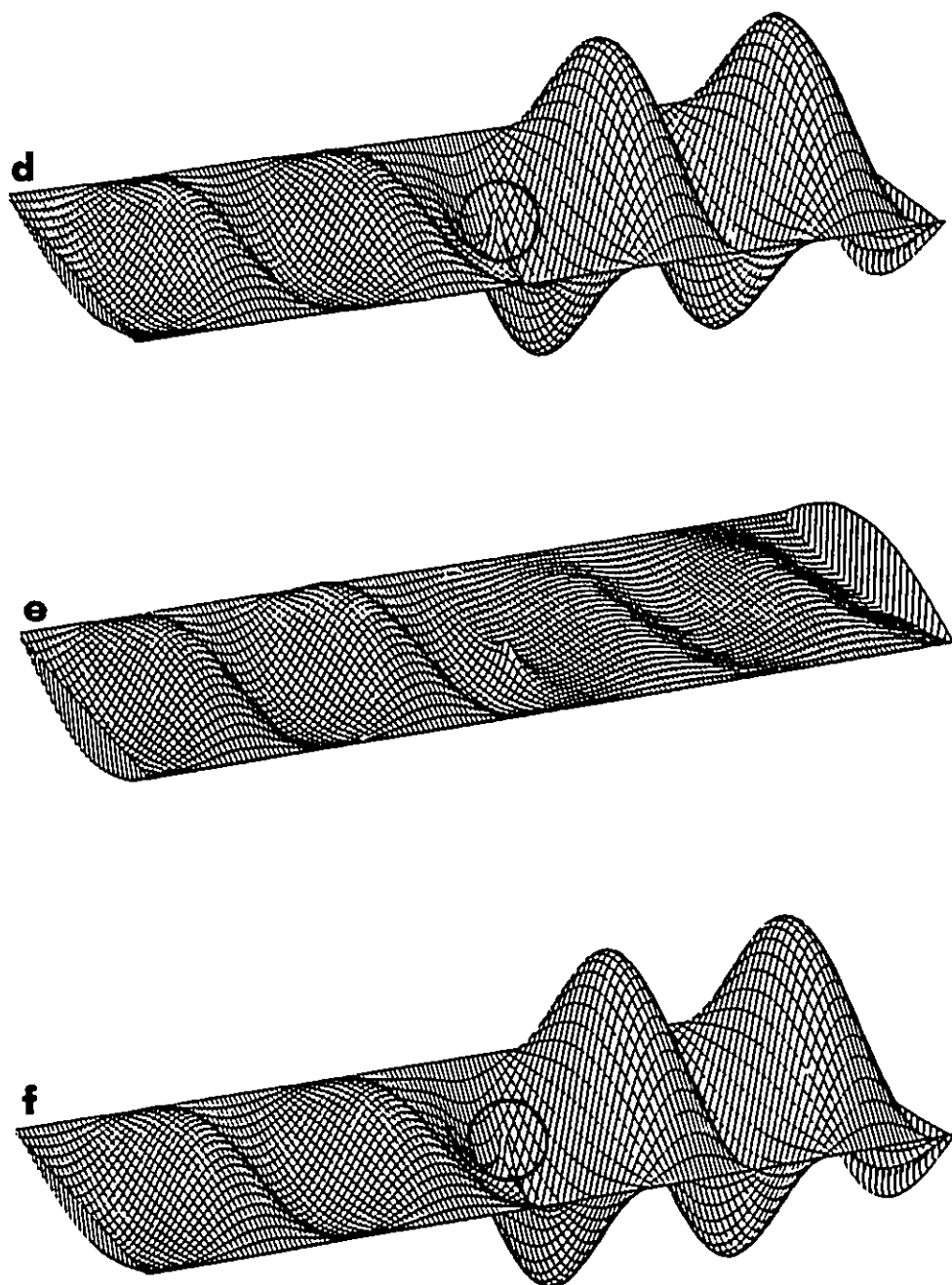


Fig. 6.2.3 Numerical wave propagation in a standard homogeneous rectangular waveguide with an inductive metal strip at iterations (d) 1000, (e) 1200, and (f) 1900. Excitation : CW.

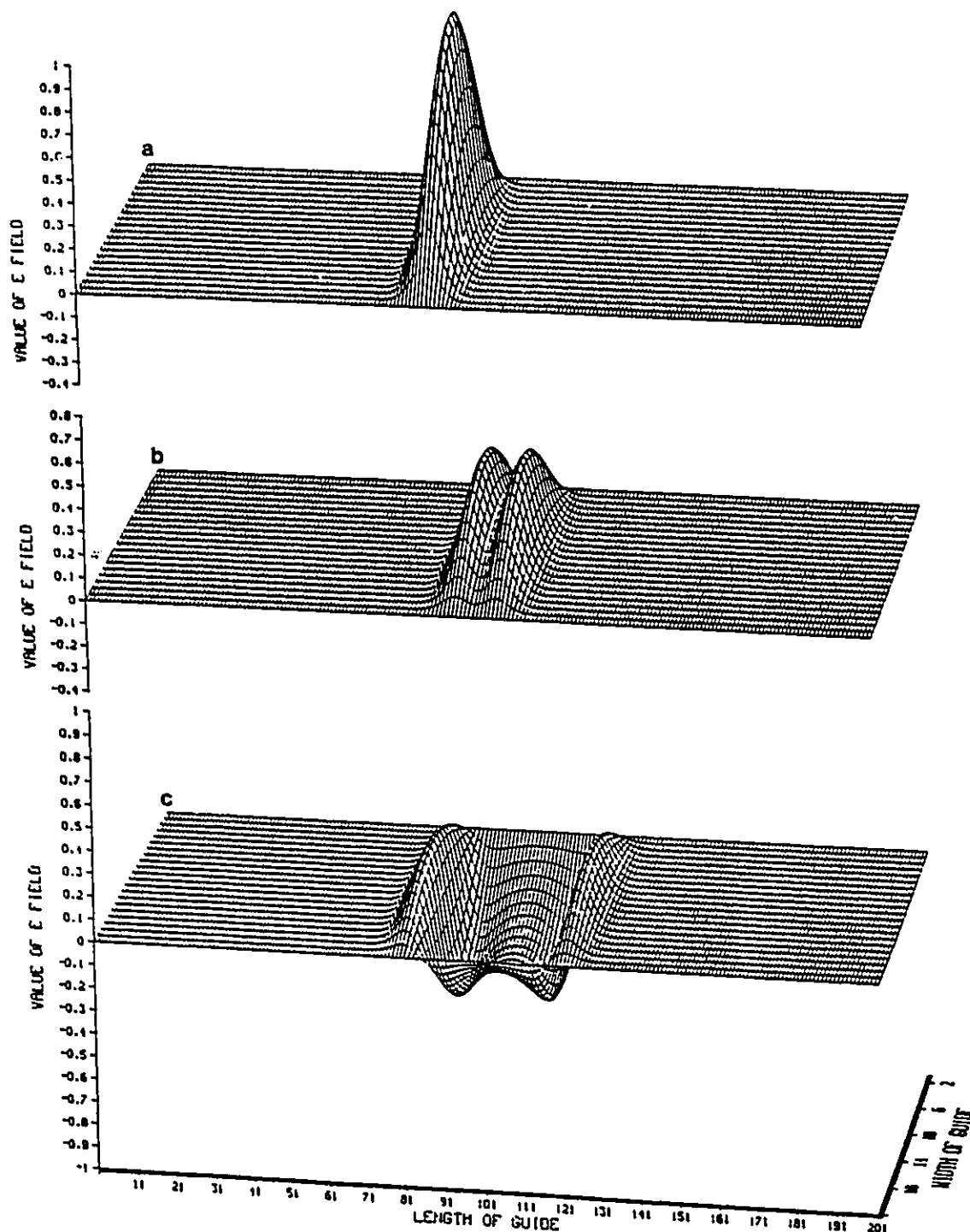


Fig. 6.2.4 Numerical pulse wave propagation in a standard homogeneous rectangular waveguide at iterations (a) 0, (b) 5, and (c) 25. Excitation : Gaussian pulse.

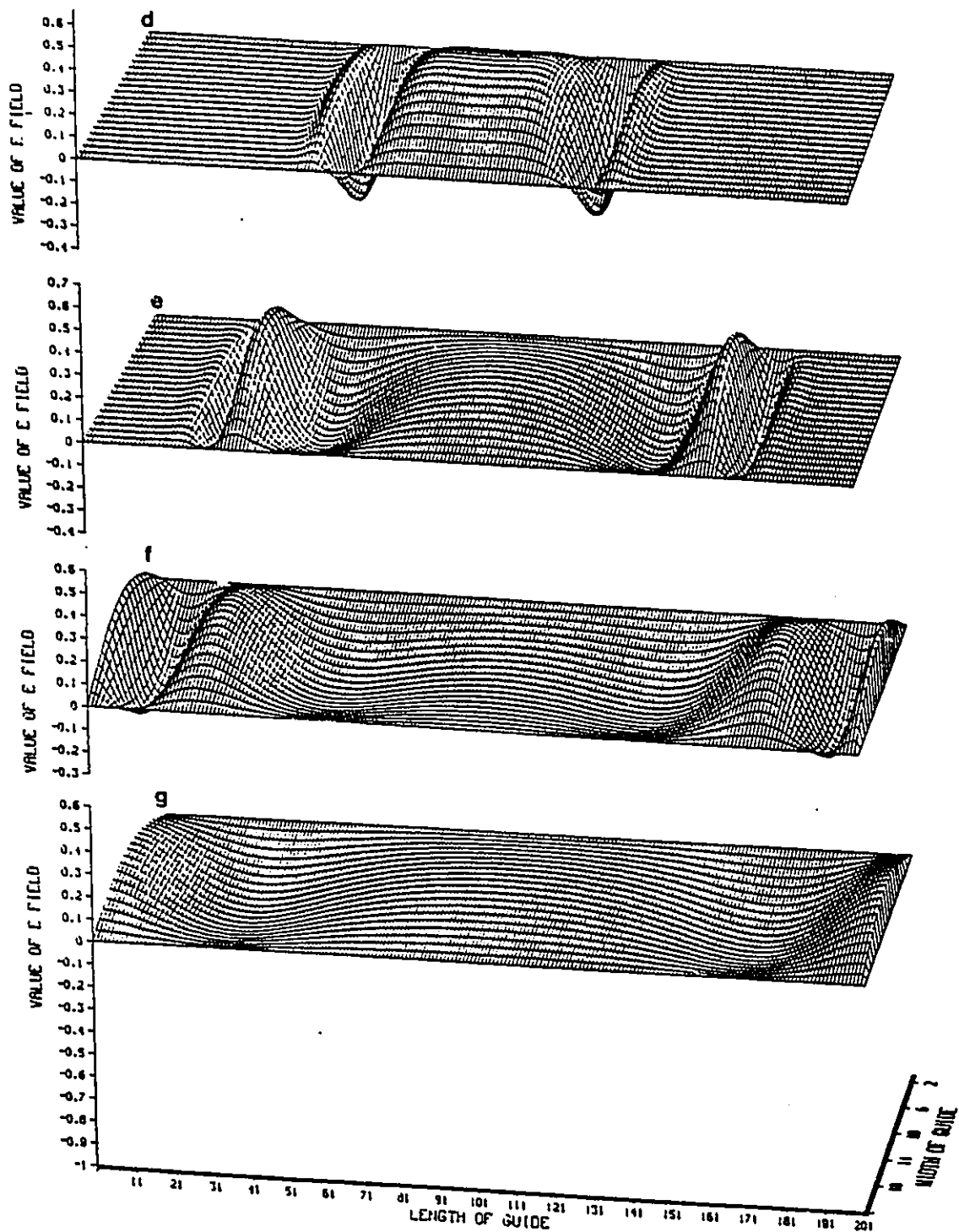


Fig. 6.2.4 Numerical pulse wave propagation in a standard homogeneous rectangular waveguide at iterations (d) 50, (e) 100, (f) 150, and (g) 220. Excitation : Gaussian pulse

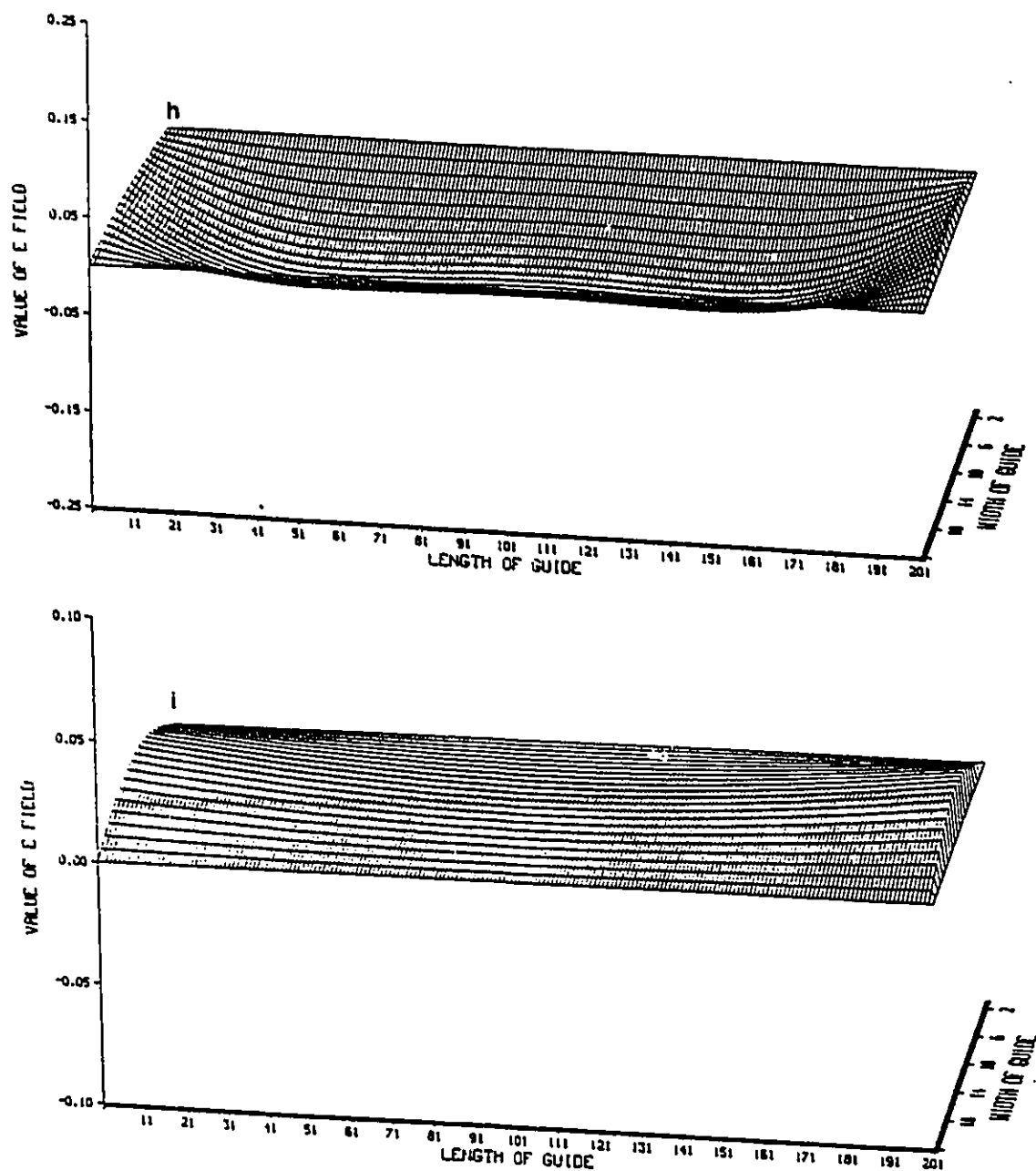


Fig. 6.2.4 Numerical pulse wave propagation in a standard homogeneous rectangular waveguide at iteration(h) 500 and (i) 2500. Excitation : Gaussian pulse.

6.3 Analysis results Several 2-D and 3-D waveguide discontinuity problems are analyzed in this section. The standard rectangular waveguide has been chosen as the computational domain ($28\Delta\ell \times 340\Delta\ell$). The initial condition was a propagating TE_{10} mode wave. All the analyses were carried out in single precision. First the propagation constant of the TE_{10} mode in WR-28 rectangular waveguide was calculated. The result is shown in Fig. 6.3.1 and is compared with the theoretical calculation. The simulated and theoretical results are in excellent agreement, but at the higher frequencies, differences between computed and theoretical results are larger than at lower frequencies. This implies that a smaller $\Delta\ell$ should be employed in the simulation. Next, a symmetrical inductive iris discontinuity in WR-90 was introduced, (as shown in the right hand corner at the top of Fig. 6.3.2) and analyzed. $|S_{11}|$ of the discontinuity was calculated and compared with TLM [6-1] and theoretical results [6-2], shown in Fig. 6.3.2 where the theoretical results were available for only a small portion of the whole frequency range. The results are also in good agreement. As a third example, an inductive metal strip was inserted in the middle of WR-28 waveguide. The configuration of the discontinuity is shown in Fig. 6.3.3. It has 50 mil thick. S_{11} is calculated for the metal insert discontinuity for various lengths (0.1 to 1.2mm) at a frequency of 40 GHz. The amplitude and phase of the E field, are compared with results obtained with the mode matching technique [6-2], as shown in Figs. 6.3.3(a) and (b). This comparison shows that both techniques agree well. S-parameters have also been calculated for a centered rectangular post (the discontinuity dimensions are shown in Fig. 6.3.4) in a rectangular waveguide of width $= 21\Delta\ell$. The results are compared with mode matching results in Fig. 6.3.4. Note that there is a difference between the two methods at higher frequencies (above 38 GHz). This is due to the fact that a resolution of $21\Delta\ell$ is not fine enough to calculate S-parameters (around 4 percent error was estimated.).

A band pass filter function can be created by placing two or more inductive metal strips with spaces between them as shown in Figs. 6.3.5 and 6.3.6. This is called an E-plane band pass filter. The geometry with two metal strip discontinuities and a resonant space is called a single resonator E-plane filter. The return loss and insertion loss characterizing such a single resonator E-plane filter are plotted against frequency in Fig. 6.3.5. Results obtained with the mode matching technique [6-4] agree well. The analysis of a three resonator, four-metal-strip filter is shown in Fig. 6.3.6. The insertion loss characteristic of the filter was calculated and compared with mode matching results [6-3], but they do not agree at all frequencies since the dimensions of the filter structure in the two analyses were slightly different. We can observe that tiny changes in the dimensions of the metal strip discontinuity and the length of the space between two strips can significantly influence the filter characteristics. It should be noted that it was not possible to use exactly the same dimensions as in the mode matching analysis because all lengths must be an integer multiple of $\Delta\ell$. We have seen in this chapter that the TD-FD approach produces relatively accurate results for 2-D discontinuity problems. To illustrate the accuracy of 2-D simulation quantitatively, E_{max} and E_{min} were calculated in an inhomogeneous waveguide for different $\Delta\ell$ in the waveguide width and were compared with the convergence criteria described in Chapter 3. The accuracy in percent was better than 5.16 % for 7 $\Delta\ell$, 4.16% for 14 $\Delta\ell$, 4.02 % for 21 $\Delta\ell$, and 3.39 % for 28 $\Delta\ell$.

The magnitude of S_{11} has been analyzed using a 3-D discretization for a symmetrical capacitive discontinuity and compared with Marcuvitz's results [6-5]. These are shown in Figs. 6.3.7 and 6.3.8. Fig. 6.3.7 shows $|S_{11}|$ for various values of d/b at 40 GHz, and Fig. 6.3.8 shows $|S_{11}|$ for a fixed $d/b = 0.4$ over the whole operating frequency range of the WR-28 waveguide. The computational domain for both cases is $28\Delta\ell$ in x

(for a), $14\Delta\ell$ in y (for b), and $46\Delta\ell$ in z . The structure was excited with a Gaussian pulse, and the frequency domain results were obtained via Fourier transform after 2500 iterations in both cases. In Fig. 6.3.7, it is noted that the two curves for $|S_{11}|$ disagree for d/b higher than 0.7, and for d/b lower than 0.4. Fig. 6.3.8 shows the TD-FD results fluctuating. It has been found that smaller mesh sizes were required for more accurate computation, which means that a more powerful computer was needed.

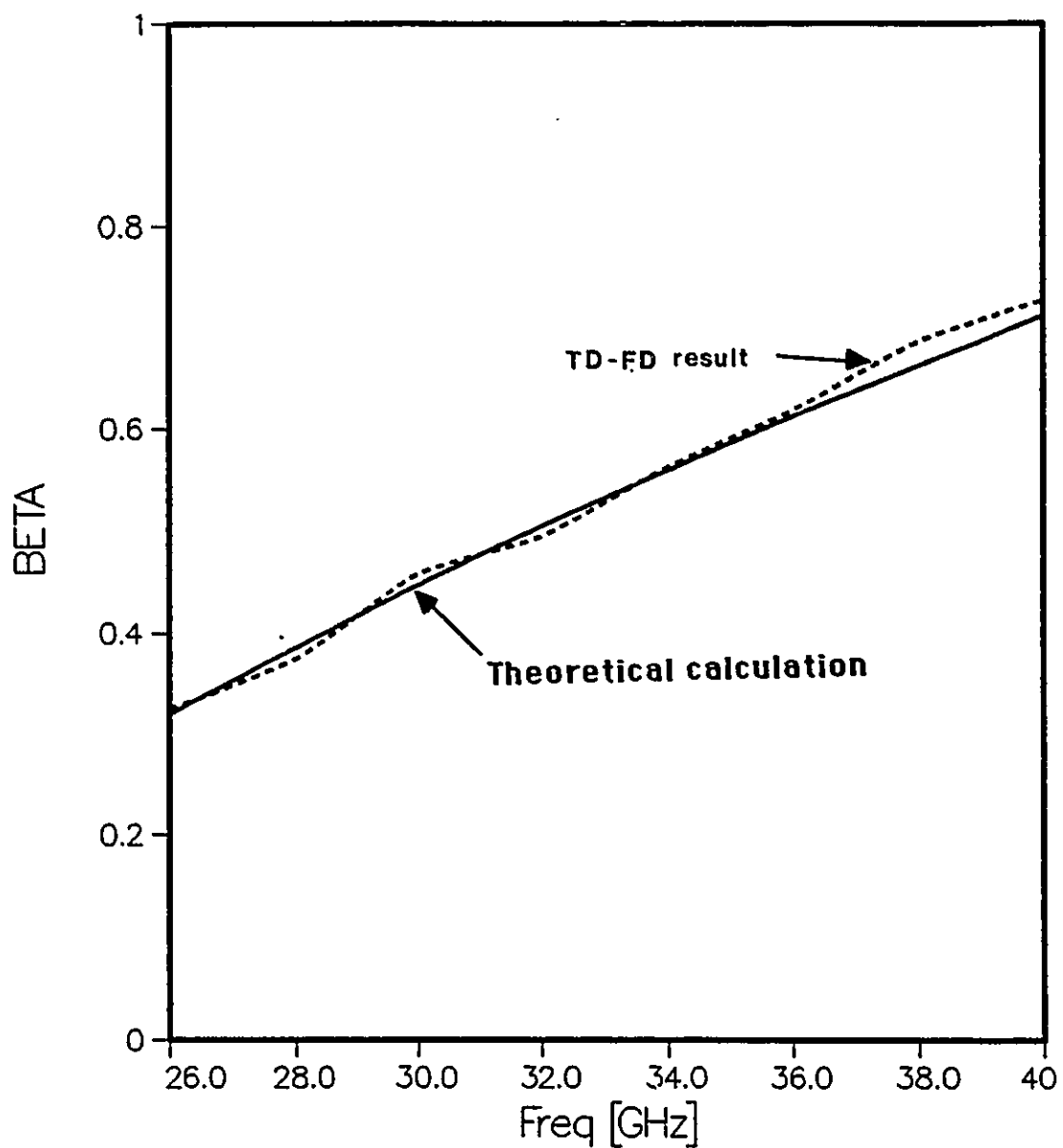


Fig. 6.3.1 Comparison of propagation constant of the TE_{10} mode in WR-28, obtained with TD-FD and theoretical analysis.

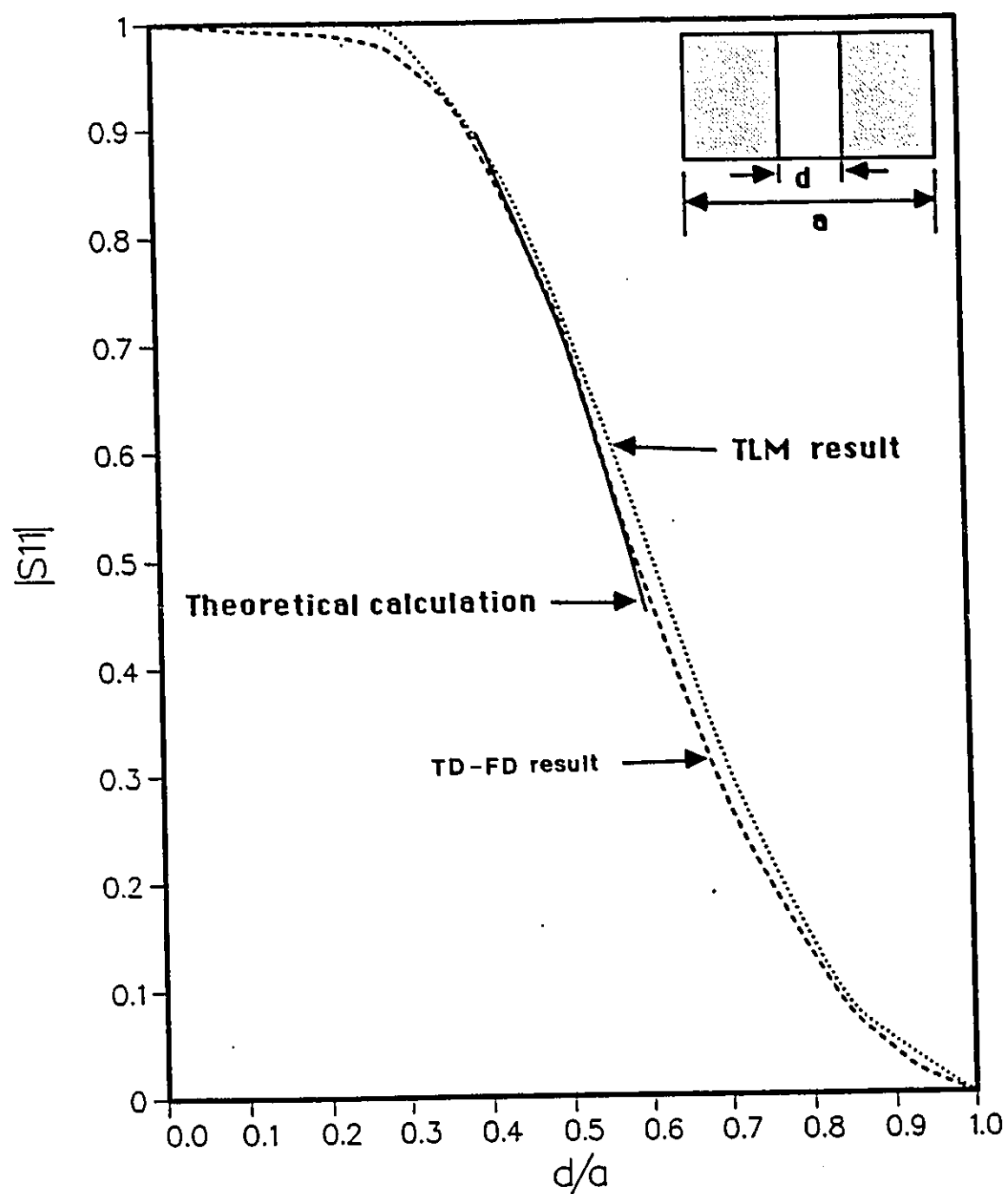


Fig. 6.3.2 Comparison of $|S_{11}|$ for the centered inductive iris in WR-90, obtained with TD-FD, TLM, and theoretical analysis. ($f=30\text{GHz}$)

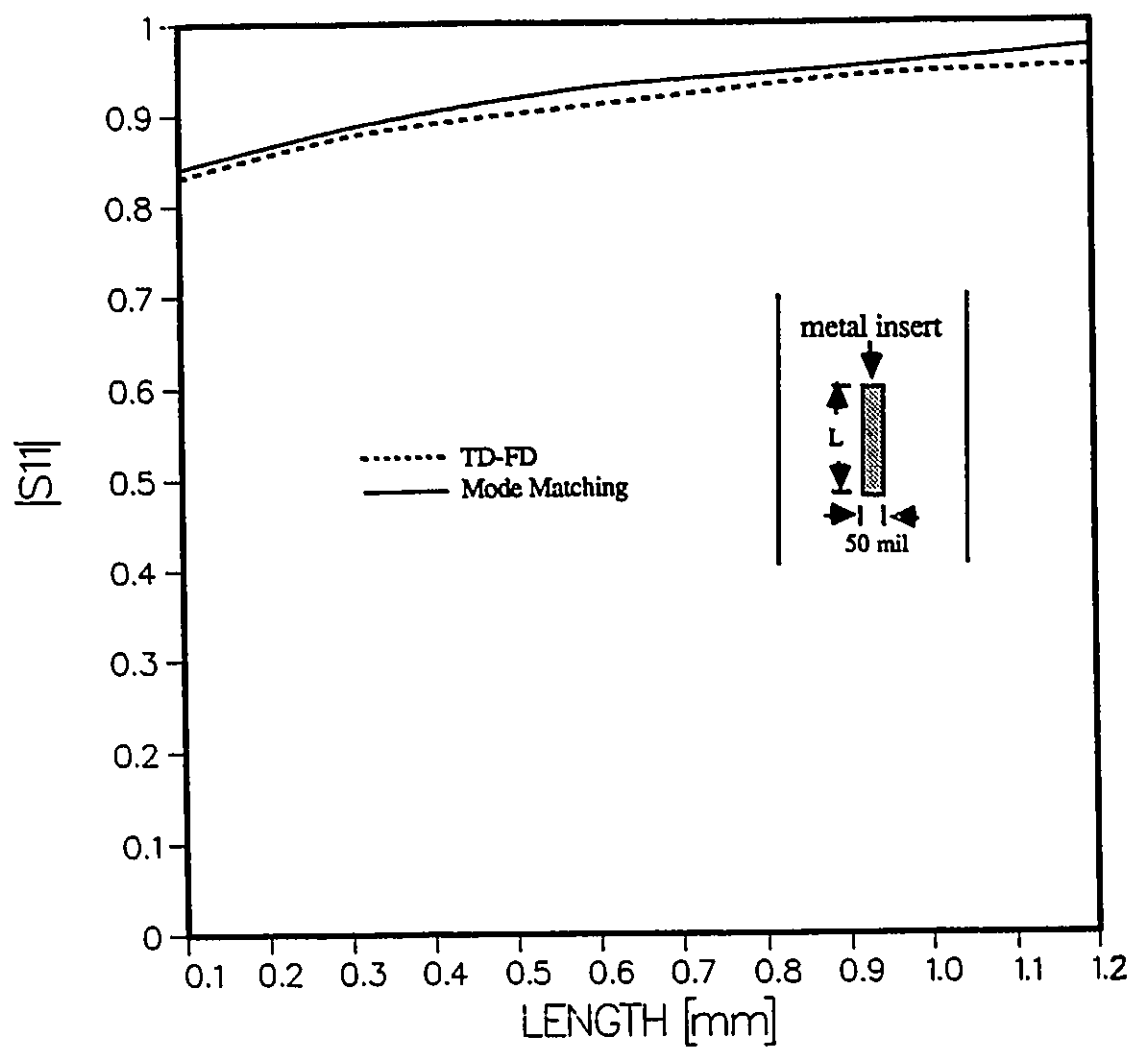


Fig. 6.3.3(a) Comparison of $|S_{11}|$ for the inductive metal strip in WR-28, calculated with TD-FD and mode matching technique. ($f=30\text{GHz}$)

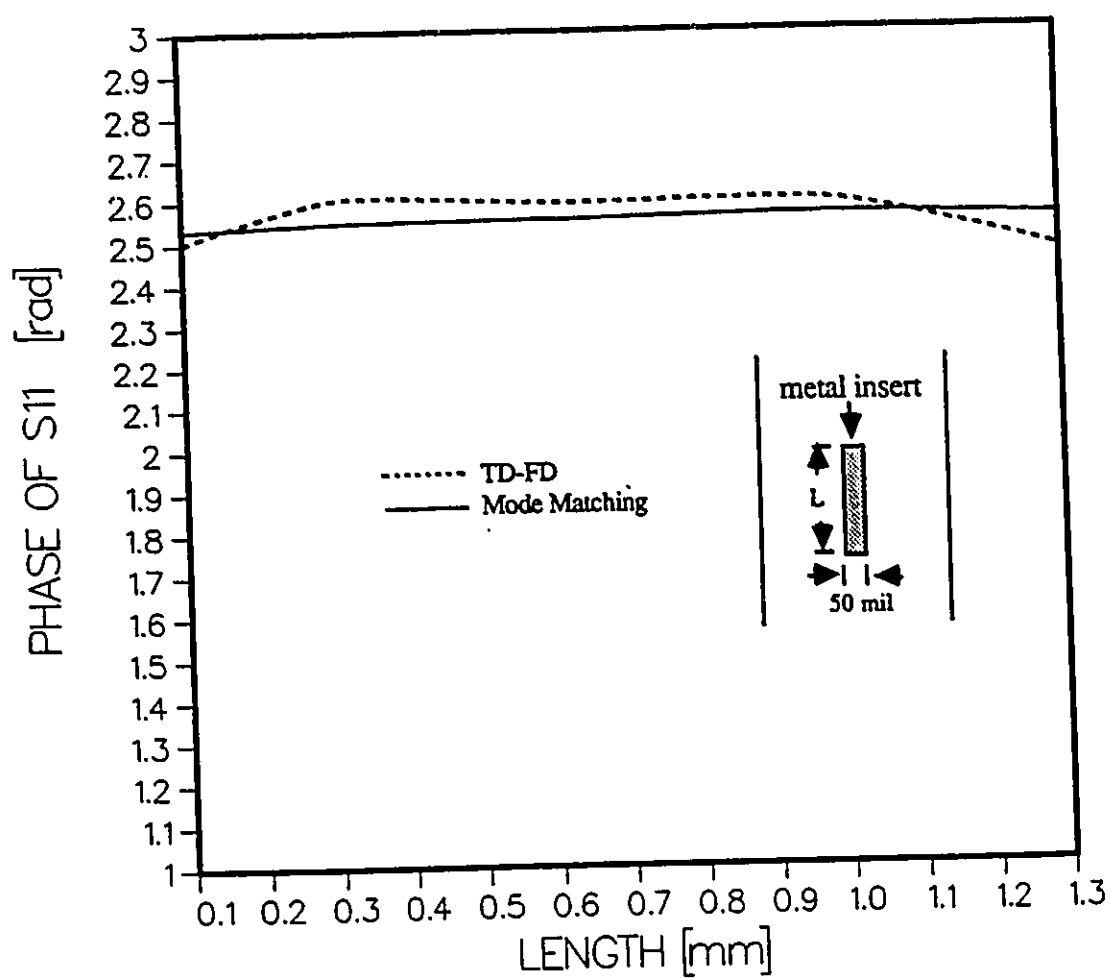


Fig. 6.3.3(b) Phase of S_{11} for the inductive metal strip in WR-28, calculated with TD-FD and mode matching technique. ($f=30\text{GHz}$)

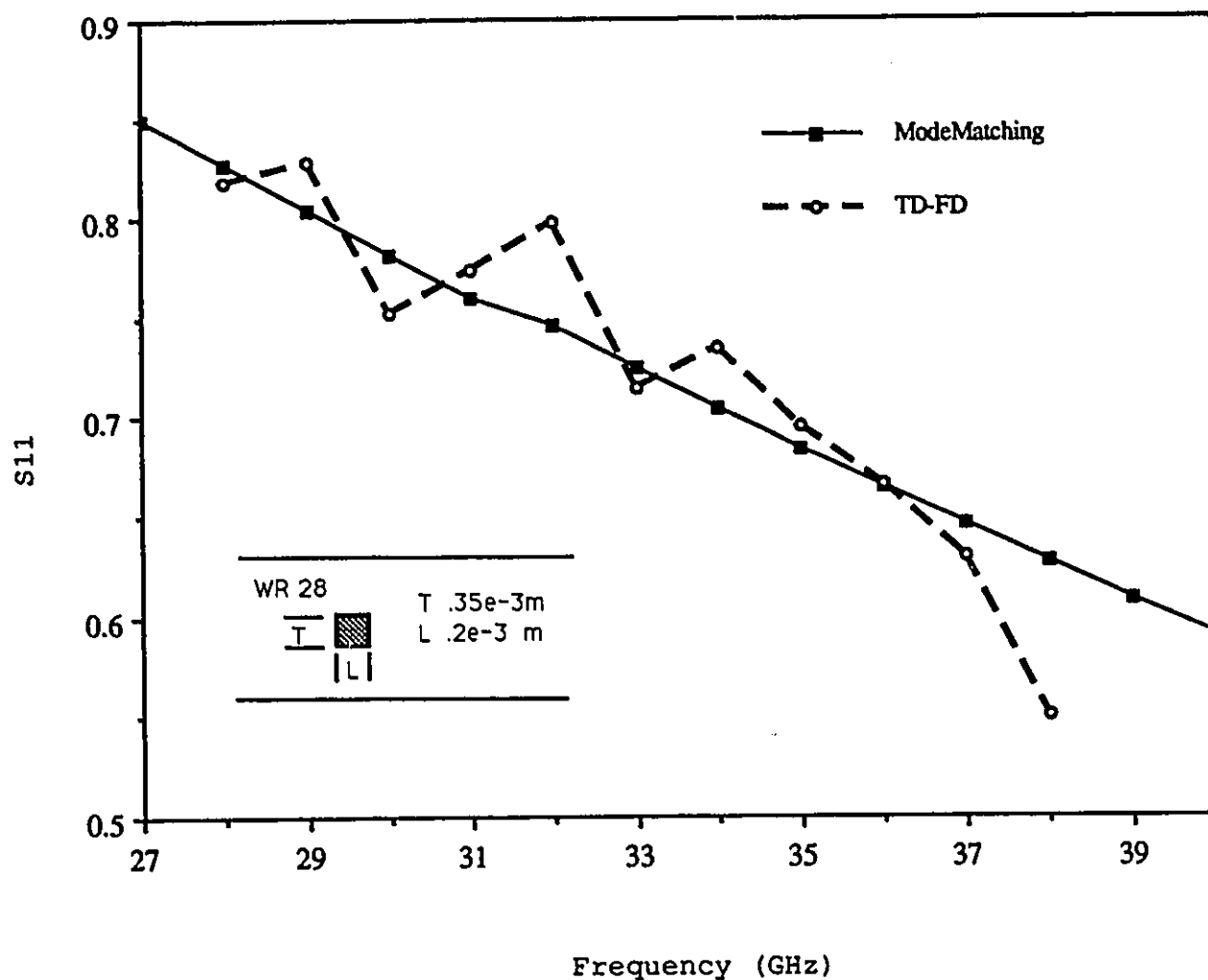


Fig. 6.3.4 Comparison of S_{11} for the rectangular metal post in WR-28, calculated with TD-FD and mode matching technique. Transition operator matching boundary condition has been used.

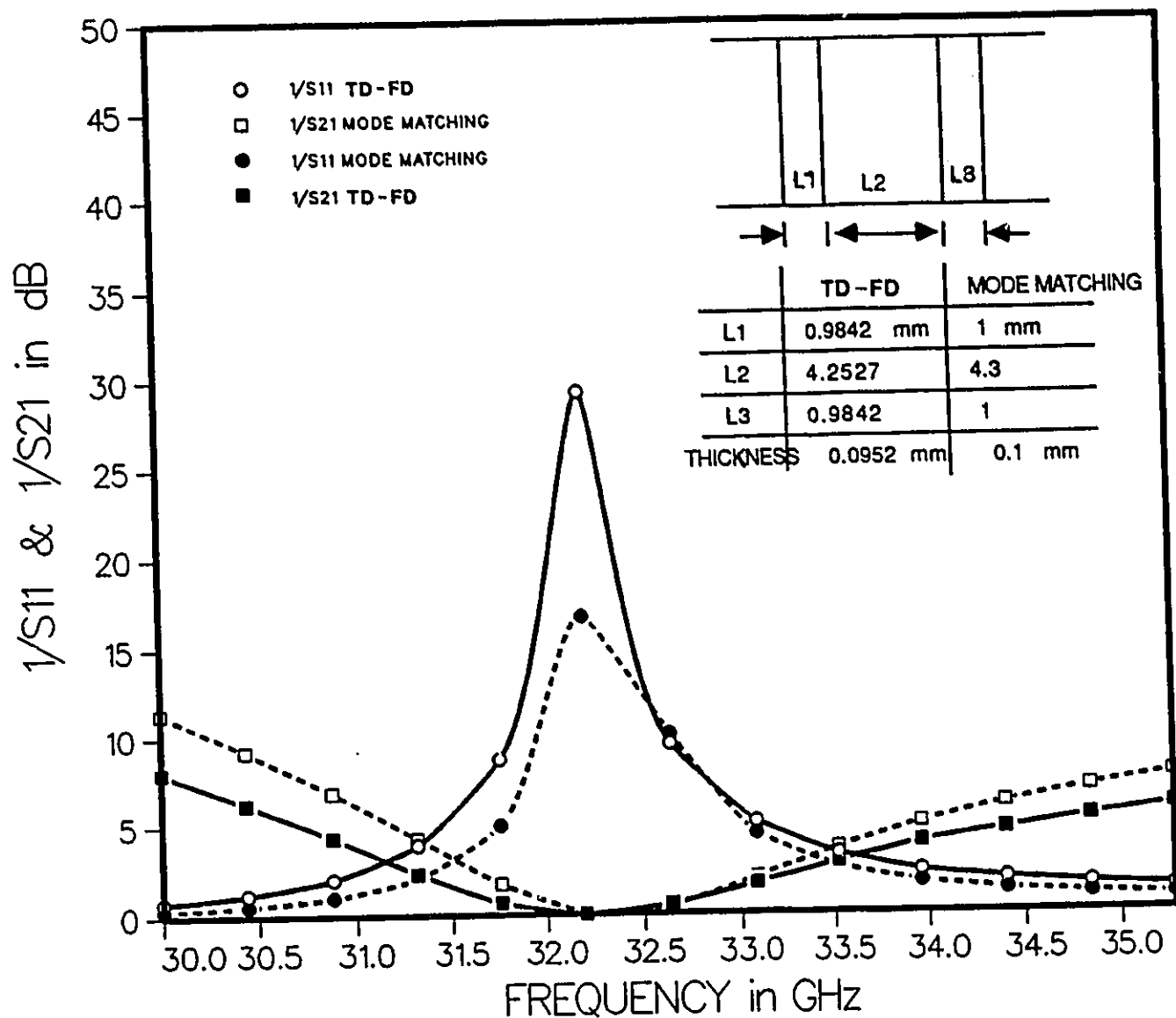


Fig. 6.3.5 Comparison of single resonator E-plane filter characteristics, calculated with TD-FD and mode matching technique.

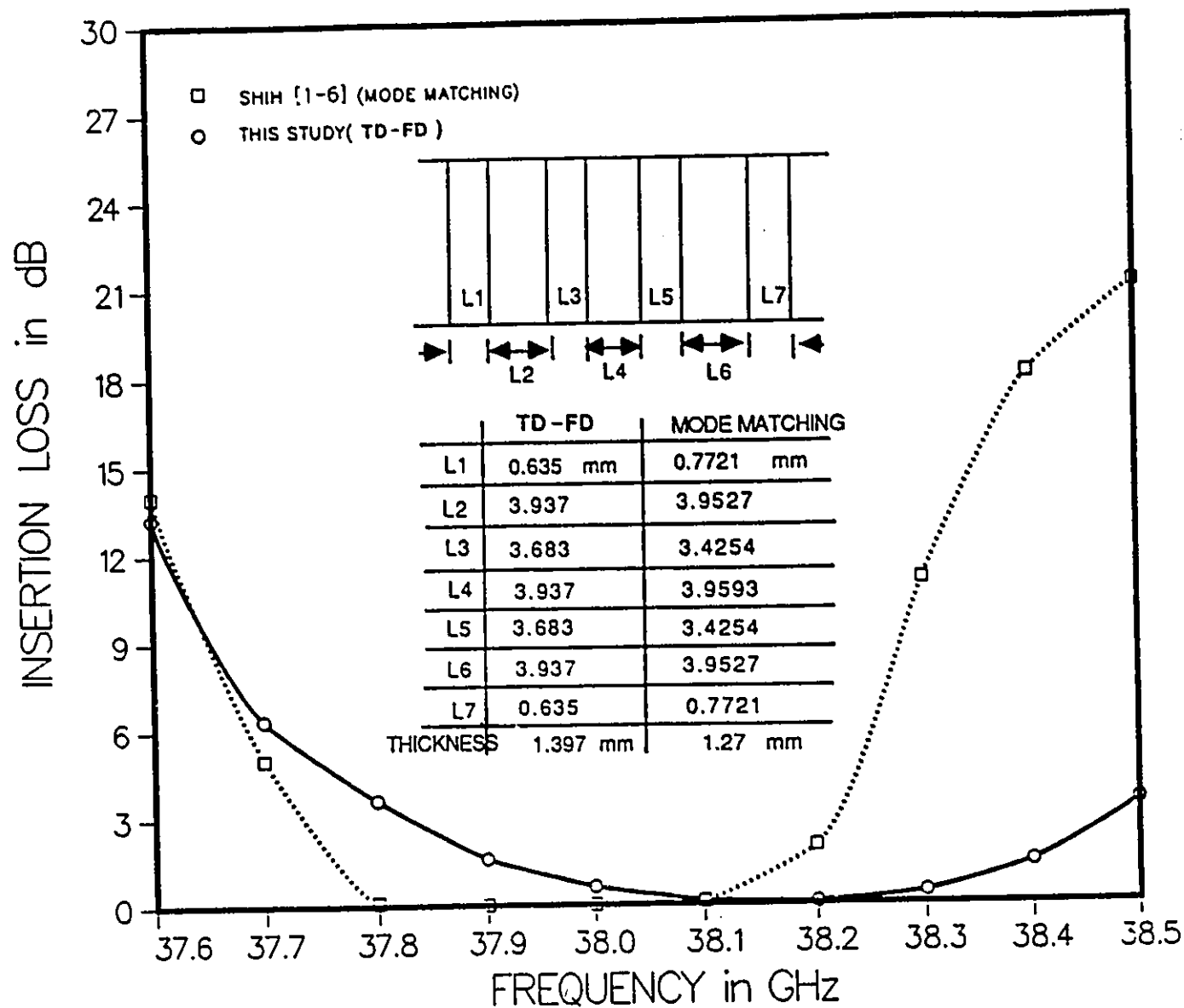


Fig. 6.3.6 Comparison of three-resonator E-plane filter characteristics, calculated with TD-FD and mode matching techniques.

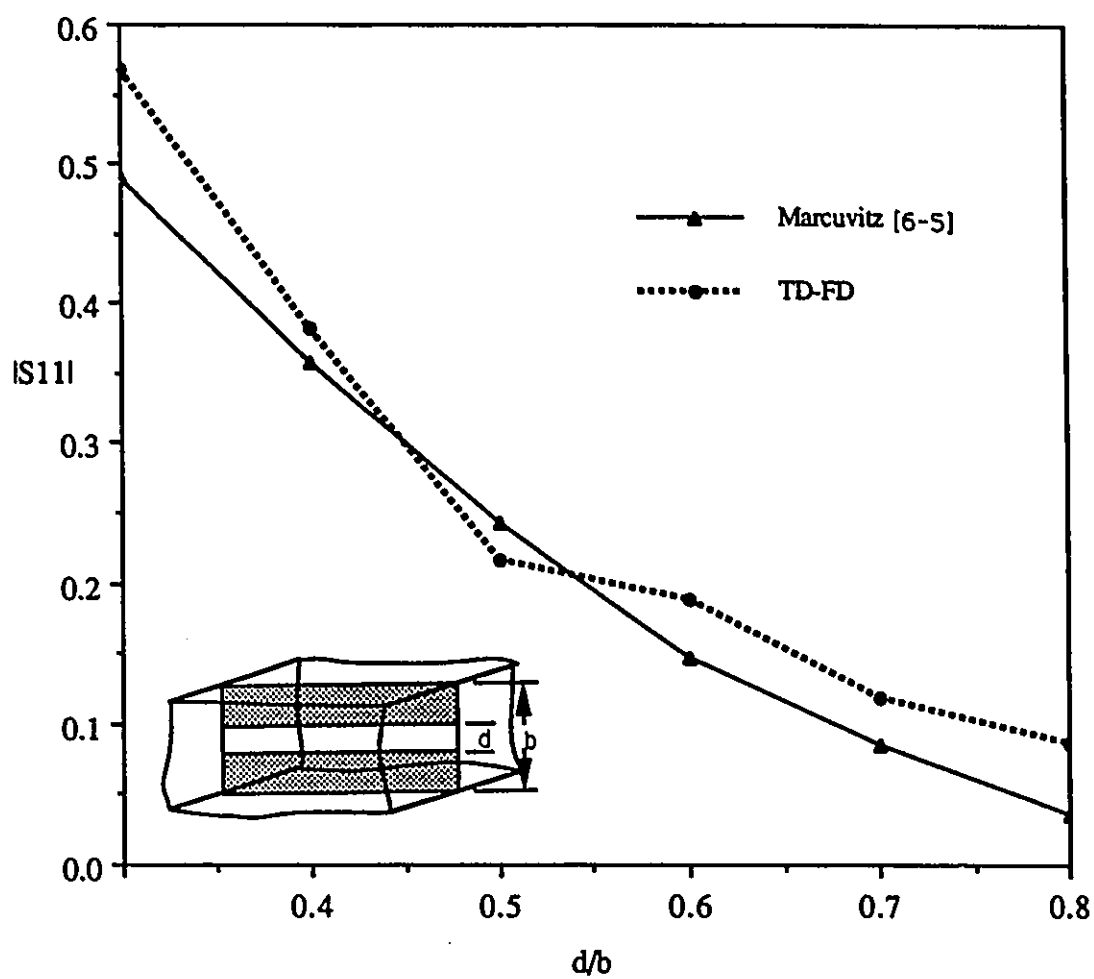


Fig. 6.3.7 $|S_{11}|$ computed with TD-FD, and Marcuvitz's result for various values of d/b in WR-28 waveguide at 40 GHz. (3D-computation)

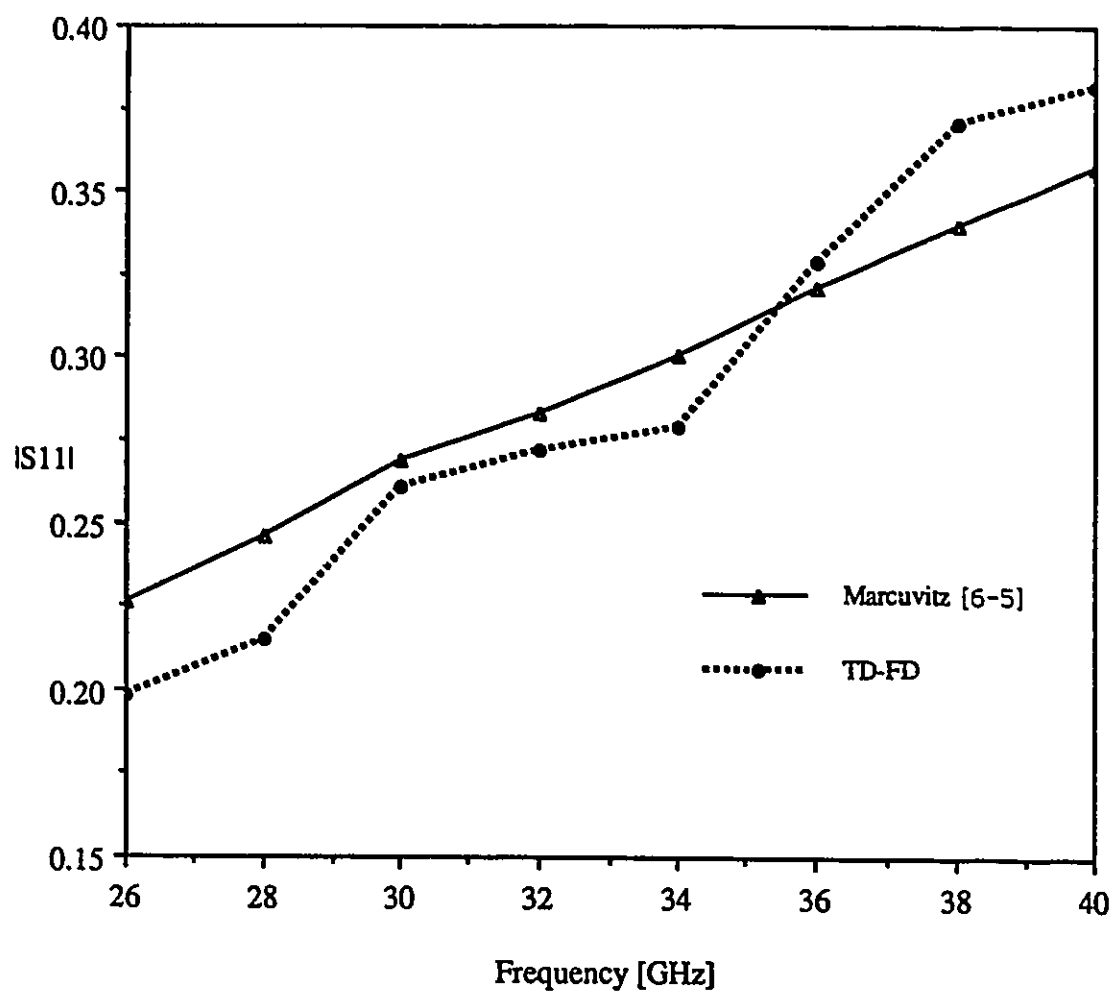


Fig. 6.3.8 $|S_{11}|$ computed with TD-FD, and Marcuvitz's result for fixed $d/b=0.4$ over the whole operating range of the WR-28 waveguide.

CHAPTER 7

Conclusions

7.1 Discussion The objective of the research described in this thesis was to develop a model with which one could accurately describe (by simulation) physical EM wave propagation. In waveguides with discontinuities, such a model could be used to determine the physical parameters which characterize the structure (such as scattering parameters). The Time Domain-Finite Difference (TD-FD) approach for both CW and pulse cases has been implemented for simulation of EM field propagation and extraction of microwave circuit parameters, especially S-parameters. The principles of the characteristic and the domain or dependence of partial differential equations were introduced to help understand the properties (simulating nature) of numerical wave propagation. Any physical parameter in the frequency domain can be predicted from the field description (field distribution). Errors introduced by the numerical approximation were examined both qualitatively and quantitatively, and remedies for minimizing their effect were evaluated and discussed. An algorithm which was used to extract the S-parameters from the discrete EM field distribution was developed for the CW and pulse propagation

cases. The simulating property of the model was interpreted with the basis of discrete numerical wave propagation. The leap-frog approximation scheme was a model which could be used to describe local wave propagation. In an effort to relate the discrete model of wave propagation to the continuous one, the geometrical meaning of the stability factor was introduced. By understanding the effects of the stability factor on the numerical dispersion, the accuracy of the results, and the economy of computation, significant insight was obtained with regard to the mechanics of the TD-FD method. It is interesting to note that the physical interpretation of the discrete wave propagation is possible since the leap-frog approximation simulates the characteristic lines (directions) of the continuous cases in a discrete fashion. By analyzing the leap-frog approximation, it was shown that the TD-FD method is non-dissipative which means that energy is conserved during the simulated wave propagation.

To accurately model EM wave propagation phenomena, convergence criteria were introduced to check the global errors involved in the numerical procedure. These criteria were based on the physical parameters, phase linearity and matching condition (standing wave ratio) along any segment of lossless guiding structures. The matching condition can be accurately realized at a single frequency since the leap-frog scheme is non-dissipative. It is interesting to note that the convergence criteria confirm the fact that Maxwell's equations can be separated into transverse and longitudinal parts in any guide with uniform cross-section. The criteria must be met in order to ensure the accurate analysis of complex guiding structures.

In the formulation of a computational domain for EM wave propagation solutions, artificial matching boundary conditions (MBC) are necessary to make the domain compact. The existing matching boundary conditions (MBC's) studied in Chapter 4

were not perfect and always produced some reflections of the incident wave. The error wave reflected from the MBC made it difficult to extract the S-parameters accurately (better than 30 dB return loss is required for accurate results). In order to reduce the reflection error and improve the bandwidth limitation of the MBC property, a new wideband MBC was developed. It is based on the concept of the transition operator in modern control theory as explained in Chapter 4. The MBC works fine, but the number of iterations is inversely proportional to the distance between the source and the boundary.

The main obstacle in this numerical modeling algorithm is the required computer resources. It is very expensive in terms of computer memory and CPU time to utilize a fine mesh over the whole computational domain, and in some cases, usage could easily exceed the capacity of the system. Thus, a local mesh refinement algorithm was developed to resolve the behaviour of extremely non-uniform fields near a local discontinuity using a fine mesh, and as well to resolve smoothly varying fields using a coarse mesh. This refinement algorithm produces results of satisfactory accuracy, while reducing the computing time by around 70 times over a scheme which uses only fine mesh.

Our contributions to the analysis of EM propagation problems using TD-FD method (a physical interpretation, convergence criteria, effects of the stability factor, MBC's and local mesh refinement algorithm) were combined with the basic TD-FD procedures to create an algorithm. This algorithm was designed to simulate EM field propagation and extraction of microwave circuit parameters. To check the ability of the program to describe qualitatively how numerical waves propagate in homogeneous and discontinuous waveguides with CW and pulse excitations, the program was used to

solve several problems for which the physical response was understood. The qualitative observations obtained from the program were consistent with the physical interpretation of the real solutions. In order to validate the accuracy of solutions in discontinuous waveguide problems, the results were compared with analytical solutions and with those calculated by other techniques such as TLM and mode matching. The good agreement of the qualitative response, and the quantitative results, leads me to say that the algorithm developed is a good numerical model in terms of its ability to simulate EM propagation and to extract microwave circuit parameters. A model which simulates the response of a propagating EM wave in the frequency domain can only predict the structure's response for the steady state condition and does not provide clues to the response for transient or pre-steady state conditions. Thus, such a model could not be used to generate a physical picture of the propagation phenomena. On the other hand, a model which simulates a propagating wave in the time domain can be used to obtain pictures of the EM wave as it propagates in an arbitrary structure, thus making it easy to see directly the immediate physical interactions of the EM wave with the structure.

7.2 Future research direction A new matching boundary condition (MBC) based on the transition operator concept has been developed. The procedure of obtaining the transition operator, $\bar{T}$, can be treated as a deconvolution for the impulse response (or time domain Green's function) of the system under study. Unfortunately, deconvolution is not a unique mathematical function [1-4]. In this regard, the next approach to improving the MBC is to modify the model approximating Maxwell's equations in such a way that it accepts an impulse excitation like the TLM method. To be able to produce an impulse response, the numerical scheme should be non-dispersive and non-dissipative

and this could be developed by inserting a new term into the leap-frog approximation of Maxwell's equations. This approach follows an idea suggested by Watanabe [7-1] for simple hyperbolic PDE's. Another promising idea is a hybridization of the TD-FD and the TLM methods, i.e., introducing the impulse excitation property from the TLM method into the TD-FD method. Development of a TD-FD scheme allowing characterization of structures excited with an impulse, the scheme would free us from restrictions of the initial condition and the band limited response. With the impulse response computable, the DIAKOPTIC approach that is used in the TLM method, could be used to develop a new MBC for the modified TD-FD approach. By including electric and magnetic loss terms σ_E and σ_H into the approximated Maxwell's equations, an absorbing material matching boundary condition can be developed which acts like a practical waveguide termination, but this approach requires more memory size.

In Chapter 5, an efficient local mesh refinement algorithm was developed to resolve strong non-uniform field behaviour around a fine discontinuity. The optimum variation of the mesh size could be determined, provided an analytical prediction of the reflection property at an interface of two different mesh sizes is developed. Hence, a future research topic could be the development of a procedure or expression to predict the reflection properties at an interface.

As was described in Chapter 3, the leap-frog approximation produces some numerical dispersion if a mesh size that is coarse with respect to the wavelength is used ($\frac{\lambda}{\Delta t} > 10$). Fang [7-2] introduced a fourth order scheme to reduce this numerical dispersion in the one-dimensional case. More research effort on this aspect could allow us to minimize the numerical dispersion of two- and three-dimensional cases and allow us to use a smaller computer.

Monolithic microwave integrated circuits contain passive and active elements. In order to analyze and synthesize these circuits, TD-FD models for active and non-linear elements are required. This aspect will stimulate research interest in non-linear modeling work. A recent paper by Voelker and Lomax [7-3] developed a hybrid method called FDTLM method, which used the two methods to model non-linear devices. For non-linear modeling, the soliton concept used in many non-linear wave propagation phenomena could be studied further in view of combining it with the TD-FD model.

APPENDIX I

Anisotropy Error

In this appendix, we want to discuss the error due to anisotropy which is another type of error that occurs in addition to that due to numerical dispersion. Anisotropy error occurs in the discretization of hyperbolic equations in two space dimensions, and can be described as follows: the velocity of propagation of the numerical solution is dependent upon direction and the direction is dependent upon the space discretization [2-38].

This problem will be illustrated with TE mode propagation:

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \frac{\partial E_y}{\partial z}, \quad (I.1)$$

$$\frac{\partial H_z}{\partial t} = -\frac{1}{\mu} \frac{\partial E_y}{\partial x}, \quad (I.2)$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_z}{\partial z} - \frac{\partial H_z}{\partial x} \right). \quad (I.3)$$

A sinusoidal plane wave solution is assumed as:

$$\begin{bmatrix} H_x \\ H_z \\ E_y \end{bmatrix} = \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(t) e^{-j\beta(x \cos \theta + z \sin \theta)}, \quad (I.4.a)$$

$$= \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(t) e^{-j\beta(\bar{r} \cdot \bar{c})}, \quad (I.4.b)$$

$$= \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(t) e^{-j\beta(\beta_x x + \beta_z z)}, \quad (I.4.c)$$

where $\bar{r}$ is the position vector in the $(x - z)$ plane,

$$\bar{r} = \begin{bmatrix} x \\ z \end{bmatrix}, \quad (I.5)$$

$\hat{a}$ is the directional vector of the wave, and is chosen parallel to the velocity vector $\bar{c}$,

$$\hat{a} = \begin{bmatrix} \sin \theta \\ \cos \theta \end{bmatrix}, \quad \bar{c} = c \cdot \hat{a} = \begin{bmatrix} c \cdot \sin \theta \\ c \cdot \cos \theta \end{bmatrix} \quad (I.6)$$

and $Z_o = \sqrt{\frac{\mu}{\epsilon}}$ is the characteristic impedance. The wavelength measured in the $\hat{a}$ direction is $\lambda = \frac{2\pi}{\beta}$. Substituting (I.4) into (I.1), (I.2), and (I.3) for H_x , H_z , and E_y , we obtain

$$\frac{d^2 a_\omega(t)}{dt^2} = -(c\beta)^2 a_\omega(t). \quad (I.7)$$

Hence the exact plane wave solution is

$$\begin{bmatrix} H_x \\ H_z \\ E_y \end{bmatrix} = \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(0) e^{\pm j\beta(x \cos \theta + z \sin \theta - ct)} \quad (I.8)$$

The constant phase lines are defined by

$$x \cos \theta + z \sin \theta \pm ct = \text{constant}. \quad (I.9)$$

They are perpendicular to the direction of propagation and are moving at the velocity $\pm c$ and in opposite directions as shown in Chapter 3. Equation (I.9) ensures that the continuous form of Maxwell's equations written as the wave equation describe a wave whose velocity is independent of θ and therefore isotropic.

But this isotropy will be changed if the differential equations are replaced by the leap-frog scheme. Let us consider (2.3.15) and the 2-D computational grid for TE mode propagation as shown in Fig.2.6.1. The plane wave solution in the discretized form will be

$$\begin{bmatrix} H_x(i, k) \\ H_z(i, k) \\ E_y(i, k) \end{bmatrix} = \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(t) e^{-j\beta(x_i \cos \theta + z_k \sin \theta)}, \quad (I.10)$$

where (i, k) is a specific node on the mesh and $x_i = i \cdot \frac{\Delta \ell}{2}$, and $z_k = k \cdot \frac{\Delta \ell}{2}$. The propagation characteristics are obtained by substituting (I.10) into the semi-discretized equations of (I.1)-(I.3). We then obtain:

$$\frac{\partial H_x}{\partial t} = \frac{c}{Z_o \cdot \Delta z} [E_y(i, k+1) - E_y(i, k)], \quad (I.11.a)$$

$$\frac{\partial H_z}{\partial t} = -\frac{c}{Z_o \cdot \Delta x} [E_y(i+1, k) - E_y(i, k)], \quad (I.11.b)$$

$$\frac{\partial E_y}{\partial t} = \frac{Z_o \cdot c}{\Delta x} [H_x(i, k + \frac{1}{2}) - H_x(i, k - \frac{1}{2}) - (H_z(i + \frac{1}{2}, k) - H_z(i - \frac{1}{2}, k))]. \quad (I.11.c)$$

After algebraic manipulation with the uniform mesh condition ($\Delta x = \Delta z = \Delta \ell$), we obtain:

$$\frac{d^2 a_\omega(t)}{dt^2} = (c\beta)^2 \{ \sin^2(\beta \Delta \ell \cos \theta) \cos^2(\beta \Delta \ell \sin \theta) + \sin^2(\beta \Delta \ell \sin \theta) \cos^2(\beta \Delta \ell \cos \theta) \}. \quad (I.12)$$

By integrating (I.12),

$$a_\omega(t) = a_\omega(0) e^{-j\beta c^* t}, \quad (I.13)$$

where

$$c^* = c \{ \sin^2(\beta \Delta \ell \cos \theta) \cdot \cos^2(\beta \Delta \ell \sin \theta) + \sin^2(\beta \Delta \ell \sin \theta) \cdot \cos^2(\beta \Delta \ell \cos \theta) \}^{\frac{1}{2}} \quad (I.14)$$

is the numerical phase velocity. So, the numerical plane wave solutions are

$$\begin{bmatrix} H_x(i, k) \\ H_z(i, k) \\ E_y(i, k) \end{bmatrix} = \begin{bmatrix} -Z_o^{-1} \sin \theta \\ Z_o^{-1} \cos \theta \\ 1 \end{bmatrix} \cdot a_\omega(0) e^{-j\beta(x_i \cos \theta + z_k \sin \theta - c^* t)} \quad (I.15)$$

Thus this phase velocity is not only a function of frequency, but also a function of the propagation direction

$$c^* = c^*(\beta, \theta).$$

It should be noted that the anisotropy of the numerical approximation is due to the directional dependence of the phase velocity. Figure 3.4.6 illustrates the dependence of

c^* on (β, θ) in the polar diagram. Equation (I.14) does not have any relationship to the stability factor. The phase and group velocities, however, are related. At the upper limit of the stability inequality, the lowest velocity error was obtained. This is shown in Sections 3.4 and 3.5

APPENDIX II

Energy Conservation and Non-dissipativity

The non-dissipativity nature of the leap-frog approximation of Maxwell's two time dependent curl equations is derived for unbounded TE mode propagation. Energy conservation property of the TD-FD method comes from this derivation. Since the derivation is based on Von Neumann's way, the stability inequality is also produced as another outcome.

To study the lossless characteristics of EM wave propagation, the dissipative terms in the continuous form of Maxwell's equations, σ_E and σ_H , have been excluded in the derivation. Thus, the numerical approximation must also be non-dissipative to simulate physical lossless EM wave propagation phenomena. For simplicity of derivation, an unbounded TE mode propagation is assumed. But the derivation can be easily extended to the general 3-D case in a similar way. The discretized Maxwell's equations for TE mode propagation are first considered as:

$$H_x^{n+\frac{1}{2}}(i, k + \frac{1}{2}) = H_x^{n-\frac{1}{2}}(i, k + \frac{1}{2}) + \frac{c\Delta t}{Z_o\Delta z\mu_r}[E_y^n(i, k + 1) - E_y^n(i, k)], \quad (II.1a)$$

$$H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, k) = H_z^{n-\frac{1}{2}}(i + \frac{1}{2}, k) - \frac{c\Delta t}{Z_o\Delta x\mu_r}[E_y^n(i + 1, k) - E_y^n(i, k)], \quad (II.1b)$$

$$\begin{aligned} E_y^{n+1}(i, k) = E_y^n(i, k) + \frac{Z_o c \Delta t}{\Delta z \epsilon_r} [H_x^{n+\frac{1}{2}}(i, k + \frac{1}{2}) - H_x^{n+\frac{1}{2}}(i, k - \frac{1}{2})] \\ - \frac{Z_o c \Delta t}{\Delta x \epsilon_r} [(H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, k) - H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, k))], \end{aligned} \quad (II.1c)$$

where the superscript n is the time step, β_x and β_z are the wave numbers in the x and z directions, and i and k are the indices for the x and z coordinates, respectively.

Since the TD-FD approach is based on the initial boundary value problem solution method, we want to describe how EM waves propagate as time goes on. For this purpose,

a plane wave solution for TE mode propagation can be assumed in the discrete space as:

$$\begin{bmatrix} H_x^n(i, k) \\ H_z^n(i, k) \\ E_y^n(i, k) \end{bmatrix} = \xi_i^n(\beta_i) e^{j(\beta_x i \Delta x + \beta_z k \Delta z)} \begin{bmatrix} H_x^o(i, k) \\ H_z^o(i, k) \\ E_y^o(i, k) \end{bmatrix}, \quad (II.2)$$

The term $\xi_i(\beta_i)$ is a complex number whose subscript i and superscript n indicate the eigenmodes and the time step, respectively. It is also a function of β_x and β_z , and H_x^o , H_z^o , and E_y^o are the initial conditions or excitations which are constant (both in space and in time) eigenvectors. ξ_i is called the amplification (or growth) factor of the leap-frog approximation and the eigenmodes. For simplicity of derivation, a uniform mesh size is employed: $\Delta x = \Delta z = \Delta \ell$. Now, substitute (II.2) into the expressions (II.1), and divide (II.1a) by $\xi_i^{n-\frac{1}{2}} e^{j[\beta_x i + \beta_z (k+\frac{1}{2})] \Delta \ell}$, (II.1b) by $\xi_i^{n-\frac{1}{2}} e^{j[\beta_x (i+\frac{1}{2}) + \beta_z k] \Delta \ell}$, and (II.1c) by $\xi_i^n e^{j[\beta_x i + \beta_z k] \Delta \ell}$. Then rearrange and write in matrix form as:

$$\begin{vmatrix} \xi_i - 1 & 0 & -2ja\xi_i^{\frac{1}{2}} \sin(\frac{\beta_x \Delta \ell}{2}) \\ 0 & \xi_i - 1 & 2ja\xi_i^{\frac{1}{2}} \sin(\frac{\beta_x \Delta \ell}{2}) \\ -2jb\xi_i^{\frac{1}{2}} \sin(\frac{\beta_z \Delta \ell}{2}) & 2jb\xi_i^{\frac{1}{2}} \sin(\frac{\beta_z \Delta \ell}{2}) & \xi_i - 1 \end{vmatrix} \cdot \begin{bmatrix} H_x^o \\ H_z^o \\ E_y^o \end{bmatrix} = 0, \quad (II.3)$$

where

$$a = \frac{c\Delta t}{Z_o \Delta \ell \mu_r},$$

$$b = \frac{c\Delta t Z_o}{\Delta \ell \epsilon_r}.$$

Equation (II.3) admits a solution only if the determinant of the first matrix on the left vanishes. Then,

$$(\xi_i - 1)[\xi_i^2 - 2(1 - 2abB)\xi_i + 1] = 0 \quad (II.4)$$

where

$$B = \sin^2(\frac{\beta_x \Delta \ell}{2}) + \sin^2(\frac{\beta_z \Delta \ell}{2})$$

The three roots are

$$\xi_{i(1)} = 1 \quad (II.5a)$$

$$\xi_{i(2)} = (1 - 2abB) + \sqrt{(1 - 2abB)^2 - 1} \quad (II.5b)$$

$$\xi_{i(3)} = (1 - 2abB) - \sqrt{(1 - 2abB)^2 - 1} \quad (II.5c)$$

The solutions $\xi_{i(2)}$ and $\xi_{i(3)}$ can be obtained with the Von Neumann's criterion for stability

$$|\xi_i| \leq 1 + O(\Delta t).$$

where the term of order $O(\Delta t)$ must remain bounded if $\Delta t \rightarrow 0$ and $\Delta \ell \rightarrow 0$. This term permits an exponential growing or damping solution. If

$$1 - 2abB > 1, \quad \text{then} \quad |\xi_{i(2)}| > 1; \quad (II.6a)$$

if

$$1 - 2abB < -1, \quad \text{then} \quad |\xi_{i(3)}| > 1; \quad (II.6b)$$

and if

$$|1 - 2abB| \leq 1, \quad \text{then} \quad |\xi_{i(2)}| = |\xi_{i(3)}| = 1. \quad (II.6c)$$

The condition (6c) results in

$$-1 \leq 1 - 2 \frac{c^2 \Delta t^2}{\Delta \ell^2 \mu_r \epsilon_r} [\sin^2(\frac{\beta_x \Delta \ell}{2}) + \sin^2(\frac{\beta_z \Delta \ell}{2})] \leq 1 \quad (II.7)$$

where the term, $[\sin^2(\frac{\beta_x \Delta \ell}{2}) + \sin^2(\frac{\beta_z \Delta \ell}{2})]$, is bounded by 2. The right side of the inequality (II.7) is trivial; the left side is satisfied for all β if and only if $\frac{c \Delta t}{\Delta \ell} \leq \sqrt{\frac{\mu_r \epsilon_r}{2}}$. This, then, is the criterion for stability. Courant, Friedrichs, and Lewy [2-33] encountered this condition in their study of convergence and gave the following interpretation: the region of influence of a single point for the *difference* equation is bounded by the lines

$ct = \pm \frac{c\Delta t}{\Delta \ell} \ell$ (in one space dimensional case). We introduce two basic definitions which are characteristic and domain of dependence. The lines are characteristics and the line between the projections of the characteristics is the domain of dependence. The domain of dependence is expanding as time goes on. In EM theory, this expanding is interpreted as propagated area. The numerical domain of dependence (triangular region) formed by the lines must enclose the corresponding region (analytical domain of dependence) of influence of the point for the *differential* equation, otherwise convergence of the exact solution of the partial *difference* equation to the exact solution of the partial *differential* equation is clearly impossible as $\Delta \ell$ and Δt reduce to zero (since some points which are in the limit will never be influenced though they should be). Thus, $\frac{c\Delta t}{\Delta \ell} \leq \sqrt{\mu_r \epsilon_r / n}$, (n is the number of the space dimension involved in the problem) is a necessary condition for convergence. Reference [2-33] proved that it is also a sufficient condition. It is important to note that the condition $|\xi_{i(1)}| = |\xi_{i(2)}| = |\xi_{i(3)}| = 1$ provides a non-dissipative property of the leap-frog approximation of Maxwell's equations, since the amplitude of the excitation at the initial time does not change at any late time. And from (II.7), since the condition $\frac{c\Delta t}{\Delta \ell} \leq \sqrt{\frac{\epsilon_r \mu_r}{n}}$ satisfies the Von Neuman's stability criterion, it leads to a bounded solution of the *difference* equation that is stable. If the condition $\frac{c\Delta t}{\Delta \ell} > \sqrt{\frac{\epsilon_r \mu_r}{n}}$ is met, then the root produces a solution which grows exponentially and is unstable.

Since $|\xi_i| = 1$, the leap-frog discretization of Maxwell's equations is non-dissipative, and thus energy is strictly conserved at every frequency as follows: the Poynting flux $\vec{S}$ through a surface is constant with respect to time (the rate of flow of energy is defined by the Poynting vector) and for a wave propagating in the z direction becomes

$$\vec{S}_z = E_y^o(i, k) \times H_z^{\frac{1}{2}}(i - \frac{1}{2}, k) = E_y^n(i, k + n \cdot SF) \times H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, k + n \cdot SF). \quad (II.8)$$

where energy flux through time surface coming in at the time step n and coming out at the time step $n + 1$ is locally conserved and where energy of the system is not fed in or dissipated from the boundary conditions or from forcing or damping terms. Also note that the flow of energy is proportional to the square of the amplitude. If $|\xi| \neq 1$, an amplitude modification occurs in the iteration procedure, i.e., if $|\xi| < 1$, the amplitude is decayed, and if $|\xi| > 1$, the amplitude is amplified.

This non-dissipative property is an important advantage for simulating lossless wideband EM wave propagation problems over long periods of time and it comes from the centered nature of the leap-frog approximation. The Lax-Wendroff [1-15] difference scheme does not have this non-dissipative characteristic.

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