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Time-domain Simulation of Electromagnetic Band-Gap Structures Using the TLM Method

by

Gerardo Romo Luévano, M. A. Sc.

A thesis submitted to the
Faculty of Graduate Studies and Research
in partial fulfillment of the requirements for the degree of
Doctor of Philosophy

Ottawa-Carleton Institute for Electrical Engineering
Department of Electronics
Faculty of Engineering
Carleton University
Ottawa, Canada

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Abstract

Photonic crystals can enhance the performance of various microwave and photonic devices when incorporated as part of the device's design. In this thesis, numerical techniques for the simulation of electromagnetic devices incorporating photonic crystals are developed. In addition, this work also offers optimization techniques for speeding up the proposed simulation techniques.

In summary, the transmission line matrix method is presented as an efficient simulation technique for the analysis of electromagnetic band-gap structures. The work describes important aspects for the computation of the dispersion relation of photonic crystals. It also proposes two methods for reducing the computational effort involved in the simulations. One method is based on a real-valued implementation of the periodicity condition, and the other one is based on the use of a multi-grid mesh. Depending on the physical geometry of the crystal, computational savings of over 50% can be easily achieved. The advantages and limitations of these methods are described. The suitability of the transmission line matrix method to handle photonic crystals with more general material properties such as frequency dependent metals and semiconductors is also demonstrated.

Finally, the mesh conditions that produce the least numerical dispersion error in complex meshes, are investigated. Specifically, we analyze in detail how geometrical factors influence node dispersion and obtain guidelines for use with general meshing tools. To conclude, the accuracy and efficiency of various complex meshes are evaluated by analyzing real-world problems and novel applications of electromagnetic band-gap structures.

Acknowledgments

I gratefully acknowledge the role played by many people in completing this thesis. I would like to especially express my deepest gratitude to Prof. Tom Smy, for providing motivation when I needed most, his expert insight, valuable guidance and unparalleled patience. His friendly manner and wise judgment made this thesis an enjoyable and refreshing experience.

Special thanks are extended to Prof. D. Walkey for the valuable discussions, helpful comments, ideas and suggestions.

I would like to thank and acknowledge my colleagues: G. Knight and D. Celo. The office staff of B. Zahalan, P. Piccolo, L. Duncan, N. Mikhail and J. Lemieux were always there to assist.

A special note of appreciation for my wife Martha for her loving support, care and understanding. A loving note to my sons Dante and Daniel, whose arrival has given a special meaning to my life.

Dedicated to the memory of my father

Juan Romo Cano

for teaching me the important values
of family and life.

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List of Acronyms

TLM	Transmission Line Matrix
SLN	Stub Loaded Node
SCN	Stub Condensed Node
HSCN	Hybrid Symmetrical Condensed Node
SSCN	Symmetrical Super Condensed Node
FDTD	Finite Differences Time-Domain
PWE	Plane Wave Expansion
MoM	Method of Moments
EM	Electromagnetic
PBS	Photonic Band Structure
DR	Dispersion Relation
PC	Photonic Crystals
EBG	Electromagnetic Band-Gap
PBG	Photonic Band-Gap
CEM	Computational Electromagnetics

FEM	Finite Elements Method
TE	Transverse Electric
TM	Transverse Magnetic
PML	Perfectly Matched Layers
ABC	Absorbing Boundary Condition

List of Symbols

a	Lattice constant
c	Speed of light
f	Frequency
j	$\sqrt{-1}$
$\mathbf{k}$	Propagation vector
n	Refractive index
t	Time
ω	Total energy
ω_e	Electric energy density
ω_m	Magnetic energy density
$\mathbf{B}$	Magnetic flux density
C	Capacitance
$[C]$	Connection matrix
$\mathbf{D}$	Electric displacement
$\mathbf{E}$	Electric field

G	Conductance
H	Magnetic field
I	Current
J	Current density
L	Inductance
N_e	Electron density
Q	Charge
$\mathbf{r}$	Position vector
R	Resistance
$[S]$	Scattering matrix
S	S-parameter
$\mathbf{T}$	Lattice vector
V	Voltage
Y	Admittance
Y_0	Characteristic admittance
Z	Impedance
Z_0	Characteristic impedance
Z_b	Medium impedance
Z_l	Link-line impedance
Φ	Magnetic flux
Γ	Reflection coefficient
ϵ	Absolute permittivity

ϵ^*	Complex permittivity
ϵ_0	Permittivity of free space
ϵ_r	Relative permittivity
λ	wavelength
β	Phase constant
σ	Conductivity
μ	Absolute permeability
μ_0	Permeability of free space
μ_r	Relative permeability
ρ	Charge density
ρ_l	Link-line reflection coefficient
χ	Susceptibility
ν_c	Electron collision frequency
ω	angular frequency
Δl	Generic node spacing
Δt	Time step
Δx	Node spacing in x -direction
Δy	Node spacing in y -direction
Δz	Node spacing in z -direction

Chapter 1

Introduction

1.1 Background and Motivation

In the last two decades, improvements in computer speed and memory have set the foundation for the quick development of computational electromagnetic (CEM) methods such as the finite element and finite difference methods, the method of moments (MoM), transmission line matrix (TLM) method, and others. As these computational techniques have become available, the engineering and scientific communities have relied on them for the simulation of a wide variety of electromagnetic (EM) problems. In turn, this increase in computational and simulation power has led to many technological innovations.

An interesting problem that has recently caught the attention of many researchers is that of enhancing the performance of microwave and photonic structures by incorporating periodicity as a key feature in their design. For example, a one-dimensional stack of alternating dielectric materials has been used for a long time as a frequency

selective mechanism in semiconductor lasers and thin films to produce optical filters. In recent years, the extension of periodic structures to two and three dimensions has led to what is referred to in the literature as photonic crystals (PC). The electromagnetic waves propagating in such structures have shown many interesting properties and have therefore been extensively studied in the last decade (see for example [1]). In a simplistic way, photonic crystals can be defined as infinite periodic arrays of a repeating pattern (unit cell) composed of different dielectric materials. These periodic electromagnetic structures are also referred to as electromagnetic band-gap (EBG) or photonic band-gap (PBG) materials. In the context of this work, the terms PC and EBG structures are used to refer to infinite periodic arrays, and electromagnetic structures incorporating or embedded in a finite PC, respectively.

Photonic crystals have already found many applications in microwave and millimeter-wave antenna structures [3], photonic crystal integrated circuits [4], optical waveguides [5], high- and low-Q electromagnetic resonators [6], quantum optical electromagnetic cavity effects [7], optical nano-cavities [8], etc. In all these areas, extensive research has shown that, when designed and implemented correctly, PC can considerably improve the performance of a wide variety of these devices. It should be noticed that due to the scalability of PC [9], they can be applied at both optical and microwave frequencies.

As is usually the case in modern engineering and scientific design problems, the successful achievement of the design specifications greatly depends upon simulations. It is obvious that practical applications of PC involve periodic structures of only finite extent, however, when large enough, insight into the device's behavior can be obtained by modelling infinitely large periodic structures. Thus, there are three

important simulation aspects of devices incorporating PC:

1. The simulation of an infinitely large PC to be utilized for enhancing the performance of a given EM device.
2. The simulation of the EM device under consideration as a stand-alone structure to determine its behaviour in the absence of the PC.
3. The simulation of the EM device in the presence or embedded in the PC to assess its modified performance.

One might think that the availability of high performance commercial electromagnetic software would provide the flexibility to handle the above three simulation aspects of EBG structures. However, general purpose EM software is not always suitable to real-world problems which often require customized solutions by writing original computer codes to solve them. This is particularly true for EBG structures, where the wide variety of potential applications makes development of general simulation software difficult.

It is the purpose of this work to develop numerical techniques with the required flexibility to handle the three simulation aspects described above. That is, a simulation technique capable of computing the dispersion relation of general, infinitely large PC. In addition, a simulation technique capable of simulating the EM properties of general microwave and photonic devices. Note that these two simulation aspects do not necessarily have to be implemented using the same numerical technique because the two simulation problems are, at this stage, totally independent. However, intuition indicates that the third simulation aspect follows more straightforwardly if the

first two are addressed using the same numerical technique. Therefore, that is the approach taken in this work.

Over the last few years, several methods to determine the dispersion relation of periodic structures have been used. The plane wave expansion method (PWE) and the MoM are two of the most popular. Although these numerical techniques are fast and accurate, their main drawback is that the pre-conditioning required for the simulation of arbitrary unit cells requires considerable effort. In addition, the preconditioning procedure is structure-dependent, making generalization of these methods a difficult task. Although less frequently, time-domain methods, such as finite differences time-domain (FDTD) and the TLM method, have also been applied for simulating PC. In contrast to the PWE and MoM methods, time-domain methods can easily be generalized to handle unit cells composed of arbitrary shapes and materials.

Numerical techniques such as FEM, MoM, FDTD and TLM methods have also been used for the simulation of general microwave and optical structures. In this respect, time-domain methods offer similar advantages to those described above. For example, once the method is implemented in a computational volume, it can handle arbitrary structures by simply changing boundary conditions and EM parameters, such as permittivity and permeability, at every node. In addition, time-domain methods provide information at various frequencies from a single simulation. Thus, a time-domain method has been found suitable for this work, because it provides the required flexibility to address the three simulation aspects of EBG structures described before.

After performing a thorough literature review, it has been found that the FDTD method has been much more extensively utilized for the simulation of EBG structures than the TLM method. As a matter of fact, there are only a few published papers

Figure 1.1: Comparison of papers published on EBG structures using FDTD and TLM as the analysis method.

addressing the simulation of these problems by means of the TLM method. Fig. 1.1 shows a histogram of papers published in the last years dealing with EBG structures and using FDTD and TLM as the method of analysis¹. As the figure shows, the number of papers published on this field based on TLM is very small compared with those based on FDTD. This lack of TLM-EBG documentation, motivated the possible use of the TLM method as the simulation tool for this work.

The performances of the FDTD and TLM methods have extensively been compared when applied to general EM problems [10]–[14]. It has been found that both methods yield similar results and that generally speaking, the main advantages of the TLM method over the FDTD method, are those which stem from the fact that the fields in the former method are computed in the same temporal and spatial mesh points [15].

¹Source: <http://scholar.google.com/>

In this respect, this work also aims at exploring possible advantages of TLM over FDTD for the simulation of EBG structures. In addition, given that time-domain methods are inherently slow, this work also proposes optimization techniques for speeding up the simulation aspects described before.

1.2 Contributions

Based on the previous section, the motivation and objectives that generated this work can be summarized as follows: to develop optimized simulation techniques with the flexibility to handle three simulation aspects of EBG structures. The simulation aspects were described to be, *a)* Simulation of infinitely large PC, *b)* Simulation of stand-alone microwave and photonic structures and *c)* a combination of *a)* and *b)*. Thus, in view of the objectives that originated this research work, the following contributions have been made:

1. Given that a methodology to compute the dispersion relation of PC by means of the TLM method had not been addressed in detail in literature, a methodology presenting the TLM method as a simulation technique capable of accomplishing this task was developed [16]. In this contribution, the implementation and stability aspects of the method were presented in detail.
2. The formulation presented in [16] (valid for PC crystals composed of simple dielectric materials) was expanded to handle PC composed of frequency dependant materials such as metals and semiconductors [17]. In this contribution, the necessary equations for their application in non-cubic meshes were derived.

3. It had been suggested by previous authors that a so called “Real-valued formulation” reduces the computation time by half as compared with the methodology proposed in [16]. However, previous published formulations suffered from stability problems. In Refs. [18] and [19] an unconditionally stable formulation, valid for PC and other periodic microwave structures was presented.
4. A methodology for the optimization of the formulation presented in [16] was presented in [20] and [21]. The optimization is based on a combination of the real-valued formulation and multi-gridding techniques.
5. A summary of the previous results was presented in [22].
6. A formulation that studies the dispersion characteristics of quad-tree meshes has been derived. These results are still to be published.

Chapter 2

Literature Review

2.1 General Aspects of Photonic Crystals

The main asset of PC is their ability to prevent the propagation of electromagnetic radiation at certain frequencies. The frequencies which are not allowed to propagate are said to fall within a forbidden band-gap when mapped into the dispersion relation of the PC. The dispersion curves show the relation between the light frequency ω and the propagation vector $\mathbf{k}$ of a given PC. In addition, due to symmetry and the periodic properties of PC, the propagation vector can be restricted to values within the irreducible Brillouin zone [23]. Thus, the dispersion curves are generally calculated by letting $\mathbf{k}$ take on values along the edge of the irreducible Brillouin zone. It should be noted that, in the context of PC, the dispersion relation is frequently referred to as a photonic band structure (PBS). Thus, in this work both terms are used interchangeably.

The analysis of PC generally involves the computation of the dispersion relation

when dealing with an infinite array, or the computation of the transmitted and reflected spectra when dealing with a finite array. In both cases, knowledge of the propagation properties of EM waves in the structure under consideration is indispensable to assess the structure's performance. In the next sections, a literature review of previous published work in the field of PC modelling using time-domain methods is presented.

2.2 Review of Time-domain Methods for Simulating PC

Time-domain methods have been found suitable for computing the dispersion relation of PC. Common to time domain methods is the ability to reduce the computational domain when simulating periodic structures. That is, if the right periodic boundary conditions are used, infinitely large periodic structures can be analyzed by simulating a single cell of the repeating pattern. The general procedure to calculate the dispersion relation of periodic structures in time-domain methods is to excite the reduced structure with a delta or Gaussian impulse. Then, the time-domain data is stored at randomly selected points as the simulation is carried out. At the end of the simulation, the data is Fourier transformed to identify the frequency modes that satisfy a fundamental phase shift per spatial period. By repeating this procedure for each discrete value of the k -vector around the first Brillouin zone, the PBS can be constructed.

While the FDTD method has extensively been used for the analysis and computation of the dispersion relation of PC [24]–[30], very little attention has been given

to the TLM method¹. In Ref. [31], a class of spatially looped algorithms for the analysis of microwave periodic structures was developed. In the same reference, a special form of periodic boundary conditions for the FDTD method was presented. In addition, it was pointed out that such an approach could be extended to the TLM method, although no further information was provided. It was also suggested without proof that in a complex-valued TLM algorithm, the energy remains constant in time because it is able to circulate between two space-orthogonal grids.

In Ref. [28], the issue of applying periodic boundary conditions within the framework of the real-valued TLM method was analyzed in more detail. Equations relating incident and reflected pulses at the boundaries of the periodic structure were derived. The algorithm was tested by calculating the dispersion relation of a periodically loaded rectangular microwave waveguide. The results were compared with those predicted by analytical solutions and a good agreement was found despite the appearance of high frequency components in the time-domain data.

2.3 Review of the Simulation Aspects of TLM-EBG Problems

Since its appearance in 1987 [32], the TLM method has quickly gained popularity as a simulation tool for the analysis of general electromagnetic problems. The wide variety of electromagnetic problems the TLM method has been applied to, include but are not limited to, radiation of microstrip lines and patch antennas [33]–[36], modelling of

¹The reason for this is perhaps that FDTD was introduced to the scientific community 20 years earlier than TLM.

integrated optic components [37], simulation of waveguide structures [38], analysis of the optical properties of thin films [39], far-zone and radar cross-section calculations [40]–[42], modelling of magnetized and unmagnetized plasmas [43], solving transient problems of diffusion [44], etc.

Despite the numerous applications of the TLM method to general EM problems, only a few applications of this method to EBG structures have been reported. For example, in Ref. [45], a commercial two-dimensional TLM program was used to explore the transmission properties and field distributions of localized electromagnetic modes associated with defects of a finite array of dielectric cylinders. The finite nature of the array used in this reference had two drawbacks. The fact that the computational domain was not restricted to a single cell, increased the demand for computational resources. In addition, when the dispersion relation was calculated from the phase information of the time-domain data, odd symmetry modes with respect to a mirror plane along the direction of propagation were not detected. In Ref. [46], the same commercial program was used to simulate tunneling of electromagnetic pulses through the forbidden gap of a two-dimensional PC. The results showed that pulses tunnel with a group velocity that exceeds that of light in vacuum and that the tunnelling time becomes constant once sufficient periodicity exists to create a forbidden gap. It should be noted that while Einstein’s theory of special relativity prevents mass, energy, or information from traveling faster than the speed of light c , there is nothing preventing “apparent” motion faster than c (or, in fact, with negative speeds). For example, in this case the phase velocity and group velocity of the tunneling wave exceeds the speed of light, but no energy or information is actually traveling faster than c . The observed superluminal propagation is a consequence of classical interference

between the constituent frequency components in a region of anomalous dispersion, which results in an “evanescent”, rather than in a propagating wave.

In Ref. [47], the transmission line matrix-integral equation (TLM-IE) method was used to perform full-wave analysis of optical periodic structures. The TLM-IE method is a hybrid version of the TLM method and combines the advantages of the TLM method in dense finite regions and those of the IE method in open regions where simple Green functions are available. Although this hybrid method offers a good alternative for simulating the interaction between optical components embedded in space, this type of problems are not very common. In addition, the implementation of the TLM-IE method is not very straightforward.

In Ref. [48] a simple and intuitive TLM algorithm was developed to model nonlinear optical phenomena in fiber Bragg gratings. The method was used to simulate periodic nonlinear media having a Kerr nonlinearity.

Finally, in Ref. [37] the TLM method was used to analyze the evolution of the field distribution and spectral response of an optical waveguide embedded in a photonic band-gap filter.

2.4 Review of Optimization Techniques Used in the TLM Method

In the original formulation of the TLM method presented by P.B. Johns [32], time stepping at every iteration required one inversion of a small scattering matrix per node. Thus, the computation time per node was considerably high (compared with FDTD, for example), resulting in an extremely slow method. To overcome this prob-

lem, Naylor and Ait-Sadi [49] developed a more efficient implementation of the scattering procedure based on calculation of nodal voltages and loop currents. However, despite the reduction in computation time obtained with the new scattering procedure, the TLM method remained inherently slow. The reason for this is that, in time-domain methods, every node in the computational volume is processed independently. Thus, the processing of each node at every time step requires a minimum number of mathematical operations for the implementation of the method. As a consequence, once the method is optimized to the minimum number of operations, there is virtually no room for additional optimization.

2.4.1 General Optimization Techniques Used in TLM

A common practice to alleviate the computational burden associated with time-domain methods, is to resort to multi-gridding and variable mesh techniques [50]–[55]. Not only do these techniques reduce the run-time, but they also provide a means of increasing resolution only in areas where required; for example, in regions of space where the fields have large spatial variations or where there exist small structural details. This is illustrated in Fig. 2.1, where two-dimensional versions of variable and multi-grid meshes are shown.

In a variable or graded mesh, the shape of the nodes is allowed to change throughout the simulation space. The mesh is defined by specifying the node dimensions along each of the coordinate axes. A drawback of a variable mesh is that regions of fine resolution cannot be completely localized in the problem space.

In contrast to a graded mesh, a multi-grid mesh allows one to embed regions of fine resolution into coarser ones. This is possible because the computational space

Figure 2.1: Two-dimensional examples of variable and multi-grid meshes.

is discretized into regions of different resolutions linked by a “connecting interface”. This results in two important advantages that make multi-gridding techniques more attractive than variable meshing techniques. The first one is that a multi-grid mesh requires less nodes than a graded mesh to achieve similar spatial resolutions. The second advantage is that a multi-grid mesh results in more regular (less distorted) nodes which in turn lead to lower dispersion error. On the other hand, multi-gridding techniques are, in general, more difficult to implement and prone to stability problems. The difficulties arise from the fact that the connecting interface between the fine and coarse regions must be subject to four important constraints, which ideally, must be satisfied simultaneously. The constraints are: charge and energy conservation, no reflections and zero delay. The constraints stem from the fact that the introduction in the mesh of the connecting interface must not affect the conditions met by the original mesh, which are precisely the four constraints just mentioned.

In early attempts [51], [54], it was found that strict adherence to all four constraints

was not possible and that a compromise should therefore be found. There are several implications of not meeting the four constraints. The most important ones lead to inaccurate results and stability problems.

An improved multi-grid interface was described in Ref. [50]; it makes use of matching transformers to connect the fine and coarse regions. Given that the TLM method is an equivalent circuit field representation and that this type of connecting interface is also consistent with circuit theory, stability is guaranteed. Unfortunately, despite the potential of this new connecting interface for the simulation of multi-scale problems, it has not previously received significant attention.

It should also be mentioned at this point that there is yet another type of TLM meshing technique which is called unstructured mesh [56]. In an unstructured mesh, the computational volume is discretized by means of tetrahedrons. This permits the proper discretization of circular features without using a staircase approximation and the use of diversely sized elements in multiscale problems. Nevertheless, an unstructure mesh results in nodes of different shapes whose scattering matrix need to be uniquely determined. In addition, some meshing constraints must be enforced in order to avoid the use of undesirable small time steps.

2.4.2 Optimization Techniques Used in the Simulation of PC

While the previous optimization techniques apply to the computation of general electromagnetic problems, a unique optimization approach can be applied to the simulation of PC. As it will be shown in more detail in Chapter 4, the computation of the dispersion relation of PC requires a complex-valued network. In the TLM method, the real and imaginary parts of the complex-valued network are split into two par-

allel (real-valued) networks connected only at the boundaries of the computational domain. Early attempts have been made to reduce the computation effort by half by decoupling the real and imaginary parts and computing the PBS by using only either part. In Ref. [57], this approach was used to compute the dispersion relation of a periodically loaded microwave waveguide. However, it was seen that such an approach introduced high-frequency components in the time-domain data that eventually led to unstable simulations. These high-frequency components had already been observed in Ref. [58] and dealt with by using an averaging process.

As it can be seen from this review, no assessment of the potential of the TLM method for its application to the simulation of EBG structures has been made.

Chapter 3

Background Theory

As it was pointed out in Chapter 1, there exist several methods to compute the PBS of PC, the most commonly used being the PWE method and the MoM. In the MoM, the simulation domain is discretized and the unknown equivalent electric current across the dielectric region is expanded with a linear combination of subsectional or entire domain basis functions. The equations are then tested in order to obtain an adequate number of equations for the unknown coefficients of the basis functions [59]. This allows Maxwell's equations to be recast as an eigenvalue problem which is then solved by using standard techniques.

In the PWE method, the fact that the solution is periodic is exploited by expanding both, the electromagnetic fields and the periodic dielectric structure, with a Fourier series [1]. This formulation also leads to an eigenvalue problem. Given that the PWE method is widely used in this work to validate the results obtained by the transmission line matrix method, in the following sections a quick review of this method is provided. The introduction of the PWE method is facilitated by first

reviewing Maxwell's equations.

3.1 Maxwell's Equations

The starting point for the analysis of PC is Maxwell's equations, which form the foundation for electromagnetic theory. Written in differential form, these equations are

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} \quad (3.1)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \mathbf{J} + \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} \quad (3.2)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = \rho \quad (3.3)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0 \quad (3.4)$$

where $\mathbf{E}(\mathbf{r}, t)$ is the electric field intensity, $\mathbf{B}(\mathbf{r}, t)$ is the magnetic field density, $\mathbf{H}(\mathbf{r}, t)$ is the magnetic field intensity, and $\mathbf{D}(\mathbf{r}, t)$ is the electric field density. The electric current density $\mathbf{J}$ and electric charge density ρ are the sources of the electromagnetic fields. However, because the interest is in the eigenmodes of the radiation field, it is assumed here that free charges and electric currents are absent, i.e. $\mathbf{J}=0$ and $\rho=0$.

For linear and isotropic media, $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{D}(\mathbf{r}, t)$, and $\mathbf{B}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$ are related by the so-called constitutive relations

$$\mathbf{D}(\mathbf{r}, t) = \epsilon_r \epsilon_0 \mathbf{E}(\mathbf{r}, t) \quad (3.5)$$

$$\mathbf{B}(\mathbf{r}, t) = \mu_r \mu_0 \mathbf{H}(\mathbf{r}, t), \quad (3.6)$$

where ϵ_0 , μ_0 , ϵ_r and μ_r are the free-space permittivity, free-space permeability, relative permittivity and relative permeability, respectively. In this chapter, it is assumed that the dielectric constant is real, isotropic and does not depend on frequency. Those cases in which the dielectric constant is complex or depends on frequency will be dealt with in Chapter 4.

The fields in Maxwell's equations can be decoupled. That is, they can be reduced to four equations, each involving only one type of field ($\mathbf{E}$, $\mathbf{D}$, $\mathbf{H}$ and $\mathbf{B}$). For example, by taking the curl of both sides of Eq. (3.1) and substituting from Eq. (3.2) gives the two electric field equations. Furthermore, if a similar procedure is carried out in the opposite order, the result is the two magnetic field equations. In addition, if the fields are time-harmonic

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{i\omega t} \quad (3.7)$$

$$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r})e^{i\omega t}, \quad (3.8)$$

then $\partial^2/\partial t^2 \rightarrow -\omega^2$, and the decoupled equations can be written as

$$\frac{1}{\epsilon_r(\mathbf{r})} \nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2} \mathbf{E} \quad (3.9)$$

$$\nabla \times \nabla \times \frac{1}{\epsilon_r(\mathbf{r})} \mathbf{D} = \frac{\omega^2}{c^2} \mathbf{D} \quad (3.10)$$

$$\nabla \times \frac{1}{\epsilon_r(\mathbf{r})} \nabla \times \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H} \quad (3.11)$$

$$\nabla \times \frac{1}{\epsilon_r(\mathbf{r})} \nabla \times \mathbf{B} = \frac{\omega^2}{c^2} \mathbf{B} \quad (3.12)$$

Note that because we are dealing with non-magnetic materials, μ is constant in the

equations and consequently the equations for $\mathbf{H}$ and $\mathbf{B}$ have the same form. However, it should be noted that $\epsilon(\mathbf{r})$ is a function of position (it is periodic), and thus the placement of the $\frac{1}{\epsilon_r}$ term is strict.

At this stage, the question of which equation to solve arises. Given a dielectric function, all four equations will produce a set of field distributions. From these, the other fields can be computed by simply using Maxwell's equations. There are advantages and disadvantages associated with using each equation. In this work, Eq. (3.9) is mainly used. More information about the implications of using each equation can be found in Ref. [1].

If the vector operations in Eqs. (3.9-3.12) are carried out, each of the decoupled equations will produce three component equations. For example, the expansion equations for the $\mathbf{E}$ field can be expressed as

$$\frac{1}{\epsilon_r(\mathbf{r})} \left(-\frac{\partial^2 E_x}{\partial y^2} - \frac{\partial^2 E_x}{\partial z^2} + \frac{\partial^2 E_y}{\partial x \partial y} + \frac{\partial^2 E_z}{\partial x \partial z} \right) = \frac{\omega^2}{c^2} E_x \quad (3.13)$$

$$\frac{1}{\epsilon_r(\mathbf{r})} \left(-\frac{\partial^2 E_y}{\partial x^2} - \frac{\partial^2 E_y}{\partial z^2} + \frac{\partial^2 E_z}{\partial y \partial z} + \frac{\partial^2 E_x}{\partial x \partial y} \right) = \frac{\omega^2}{c^2} E_y \quad (3.14)$$

$$\frac{1}{\epsilon_r(\mathbf{r})} \left(-\frac{\partial^2 E_z}{\partial x^2} - \frac{\partial^2 E_z}{\partial y^2} + \frac{\partial^2 E_x}{\partial x \partial z} + \frac{\partial^2 E_y}{\partial y \partial z} \right) = \frac{\omega^2}{c^2} E_z \quad (3.15)$$

This final simplification will be useful to more clearly illustrate the PWE in Sect. 3.2.

3.1.1 Propagation of Waves in a Periodic Medium

For an infinite periodic structure, we can assume that the propagating mode in the structure has the form

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_{\mathbf{p}}(\mathbf{r}, t) e^{-j\mathbf{k} \cdot \mathbf{r}}, \quad (3.16)$$

where $E_p(\mathbf{r}, t)$ is a periodic function of $\mathbf{r}$ with period $\mathbf{a}$, then

$$\mathbf{E}(\mathbf{r} + \mathbf{a}, t) = \mathbf{E}_p(\mathbf{r} + \mathbf{a}, t)e^{-j\mathbf{k} \cdot (\mathbf{r} + \mathbf{a})}. \quad (3.17)$$

Given that $E_p(\mathbf{r}, t)$ is periodic with period $\mathbf{a}$,

$$\mathbf{E}_p(\mathbf{r} + \mathbf{a}, t) = \mathbf{E}_p(\mathbf{r}, t). \quad (3.18)$$

Substituting Eq. (3.18) into Eq.(3.17) yields

$$\mathbf{E}(\mathbf{r} + \mathbf{a}, t) = \mathbf{E}_p(\mathbf{r}, t)e^{-j\mathbf{k} \cdot (\mathbf{r} + \mathbf{a})}, \quad (3.19)$$

and using Eq. (3.16),

$$\mathbf{E}(\mathbf{r} + \mathbf{a}, t) = \mathbf{E}(\mathbf{r}, t)e^{-j\mathbf{k} \cdot \mathbf{a}}. \quad (3.20)$$

Equation (3.20) is known as Bloch's theorem. It simply indicates that for propagating modes in infinite periodic dielectric structures, the field between adjacent cells is related by a complex (phase) constant.

For example, from the theory of Fourier series, a periodic electric field with period a , can be expanded as a periodic function in the direction of periodicity and prescribed phase constant β_0 . Assuming that the periodicity is in the z -direction, the field expansion is given by

$$E(x, y, z) = \sum_n E_n(x, y)e^{-j\frac{2\pi n}{a}z}e^{-j\beta_0 z} = \sum_n E_n(x, y)e^{-j\beta_n z} \quad (3.21)$$

where

$$E_n(x, y) = \frac{1}{a} \int_0^a E_n(x, y, z) e^{j \frac{2\pi n}{a} z} dz \quad (3.22)$$

are the expansion coefficients that serve to represent the dependence on x and y , and

$$\beta_n = \beta_0 + \frac{2\pi n}{a} \quad (3.23)$$

is the phase constant of the n^{th} harmonic. Thus, the field in a periodic structure can be expanded in an infinite set of harmonics through Bloch's theorem, each with phase constant β_n .

3.2 Plane Wave Expansion Method

Throughout this thesis, the PWE is extensively used as a verification tool for simple cases. For this reason, this section is intended to provide a review of this method. The implementation, limitations and computational solutions of periodic structures based on the PWE method are analyzed in some detail. For the sake of simplicity, the PWE method is presented in the context of a one-dimensional example.

Consider the one-dimensional periodic structure shown in Fig. 3.1. It consists of a dielectric slab, of width b , embedded in air. The basic structure (unit cell) repeats itself every a units of length in the x -direction. As it is well known, there are two independent polarizations for these type of structures. If the electric field only has components in the zy -plane, i.e. it does not have a component in the x -direction, the mode is denoted TE_x . Similarly, if the magnetic field does not have a component in the x -direction, the mode is denoted TM_x . For normal incidence ($\phi = 0$), the modes

Figure 3.1: One-dimensional periodic structure. The width of the slabs is b and the lattice constant (period) a .

are degenerate, i.e. the TE_x and TM_x modes are equivalent. In this case, we have chosen to solve for the TE_x modes.

3.2.1 Transverse Electric (TE_x) Modes

Without loss of generality, let us assume that the electric field propagates only in the xy -plane, i.e. $k_z = 0$. Thus, the electric field can be represented by

$$\mathbf{E}(x, y) = E_z(x, y)\hat{\mathbf{z}} = E_p(x)e^{-jk_{x0}x}e^{-jk_y y}\hat{\mathbf{z}} \quad (3.24)$$

where E_p is the periodic electric field and k_{x0} is a prescribed propagation constant in the direction of periodicity. Note that if propagation in the z -direction had been included in this formulation, then the term $e^{-jk_z z}$ would have been included in

Eq. (3.24). Also noting that the dielectric constant is a periodic function of x and assuming that the dielectric slabs are infinite in the y - and z -directions, the following equation is obtained after substituting Eq. (3.24) into Eq. (3.15)

$$\frac{1}{\epsilon_r(x)} \left(-\frac{\partial^2 E_z(x, y)}{\partial x^2} + k_y^2 E_z(x, y) \right) = \frac{\omega^2}{c^2} E_z(x, y) \quad (3.25)$$

at this point we proceed by expanding the periodic electric field in a Fourier series in x with unknown coefficients a_n , this results in the following expression

$$E_p(x) = \sum_{n=-\infty}^{+\infty} a_n e^{-j \frac{2\pi n}{a} x} \quad (3.26)$$

Given that the dielectric function is also periodic, it is appropriate to expand the term $\frac{1}{\epsilon_r(x)}$ in another Fourier series with coefficients b_m , this leads to

$$\frac{1}{\epsilon_r(x)} = \sum_{m=-\infty}^{+\infty} b_m e^{-j \frac{2\pi m}{a} x} \quad (3.27)$$

note that if this term had been sent to the right hand side of Eq. (3.25), then a Fourier series expansion for the term $\epsilon_r(x)$ would have been required instead. Although this is a valid alternative, it would lead to a *generalized* eigenvalue problem.

Substituting the Fourier expansions (3.26) and (3.27) into (3.25) and carrying out the algebraic operations results in

$$\sum_n \sum_m \left[\left(\frac{2\pi n}{a} + k_{x0} \right)^2 + k_y^2 \right] a_n b_m e^{-j \frac{2\pi n}{a} x} e^{-j \frac{2\pi m}{a} x} = \frac{\omega^2}{c^2} \sum_n a_n e^{-j \frac{2\pi n}{a} x}. \quad (3.28)$$

To simplify this equation, each side is multiplied by an orthogonal function $\left(e^{-j \frac{2\pi p}{a} x} \right)$,

where p is an integer, and integrated over a unit cell, i.e., $\left(\frac{1}{a} \int_{-a/2}^{a/2} \cdots\right)$. Due to the orthogonality between the functions, one summation on each side of the equation can be dropped. After rearranging the terms and renaming the sums to use only the indices n and m , Eq. (3.28) takes the following eigenvalue form

$$\sum_n \left[\left(\frac{2\pi n}{a} + k_{x0} \right)^2 + k_y^2 \right] b_{m-n} a_n = \frac{\omega^2}{c^2} a_m. \quad (3.29)$$

Equation (3.29) forms an ordinary eigenvalue problem. For the purpose of computation, the integers m and n are truncated symmetrically about zero, which corresponds to including only lower order plane waves in the Fourier expansions.

For illustrating how the plane wave expansion works, let us consider the case where m and n are truncated to five terms, i.e. $(m = n) \in [-2, -1, 0, 1, 2]$. The eigenvalue problem appears as follows

$$\begin{array}{c} m = -2 \\ m = -1 \\ m = 0 \\ m = 1 \\ m = 2 \end{array} \begin{array}{ccccc} n = -2 & n = -1 & n = 0 & n = 1 & n = 2 \\ \left(\begin{array}{ccccc} Q_{-2,-2} & Q_{-2,-1} & Q_{-2,0} & Q_{-2,1} & Q_{-2,2} \\ Q_{-1,-2} & Q_{-1,-1} & Q_{-1,0} & Q_{-1,1} & Q_{-1,2} \\ Q_{0,-2} & Q_{0,-1} & Q_{0,0} & Q_{0,1} & Q_{0,2} \\ Q_{1,-2} & Q_{1,-1} & Q_{1,0} & Q_{1,1} & Q_{1,2} \\ Q_{2,-2} & Q_{2,-1} & Q_{2,0} & Q_{2,1} & Q_{2,2} \end{array} \right) \end{array} \begin{pmatrix} a_{-2} \\ a_{-1} \\ a_0 \\ a_1 \\ a_2 \end{pmatrix} = \frac{\omega^2}{c^2} \begin{pmatrix} a_{-2} \\ a_{-1} \\ a_0 \\ a_1 \\ a_2 \end{pmatrix}$$

where the following definition is used

$$Q_{m,n} = \left[\left(\frac{2\pi n}{a} + k_{x0} \right)^2 + k_y^2 \right] b_{m-n}. \quad (3.30)$$

The only remaining problem is to find the dielectric expansion coefficients b_{m-n} , which can be found by means of an inverse Fourier transform:

$$b_n = \frac{1}{a} \int_{-a/2}^{a/2} \frac{1}{\epsilon_r(x)} e^{j \frac{2\pi n}{a} x} dx. \quad (3.31)$$

Based on Fig. 3.1, we can see that the integral can be split into three integration regions where the permittivity is a constant

$$b_n = \frac{1}{a} \int_{-a/2}^{-b/2} e^{j \frac{2\pi n}{a} x} dx + \frac{1}{a} \int_{-b/2}^{b/2} \frac{1}{\epsilon_r} e^{j \frac{2\pi n}{a} x} dx + \frac{1}{a} \int_{b/2}^{a/2} e^{j \frac{2\pi n}{a} x} dx \quad (3.32)$$

which results in

$$b_n = \frac{1}{\epsilon_r} \delta_n + \left(1 - \frac{1}{\epsilon_r}\right) \frac{b}{a} \text{sinc} \left(\frac{\pi n b}{a} \right). \quad (3.33)$$

The basic approach for calculating the field distributions and eigenfrequencies using the PWE method can be summarized as follows: given a periodic dielectric function and a prescribed propagation vector, expand the term $\frac{1}{\epsilon(\mathbf{r})}$ and the three components of the appropriate field vector in Fourier series. These series are then substituted into the decoupled Maxwell's equations and the terms reorganized into an eigenvalue problem. This approach can be generalized to two and three-dimensions in a straightforward way.

3.2.2 Solving the Eigenvalue Problem

The eigenvalue equation (3.29) is now complete and can be solved using a software package or computational technique of choice. For the work in this thesis, the commercial software package MATLAB is used. After diagonalization, the eigenvalues

(ω^2/c^2) and eigenvectors (a_n) will be known. The eigenvalues determine the frequencies of the modes that can propagate in the structure and are found for specific values of prescribed phase shift. For example, in one-dimension $k_{x0}a \in [0, 2\pi]$. For each prescribed phase shift, one obtains as many solution frequencies as the number of space harmonics that are used in the expansion of the field in (3.26). When the resulting eigenvalues are sorted from smallest to largest and plotted versus the prescribed phase shift, the dispersion diagram is formed. In the general case, the band diagram is constructed by varying values of k_x , k_y and k_z along the boundaries of the first Brillouin zone.

The eigenvectors, when substituted back into the Fourier expansion for $\mathbf{E}$, determine the field distribution at any given frequency. It should be mentioned that in studies of photonic crystals, the main interest is not in the electric or magnetic field distributions themselves, but in the eigenvectors that contain information on the location of the modes in k -space.

3.3 The Transmission-Line Modelling Method

Traditionally, the TLM method has been regarded as the application of a discrete version of Huygen's principle to the modelling of electromagnetic fields [60]. The method is based on a lumped-element model of Maxwell's equations from which a transmission line model is extracted. In simple words, the TLM method basically models an electromagnetic field in a computational domain by means of voltage impulses that travel in a network of interconnected transmission lines. More fundamentally, the TLM network is able to model Maxwell-Ampere and Maxwell-Faraday laws in the

presence of electric and magnetic current densities in lossy media.

The analogy between circuits and fields can be understood by considering the transmission line system shown in Fig. 3.2(a). After discretizing the line into infinitesimal sections of length Δx , Fig. 3.2(b) results. Assuming uniform per unit length param-

(a) A transmission line system

(b) An infinitesimal section of the transmission line

Figure 3.2: Transmission line system.

eters of resistance (R), inductance (L), conductance (G), and capacitance (C), each section includes a resistance $R\Delta x$, inductance $L\Delta x$, conductance $G\Delta x$, and capacitance $C\Delta x$. Using Kirchhoff's current and voltage laws for the infinitesimal section

described above and taking the limit $\Delta x \rightarrow 0$, the following equations are obtained:

$$\Delta x \frac{\partial}{\partial x} v(x, t) = -Ri(x, t) - L \frac{\partial}{\partial t} i(x, t) \quad (3.34a)$$

$$\Delta x \frac{\partial}{\partial x} i(x, t) = -Gv(x, t) - C \frac{\partial}{\partial t} v(x, t) \quad (3.34b)$$

By differentiating Eq. (3.34a) with respect to t , and (3.34b) with respect to x and combining them for the case when $R = 0$, we get

$$\frac{\partial^2}{\partial x^2} v(x, t) = \frac{LC}{\Delta x^2} \frac{\partial^2}{\partial t^2} v(x, t) + \frac{GL}{\Delta x^2} \frac{\partial}{\partial t} v(x, t). \quad (3.35)$$

In order to find the analogy with Maxwell's equations, consider now the following one-dimensional EM problem. For a wave propagating along $+x$, the only non-zero field components must be E_y and B_z . Under these conditions, Eqs. (3.1) and (3.2) simplify to

$$\frac{\partial E_y}{\partial x} = -\frac{\partial B_z}{\partial t} \quad (3.36)$$

$$-\frac{\partial H_z}{\partial x} = j_y + \frac{\partial D_y}{\partial t}, \quad (3.37)$$

multiplying Eq. (3.37) by μ and using $j_y = \sigma E_y$, gives

$$-\frac{\partial B_z}{\partial x} = \mu\sigma E_y + \mu\epsilon \frac{\partial E_y}{\partial t}. \quad (3.38)$$

Taking the derivative of this equation with respect to t , differentiating Eq. (3.36) with respect to x and eliminating B_z gives

$$\frac{\partial^2}{\partial x^2} E_y = \mu\epsilon \frac{\partial^2}{\partial t^2} E_y + \mu\sigma \frac{\partial}{\partial t} E_y. \quad (3.39)$$

The analogy between the circuit and field problems is based on the similarities between Eqs. (3.35) and (3.39). By comparing these equations, the following equivalences are obtained:

$$E_y \Leftrightarrow v(x, t), \quad \frac{C}{\Delta x} \Leftrightarrow \epsilon, \quad \frac{L}{\Delta x} \Leftrightarrow \mu, \quad \frac{G}{\Delta x} \Leftrightarrow \sigma$$

Similarly, B_z may be associated with the current on the line.

As shown in Ref. [61], a complete circuit representation of Maxwell's equations (Eqs. 3.1 and 3.2) in three-dimensions can also be derived. In this case, the complete mapping between circuit and field quantities requires twelve transmission (or link-) lines connected as shown in Fig. 3.3(a). The point where the transmission lines meet is referred to as a *node*.

In the TLM method, the entire propagation space is quantized into nodes as that shown in Fig. 3.3(a). The node shown in the figure is known as symmetrical condensed node (SCN) and shows the original voltage numbering scheme introduced by P.B. Johns [32]. At this point, it is convenient to introduce an alternative notation also used in this thesis to identify the link-lines and their respective voltage pulses in the node. This notation was originally introduced in Ref. [62] and is shown in Fig. 3.3(b). As can be seen from this figure, each link-line is assigned a three-character name: the first character indicates the direction parallel to the link-line, the second indicates whether the link-line is on the positive or negative side of the node, and the third character indicates the polarization of the voltage pulses travelling in the link-line. For example, the impedance of a link-line parallel to the z -axis, on the negative of the node, and with a voltage pulse polarized in the x -direction is indicated by Z_{-zx} .

Figure 3.3: Symmetrical condensed node. a) Original voltage pulse notation, b) Alternative notation also used in this thesis.

Correspondingly, the voltage pulse travelling in this link-line is identified as V_{znx} .

The SCN is the result of earlier expanded [63] and asymmetrical nodes [64]. In each node (c.f. Fig. 3.3), the voltage pulses and related currents provide information of the electric and magnetic tangential field components at the center of every face as well as total (average) field components at the center of each node.

From the processing point of view, each node can be viewed as a scattering zone. At a given time step, n , voltage pulses are *incident* $_n[V^i]$ upon the node from each of the link-lines. These voltage pulses are then scattered at the node producing a set of *reflected* or scattered pulses $_n[V^r]$. Thus, the incident and reflected voltage pulses are related by a scattering matrix $[S]$ unique to each node. The scattering matrix contains key information about the physical and EM properties of each node such as

its dimensions and permittivity and permeability tensors. In mathematical form, the incident and reflected pulses are then related by ${}_n[V^r] = [S]_n[V^i]$.

After the reflected pulses from a node have been determined, they are used in a connect procedure $[C]$ to determine the incident voltage pulses on adjacent nodes at the next time step $(n + 1)\Delta t$. In the simple case when the link-line impedances of adjacent nodes are equal, the connect procedure is accomplished by simply swapping reflected voltage pulses between adjacent nodes. However, whenever there are discontinuities between the link-line impedances or the connection is made between nodes of different sizes in a multi-grid mesh, a more elaborate connect procedure is required. In either case, the mathematical form of the connect procedure is given by ${}_{n+1}[V^i] = [C]_n[V^r]$.

After introducing the scattering and connect matrices, the TLM method can be viewed as an iterative process where voltage pulses are incident, scattered and connected at every iteration. For the first iteration, the incident voltage pulses are chosen such that they are consistent with the desired excitation. In this respect, a Gaussian pulse with the spectral content of interest, is the most common form of excitation. A detailed explanation of the TLM method is provided in the next sections.

3.3.1 General Constitutive Relations in TLM

In this section, the fundamental equations governing the TLM method are derived. The derivation results in a general system of equations that holds for any type of TLM node. Consider a node of space with arbitrary dimensions Δx , Δy and Δz . The material properties, $\bar{\epsilon}$, and $\bar{\mu}$, of the node modelling symmetric anisotropic media are

given by the following diagonal tensors

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_x & 0 & 0 \\ 0 & \epsilon_y & 0 \\ 0 & 0 & \epsilon_z \end{bmatrix} = \epsilon_0 \begin{bmatrix} \epsilon_{rx} & 0 & 0 \\ 0 & \epsilon_{ry} & 0 \\ 0 & 0 & \epsilon_{rz} \end{bmatrix} \quad (3.40)$$

$$\bar{\mu} = \begin{bmatrix} \mu_x & 0 & 0 \\ 0 & \mu_y & 0 \\ 0 & 0 & \mu_z \end{bmatrix} = \mu_0 \begin{bmatrix} \mu_{rx} & 0 & 0 \\ 0 & \mu_{ry} & 0 \\ 0 & 0 & \mu_{rz} \end{bmatrix} \quad (3.41)$$

The total capacitance C_t of this block of space is obtained from the general definition of capacitance

$$C_t = \frac{Q}{V} = \frac{\int_s \bar{\epsilon} \mathbf{E} \cdot d\mathbf{S}}{\int \mathbf{E} \cdot d\mathbf{l}} \quad (3.42)$$

giving, for each of the three principal directions, the following total capacitances [65]

$$C_t^x = \epsilon_x \frac{\Delta y \Delta z}{\Delta x} \quad (3.43)$$

$$C_t^y = \epsilon_y \frac{\Delta x \Delta z}{\Delta y} \quad (3.44)$$

$$C_t^z = \epsilon_z \frac{\Delta x \Delta y}{\Delta z} \quad (3.45)$$

Similarly, from the general definition of inductance, the total inductance L_t of the block of space can be calculated from

$$L_t = \frac{\Phi}{I} = \frac{\int_s \bar{\mu} \mathbf{H} \cdot d\mathbf{S}}{\oint \mathbf{H} \cdot d\mathbf{l}} \quad (3.46)$$

giving, for each of the three principal directions, the following total inductances [65]

$$L_t^x = \mu_x \frac{\Delta y \Delta z}{\Delta x} \quad (3.47)$$

$$L_t^y = \mu_y \frac{\Delta x \Delta z}{\Delta y} \quad (3.48)$$

$$L_t^z = \mu_z \frac{\Delta x \Delta y}{\Delta z} \quad (3.49)$$

Equations (3.43)-(3.45) and (3.47)-(3.49) represent the total capacitance and inductance of an arbitrary discretized block of space. These equations are the general starting point for the TLM method and are therefore referred to as the *general TLM constitutive relations*.

3.3.2 TLM Representation of Space Parameters

In TLM, the total capacitance (3.43-3.45) and inductance (3.47-3.49) of each discrete node has to be supplied by the capacitance and inductance of the link-lines (transmission lines) and stubs at each node. It should be mentioned at this point that stubs are nothing but a convenient way to add extra capacitance (open-circuit) or inductance (short-circuit) to the node. Of course, the extra capacitance and inductance is in addition to that already modelled by the transmission lines. Thus, it becomes obvious that modelling of the total capacitance and inductance can be accomplished by arbitrary combinations of link-lines and stubs, which results in different TLM node types.

Figure 3.4 shows how, in general, the total capacitance in the y -direction is modelled by a symmetrical condensed node. As the figure shows, the total capacitance of

Figure 3.4: Modelling capacitance in the y -direction in TLM

the node in the y -direction C_t^y is modelled by the distributed capacitance of two y -polarized link-lines C_{xy} , C_{zy} of length Δx and Δz and the capacitance of an open-circuit stub C_o^y . Note that these are the only transmission lines contributing to the y -directed electric field. Thus, the following equation must be satisfied

$$C_t^y = C_{xy}\Delta x + C_{zy}\Delta z + C_o^y. \quad (3.50)$$

Note that in this notation, the second subscript has been dropped because the position of the link-lines with respect to the node is not relevant for this analysis.

In a similar way, the total inductance in the z -direction of a block of space is modelled in TLM as shown in Fig. 3.5. As the figure shows, the total inductance of the node in the z -direction L_t^z is represented by the distributed inductance of two link-lines L_{xy} , L_{yx} of length Δx and Δy contributing to the z -component of the

Figure 3.5: Modelling inductance in the z -direction in TLM

magnetic field plus the inductance of a short-circuit stub L_s^z . As in the previous case, it should be noted that these are all the link-lines contributing to the z -component of the magnetic field. In this case, the following equation must be satisfied

$$L_t^z = L_{xy}\Delta x + L_{yx}\Delta y + L_s^z \quad (3.51)$$

Following a similar procedure for the other components of capacitance and inductance, the following equations are obtained

$$C_t^x = C_{zx}\Delta z + C_{yx}\Delta y + C_o^x \quad (3.52)$$

$$C_t^z = C_{yz}\Delta y + C_{xz}\Delta x + C_o^z \quad (3.53)$$

$$L_t^x = L_{yz}\Delta y + L_{zy}\Delta z + L_s^x \quad (3.54)$$

$$L_t^y = L_{zx}\Delta z + L_{xz}\Delta x + L_s^y \quad (3.55)$$

After substituting the total inductances and capacitances in each direction given by Eqs. (3.43)-(3.45) and (3.47)-(3.49) into these equations, the following six equations are obtained

$$C_{zx}\Delta z + C_{yx}\Delta y + C_o^x = \epsilon_x \frac{\Delta y \Delta z}{\Delta x} \quad (3.56)$$

$$C_{xy}\Delta x + C_{zy}\Delta z + C_o^y = \epsilon_y \frac{\Delta x \Delta z}{\Delta y} \quad (3.57)$$

$$C_{yz}\Delta y + C_{xz}\Delta x + C_o^z = \epsilon_z \frac{\Delta x \Delta y}{\Delta z} \quad (3.58)$$

$$L_{yz}\Delta y + L_{zy}\Delta z + L_s^x = \mu_x \frac{\Delta y \Delta z}{\Delta x} \quad (3.59)$$

$$L_{zx}\Delta z + L_{xz}\Delta x + L_s^y = \mu_y \frac{\Delta x \Delta z}{\Delta y} \quad (3.60)$$

$$L_{xy}\Delta x + L_{yx}\Delta y + L_s^z = \mu_z \frac{\Delta x \Delta y}{\Delta z} \quad (3.61)$$

These equations represent the basis for all forms of the TLM method. They contain eighteen unknowns to be determined: six distributed capacitances C_{ij} , six distributed inductances L_{ij} , three total capacitances of the open-circuit stubs C_o^i and three total inductances of the short-circuit stubs L_s^i . Because we only have six equations, there are twelve degrees of freedom in the way the parameters of link-lines and stubs can be determined. It should be noted that, in transmission line theory, the capacitance and inductance values are not used directly; instead they are translated into the more commonly used parameter of characteristic impedance (or admittance).

3.3.3 Time Synchronism in TLM

An important feature of the TLM method is time synchronism, which must be maintained in the mesh. That is, the voltage pulses must arrive at the center of the nodes, where they will be scattered, simultaneously. For this condition to be met, additional equations must be derived. For example, basic transmission line theory indicates that the velocity of propagation of an x -directed, y -polarized link-line with distributed capacitance C_{xy} and inductance L_{xy} , is given by:

$$v_{xy} = \frac{1}{\sqrt{C_{xy}L_{xy}}} \quad (3.62)$$

On the other hand, pulses must travel the node distance Δx in one time step Δt . Thus,

$$v_{xy} = \frac{\Delta x}{\Delta t} \quad (3.63)$$

combining Eqs. (3.62) and (3.63), the following condition must be satisfied for synchronicity to be maintained in the xy link-line

$$\Delta t = \Delta x \sqrt{C_{xy}L_{xy}} \quad (3.64)$$

Similarly, the following conditions apply to the other link-lines

$$\Delta t = \Delta x \sqrt{C_{xz}L_{xz}} \quad (3.65)$$

$$\Delta t = \Delta y \sqrt{C_{yz}L_{yz}} \quad (3.66)$$

$$\Delta t = \Delta y \sqrt{C_{yx}L_{yx}} \quad (3.67)$$

$$\Delta t = \Delta z \sqrt{C_{zx} L_{zx}} \quad (3.68)$$

$$\Delta t = \Delta z \sqrt{C_{zy} L_{zy}} \quad (3.69)$$

These equations, together with equations (3.56)-(3.61), form a system of twelve equations with eighteen unknowns and six degrees of freedom. From this formulation and by applying additional constraints, the different versions of TLM node types are derived in Sect. 3.4.

3.3.4 General TLM Equations

The system of equations (3.56)-(3.61), when combined with Eqs. (3.64)-(3.69), can be written in terms of the characteristic impedances and admittances of the link-lines and stubs, which results in a set of equations more amenable to transmission line theory.

For example, the characteristic admittances of a y -directed, x -polarized (Y_{yx}) and a z -directed, x -polarized (Y_{zx}) link-lines are defined, respectively, as

$$Y_{yx} = \frac{1}{Z_{yx}} = \sqrt{\frac{C_{yx}}{L_{yx}}} \quad (3.70)$$

$$Y_{zx} = \frac{1}{Z_{zx}} = \sqrt{\frac{C_{zx}}{L_{zx}}} \quad (3.71)$$

Combining these expressions with the time synchronism conditions (3.67) and (3.68), the characteristic admittances of the link-lines can be written as functions of the time step

$$Y_{yx} = \frac{C_{yx} \Delta y}{\Delta t} \quad (3.72)$$

$$Y_{zx} = \frac{C_{zx}\Delta z}{\Delta t} \quad (3.73)$$

The characteristic admittance of the open-circuit stubs contributing to the x -directed electric field is determined from the condition that pulses must make a round trip during the time step Δt . This requires that the effective transit time of a pulse along the length of the stub be equal to $\Delta t/2$. From basic transmission line theory, this results in the following conditions [61]

$$Y_{ox} = \frac{2C_o^x}{\Delta t}. \quad (3.74)$$

Substituting Eqs. (3.72), (3.73) and (3.74) into Eq. (3.56), the following equation is obtained

$$Y_{zx} + Y_{yx} + \frac{Y_o^x}{2} = \epsilon_x \frac{\Delta y \Delta z}{\Delta x \Delta t}. \quad (3.75)$$

Following similar procedures, Eqs. (3.57) and (3.58) can be written as

$$Y_{xy} + Y_{zy} + \frac{Y_o^y}{2} = \epsilon_y \frac{\Delta x \Delta z}{\Delta y \Delta t} \quad (3.76)$$

$$Y_{yz} + Y_{xz} + \frac{Y_o^z}{2} = \epsilon_z \frac{\Delta x \Delta y}{\Delta z \Delta t} \quad (3.77)$$

Similarly, equations (3.59)-(3.61) can also be rewritten in terms of characteristic impedances as follows. For example, the characteristic impedances of a y -directed, z -polarized (Z_{yz}) and a z -directed, y -polarized (Z_{zy}) link-line are defined, respectively, as

$$Z_{yz} = \frac{1}{Y_{yz}} = \sqrt{\frac{L_{yz}}{C_{yz}}} \quad (3.78)$$

$$Z_{zy} = \frac{1}{Y_{zy}} = \sqrt{\frac{L_{zy}}{C_{zy}}} \quad (3.79)$$

Combining these expressions with the time synchronism conditions (3.66) and (3.69), the characteristic impedances of the link-lines can be written as functions of the time step

$$Z_{yz} = \frac{L_{yz}\Delta y}{\Delta t} \quad (3.80)$$

$$Z_{zy} = \frac{L_{zy}\Delta z}{\Delta t} \quad (3.81)$$

As before, the characteristic impedance of the short-circuit stubs contributing to the x -directed magnetic field is determined from the condition that pulses must make a round trip during the time step Δt . This results in the following condition [61]

$$Z_{sx} = \frac{2L_s^x}{\Delta t} \quad (3.82)$$

Substituting Eqs. (3.80), (3.81) and (3.82) into Eq. (3.59), the following equation is obtained

$$Z_{yz} + Z_{zy} + \frac{Z_s^x}{2} = \mu_x \frac{\Delta y \Delta z}{\Delta x \Delta t}. \quad (3.83)$$

Following similar procedures, Eqs. (3.60) and (3.61) can be written as

$$Z_{zx} + Z_{xz} + \frac{Z_s^y}{2} = \mu_y \frac{\Delta x \Delta z}{\Delta y \Delta t} \quad (3.84)$$

$$Z_{xy} + Z_{yx} + \frac{Z_s^z}{2} = \mu_z \frac{\Delta x \Delta y}{\Delta z \Delta t} \quad (3.85)$$

The system of Eqs. (3.75)-(3.77) and (3.83)-(3.85) is a more compact representation of the basic TLM equations. In these equations, the time synchronization condition

has been merged and is now implicit. The fact that the equations have been written in terms of characteristic impedances and admittances as unknowns has an additional advantage. Specifically, these quantities can be used directly for describing scattering and propagation in a network of interconnected transmission lines.

3.3.5 Modelling Losses in TLM

In the TLM method, electric and magnetic losses are incorporated into the formulation by adding lossy stubs at those nodes where modelling of losses is required. Lossy stubs can be thought of as either being infinitely long, or terminated in a perfectly matched load. In either case, the stubs do not produce reflected pulses because the energy scattered into them, is removed from the system. Losses are calculated as follows. The complex permittivity ϵ^* of a material is described by

$$\epsilon^* = \epsilon_0 \epsilon_r - j \frac{\sigma_{ei}}{\omega} \quad (3.86)$$

where σ_{ei} is the conductivity associated with electric losses in the i^{th} -direction. From this equation, the loss tangent ($\tan \delta_e$) is obtained as the ratio between the imaginary and real parts of (3.86)

$$\tan \delta_e = \frac{\sigma_e}{\omega \epsilon_0 \epsilon_r} \quad (3.87)$$

From Eq. (3.87) and the fact that the loss tangent can also be defined as the ratio between the resistance and the reactance of a parallel equivalent circuit for the material, the following expression is obtained, for example, for the lossy stub in the y -direction

$$G_y = \sigma_{ey} \frac{\Delta x \Delta z}{\Delta y} \quad (3.88)$$

similar expressions apply for G_x and G_z . Thus, to account for electric losses in the y -direction, the lossy stub G_y would be connected at the center of the node and in parallel with the transmission lines representing C_t^y in Fig. 3.4.

In a similar way, we can account for magnetic losses associated with, say H_z , by adding a resistance in series with L_t^z . For a lossy magnetic medium, the complex magnetic permeability is given by

$$\mu^* = \mu_0\mu_r - j\frac{\sigma_{mi}}{\omega} \quad (3.89)$$

where σ_{mi} represents a “magnetic” conductivity in the i^{th} -direction. Proceeding as before, the magnetic loss tangent ($\tan \delta_m$) is given by the ratio between the imaginary and real parts of (3.89)

$$\tan \delta_m = \frac{\sigma_m}{\omega\mu_0\mu_r}. \quad (3.90)$$

From Eq. (3.90) and the fact that the loss tangent can, in this case, be defined as the ratio between the resistance and the reactance of a series equivalent circuit for the material, the following expression is obtained for the lossy stub in the z -direction

$$R_z = \sigma_{mz} \frac{\Delta x \Delta y}{\Delta z} \quad (3.91)$$

similar expression apply for R_x and R_y . Thus, to account for magnetic losses in the z -direction, the lossy stub R_z would be connected in series with the transmission lines representing L_t^z in Fig. 3.5.

3.4 Types of TLM Nodes

In section 3.3.4, the fundamental equations governing the TLM method were derived. As it was mentioned there, the system of Eqs. (3.75)-(3.77) and (3.83)-(3.85) is overdetermined because there are more unknowns than equations. Thus, in order to solve the system, other constraints need to be enforced. As it can be anticipated, there are various ways in which these extra constraints can be imposed. This is the origin of the different TLM node types presented in this section.

It must be noted that the mathematical constraints needed to solve Eqs. (3.75)-(3.77) and (3.83)-(3.85) can be related to a more physical interpretation. It has already been discussed that each discrete node in the computational volume has an associated capacitance and inductance. Based on the discussion in Sect. 3.3.2, the total capacitance and inductance at each node is, in general, modelled by twelve link-lines, three short-circuit stubs, and three open-circuit stubs. Thus, it can be anticipated that the different TLM node types will differ from each other in the way in which the total capacitance and inductance associated with each node are distributed among these link-lines and stubs.

3.4.1 Stub Loaded Symmetrical Condensed Node (SL-SCN)

The stub loaded node was the first TLM node type to appear in the literature [32]. For this node, the additional constraints are imposed by demanding that all link-lines have the same characteristic impedance (and therefore admittance). The characteristic impedance of the link-lines is chosen to be equal to the characteristic impedance of the background material, which is usually free-space. Thus, this impedance value is

given by $Z_0 = 1/Y_0 = \sqrt{\mu_o/\epsilon_0}$. This results in six extra equations of the form

$$Z_{xy} = Z_{yx} = Z_{zx} = Z_{xz} = Z_{yz} = Z_{zy} \equiv Z_0 \quad (3.92)$$

which are introduced into the system of Eqs. (3.75)-(3.77) and (3.83)-(3.85). With these equations, the original system of equations is reduced to

$$2Y_0 + \frac{Y_o^x}{2} = \epsilon_x \frac{\Delta y \Delta z}{\Delta x \Delta t} \quad (3.93)$$

$$2Y_0 + \frac{Y_o^y}{2} = \epsilon_y \frac{\Delta x \Delta z}{\Delta y \Delta t} \quad (3.94)$$

$$2Y_0 + \frac{Y_o^z}{2} = \epsilon_z \frac{\Delta x \Delta y}{\Delta z \Delta t} \quad (3.95)$$

$$2Z_0 + \frac{Z_s^x}{2} = \mu_x \frac{\Delta y \Delta z}{\Delta x \Delta t} \quad (3.96)$$

$$2Z_0 + \frac{Z_s^y}{2} = \mu_y \frac{\Delta x \Delta z}{\Delta y \Delta t} \quad (3.97)$$

$$2Z_0 + \frac{Z_s^z}{2} = \mu_z \frac{\Delta x \Delta y}{\Delta z \Delta t} \quad (3.98)$$

In these equations, the unknowns to be determined are Y_o^i and Z_s^i , where $i \in \{x, y, z\}$. By straightforward manipulation of Eq. (3.93), the admittance of the open-circuit stub contributing to the x -directed electric field is found to be

$$Y_o^x = 2Y_0 \left(\frac{\epsilon_{rx}}{c\Delta t} \frac{\Delta y \Delta z}{\Delta x} - 2 \right). \quad (3.99)$$

Similar equations are obtained for Y_o^y and Y_o^z . Similarly, by straightforward manipulation of Eq. (3.96), the impedance of the short-circuit stub contributing to the

x -directed magnetic field is found to be

$$Z_s^x = 2Z_0 \left(\frac{\mu_{rx}}{c\Delta t} \frac{\Delta y \Delta z}{\Delta x} - 2 \right) \quad (3.100)$$

similar equations are obtained for Z_s^y and Z_s^z . In Eqs. (3.99) and (3.100), $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light in free-space.

There is one more constraint that needs to be imposed. For unconditional stability, the stubs must represent real and positive component values. Since all terms, except the time step (Δt), in Eqs. (3.99) and (3.100) are fixed for a given node, the stability condition is guaranteed by choosing a time step that makes the stubs Y_o^i and Z_s^i , where $i \in \{x, y, z\}$, non-negative. This leads to the following condition for the time step

$$\Delta t \leq \min \left\{ \frac{\epsilon_{rx}\Delta y \Delta z}{2c\Delta x}, \frac{\epsilon_{ry}\Delta x \Delta z}{2c\Delta y}, \frac{\epsilon_{rz}\Delta x \Delta y}{2c\Delta z}, \frac{\mu_{rx}\Delta y \Delta z}{2c\Delta x}, \frac{\mu_{ry}\Delta x \Delta y}{2c\Delta y}, \frac{\mu_{rz}\Delta x \Delta z}{2c\Delta z} \right\} \quad (3.101)$$

From equation (3.101), two important observations can be made. Firstly, when the space to be modelled is composed of non-magnetic media ($\mu_{rx} = \mu_{ry} = \mu_{rz} = 1.0$) and is discretized using a uniform mesh ($\Delta x = \Delta y = \Delta z = \Delta L$), the maximum time step (Δt_{max}) reduces to the well-known relation in FDTD

$$\Delta t_{max} = \frac{\Delta L}{2c}. \quad (3.102)$$

The second observation is related to the time constraint found in meshes composed of non-cubic nodes, such as the ones widely used in this thesis. Consider a node of space whose x -dimension is stretched such that: $\Delta x > \Delta y = \Delta z = \Delta L$. In this case,

the maximum time step is given by

$$\Delta t_{max} = \frac{\Delta L}{2c} \cdot \frac{\Delta L}{\Delta x} \quad (3.103)$$

Thus, the time step is no longer determined by the smallest node dimension, but is further decreased by the ratio between the largest and smallest node dimensions. This has a very important implication for the meshes used in this thesis, where large block aspect ratios are prone to occur. As a consequence, if the resulting time step is too small, more time steps would be needed to find the resonances of the simulated system. This is one of the main drawbacks of the SL-SCN.

It should also be noted at this point that in a general mesh, the stability condition (3.101) must be tested for all nodes. After the possible time steps that guarantee stability for each node are found, the *smallest* one must be used as the maximum time step throughout the mesh. In other words, the maximum time step is determined by the ratio of the largest and smallest mesh dimensions.

In summary, in the SLN the characteristic impedance of all transmission lines is equal and chosen to represent the capacitance and inductance of the background material (usually free-space). If extra capacitance or inductance is required at the node, capacitive or inductive stubs are added at the center of the node.

3.4.2 Hybrid Symmetrical Condensed Node (HSCN)

The previous section showed that, for stability reasons, the SL-SCN constraints the maximum permissible time step over which the mesh can be operated. The implications of this constraint diminish the benefits resulting from using blocks with large

aspect ratios for discretizing a large computational volume because there is a corresponding increase in run time. As already mentioned, this constraint is particularly detrimental for the meshes used in this thesis, which are generally composed of blocks whose dimensions can easily vary by an order of magnitude.

These constraints can be overcome if the condition that all the link lines have the same characteristic impedance is relaxed. This is the main idea behind the HSCN. In the HSCN, the link-lines model all the required inductance at the node, and hence additional short-circuit stubs are not needed. This is achieved by letting the link-lines associated with different components of the magnetic field, take different values. As in the SL-SCN, any deficit in capacitance modelled by these link-lines, is accounted for by adding open-circuit (capacitive) stubs to the node. Thus, compared with the SL-SCN, the HSCN has three fewer stubs. This translates into reduced variable storage and better dispersion properties. Even more importantly, for a given mesh discretization, the HSCN can, in general, be operated at a higher time step than the SL-SCN.

The absence of the three short-circuit stubs introduces three equations into the system of the form

$$Z_s^x = Z_s^y = Z_s^z = 0 \quad (3.104)$$

In addition, the requirement that all lines contributing to the inductance associated with a particular component of the magnetic field have the same characteristic

impedance, imposes three more conditions of the form

$$Z_{zy} = Z_{yz} \equiv Z_x \quad (3.105)$$

$$Z_{zx} = Z_{xz} \equiv Z_y \quad (3.106)$$

$$Z_{xy} = Z_{yx} \equiv Z_z \quad (3.107)$$

The characteristic impedances in these equations are those associated with the H_x , H_y , and H_z components, respectively. For example, in Fig. 3.5 the link-lines associated with the H_z component are shown.

Substituting the appropriate condition from (3.104) and Eq. (3.105) into (3.83), the characteristic impedance of the link-lines associated with the H_x component is found to be

$$Z_x = \frac{1}{Y_x} = Z_0 \frac{\mu_{rx} \Delta y \Delta z}{2c \Delta t \Delta x} \quad (3.108)$$

following a similar procedure, the equations for Z_y and Z_z are obtained as

$$Z_y = \frac{1}{Y_y} = Z_0 \frac{\mu_{ry} \Delta x \Delta z}{2c \Delta t \Delta y} \quad (3.109)$$

$$Z_z = \frac{1}{Y_z} = Z_0 \frac{\mu_{rz} \Delta x \Delta y}{2c \Delta t \Delta z} \quad (3.110)$$

At this point, an expression for the characteristic admittance of the open-circuit stubs remains to be found. For this purpose, having in mind that from Eqs. (3.106) and (3.107) $Y_{zx} = 1/Z_y$ and $Y_{yx} = 1/Z_z$, it follows that

$$Y_o^x = Y_0 \left[\frac{2\epsilon_{rx}}{c \Delta t} \frac{\Delta y \Delta z}{\Delta x} - \frac{4c \Delta t}{\Delta x} \left(\frac{\Delta y}{\mu_{ry} \Delta z} + \frac{\Delta z}{\mu_{rz} \Delta y} \right) \right] \quad (3.111)$$

after inserting (3.109) and (3.110) into (3.75). Similar equations are found for Y_o^y and Y_o^z .

Finally, the derivation of the maximum allowed time step for the HSCN can be achieved by demanding that the open-circuit stubs represent passive components. As in the SL-SCN, this condition is met by choosing a time step that satisfies $\{Y_o^x, Y_o^y, Y_o^z\} > 0$. By straightforward manipulation of the equations for the stubs, it is found that stability is guaranteed if the maximum time step is chosen as

$$\Delta t_{max} = \frac{\Delta L_{min}}{2c} \quad (3.112)$$

where ΔL_{min} is the smallest node dimension present in the mesh.

From this analysis, it can be seen that the time step in the HSCN is, in general, higher than that in the SL-SCN. This is advantageous in that one is no longer limited by the ratio of the smallest to the biggest node dimension. This translates into the possibility of using larger blocks in the mesh without having to decrease the time step used for the simulations.

In summary, in the HSCN up to three different values of characteristic impedances can be used for the transmission lines. Each value represents the total inductance of the node in each direction. As a consequence, short-circuit stubs are not required. This reduces the demand for computation time and storage resources. When extra capacitance is required at the node, it is added in the form of open-circuit stubs at the center of the node as in the SLN.

3.4.3 The Symmetrical Super Condensed Node (SSCN)

There exists a third type of node called the symmetrical super condensed node (SSCN) [66]. This type of node is not used intensively for the work in this thesis and is only briefly mentioned here. In this node, the characteristic impedances of the transmission lines are chosen to represent the total capacitance and inductance of the node such that stubs are not required. The absence of the three short-circuit stubs introduces three equations into the original system of equations of the form

$$Z_s^x = Z_s^y = Z_s^z = 0. \quad (3.113)$$

The absence of the three open-circuit stubs introduces equations of the form

$$Z_o^x = Z_o^y = Z_o^z = 0. \quad (3.114)$$

In the absence of stubs, six possible different values of characteristic impedances for the transmission lines are needed to accomodate the total inductance and capacitance of the node.

To conclude this section, it must be noted that there are various factors that influence the choice of node type to be used in simulations. Each node exhibits different dispersion properties [67], allows for a different time step [66], and has different memory requirements for variable storage. For the simulations presented in this work, all nodes have been explored; however, the HSCN has primarily been used because it has been found to provide good accuracy and offers a good compromise between the trade-offs just mentioned. However, it must be kept in mind that the fact that the

SSCN does not require any stubs at nodes, can be exploited for obtaining further memory optimization.

3.5 Scattering in TLM

The scattering procedure is the “heart” of the TLM method. Voltage pulses traveling in the link-lines are incident at the center of the node at every time step. Upon incidence, the voltage pulses are scattered (or reflected) back into the link-lines by the node. In simple words, scattering is the process whereby a set of reflected voltage pulses (from a node) is determined from a set of incident voltage pulses. Although in principle this scattering procedure is rather simple, in practice, there are a few issues that need to be carefully considered. For example, in the original derivation of the TLM method, the scattering procedure was described by a scattering matrix which was obtained from Maxwell’s equations and by resorting to the principles of charge and energy conservation [32]. This approach was required because an equivalent circuit for the node was not available.

Over the years, there have been attempts to obtain an equivalent circuit for the SCN node, but given the complexity of the task, a general equivalent circuit has not been obtained [68]. In this regard, the center of a TLM node is undefined and the node itself can be regarded more as a mathematical object than as a “node” where transmission lines interconnect. It should be said, however, that the scattering process is well understood and that it has been derived in various ways by using first principles [69]. In this section, we briefly outline the principles behind the derivation of the scattering properties of the TLM method. Contrary to the results in Ref. [32]

Figure 3.6: Equivalent total a) voltage b) current

where the scattering process is described by a matrix, the approach taken here results in a set of equations which is more computationally efficient because a matrix inversion is not required. Nevertheless, the matrix formulation of scattering will be used in Chapter 6 to study the dispersion properties of TLM meshes.

3.5.1 Scattering Into Link-lines

The total voltage on an individual transmission line at a scattering point, such as the center of a node, is equal to the sum of the incident and reflected voltage pulses on this line. This situation is illustrated schematically in Fig. 3.6(a) for an x -directed, y -polarized link-line. In the figure, an equivalent total voltage in the center of the node V_y has been introduced as the average value of V_{xny} and V_{xpy} . The averaging can be done by imposing charge balance on the respective lines and by demanding that the charge flow across the line be continuous. After some algebraic manipulations, it follows that

$$V_y = \frac{Y_{xny} V_{xny} + Y_{xpy} V_{xpy}}{Y_{xny} + Y_{xpy}} \quad (3.115)$$

Similarly, the total current on an individual transmission line at a scattering point,

such as the center of a node, can be defined as the difference between the incident and reflected currents on a link-line. Similarly as for the equivalent total voltage, an equivalent total current, I_z , can be introduced as the average of I_{xny} and I_{xpy} , as shown in Fig. 3.6(b). In this case, the averaging is done by imposing magnetic flux balance on the lines and by demanding that the magnetic flux across the line be continuous. After some algebra, the following expression results

$$I_z = \frac{Z_{xpy}I_{xpy} - Z_{xny}I_{xny}}{Z_{xny} + Z_{xpy}}. \quad (3.116)$$

Given that transmission line current and voltage are related by $I = Y_0(V^i - V^r)$, Eqs. (3.115) and (3.116) can be written as

$$V_y = \frac{Z_{xpy}}{Z_{xny} + Z_{xpy}}(V_{xny}^i + V_{xny}^r) + \frac{Z_{xny}}{Z_{xny} + Z_{xpy}}(V_{xpy}^i + V_{xpy}^r) \quad (3.117)$$

$$I_z = \frac{1}{Z_{xny} + Z_{xpy}}(V_{xpy}^i - V_{xpy}^r) - \frac{1}{Z_{xny} + Z_{xpy}}(V_{xny}^i - V_{xny}^r). \quad (3.118)$$

Multiplying equation (3.118) by Z_{xny} , adding it to equation (3.117), and solving for V_{xny}^r gives

$$V_{xny}^r = V_y + I_z Z_{xny} - V_{xpy}^i + O_{xy}. \quad (3.119)$$

Similarly, by multiplying equation (3.118) by Z_{xpy} , subtracting it from equation (3.117) and solving for V_{xpy}^r gives

$$V_{xpy}^r = V_y - I_z Z_{xpy} - V_{xny}^i + O_{xy} \quad (3.120)$$

in these equations, O_{xy} is defined as

$$O_{xy} = \frac{Z_{xny} - Z_{xpy}}{Z_{xny} + Z_{xpy}}(V_{xny}^i - V_{xpy}^i). \quad (3.121)$$

Note that for a *symmetrical* node, $Z_{xny} \equiv Z_{xpy} \equiv Z_{xy}$ and it follows that $O_{xy} = 0$. Following identical procedures for the remaining five transmission lines, the following equations for the reflected voltage pulses are obtained

$$\begin{aligned} V_{xny}^r &= V_y + I_z Z_{xny} - V_{xpy}^i \\ V_{xpy}^r &= V_y - I_z Z_{xpy} - V_{xny}^i \\ V_{ynz}^r &= V_z + I_x Z_{ynz} - V_{ypz}^i \\ V_{ypz}^r &= V_z - I_x Z_{ypz} - V_{ynz}^i \\ V_{znx}^r &= V_x + I_y Z_{znx} - V_{zpx}^i \\ V_{zpx}^r &= V_x - I_y Z_{zpx} - V_{znx}^i \\ V_{zny}^r &= V_y - I_x Z_{zny} - V_{zpy}^i \\ V_{zpy}^r &= V_y + I_x Z_{zpy} - V_{zny}^i \\ V_{xnz}^r &= V_z - I_y Z_{xnz} - V_{xpz}^i \\ V_{xpz}^r &= V_z + I_y Z_{xpz} - V_{xnz}^i \\ V_{ynx}^r &= V_x - I_z Z_{ynx} - V_{ypx}^i \\ V_{ypx}^r &= V_x + I_z Z_{ypx} - V_{ynx}^i \end{aligned} \quad (3.122)$$

These are general equations that describe the scattering process of any type of TLM node; however, equations such as (3.115) and (3.116) cannot be used to calculate

the equivalent nodal voltages V_i and currents I_i , for $i \in \{x, y, z\}$ because they are written in terms of total voltages (incident+reflected). To completely formulate the scattering equations, the equivalent voltages and currents must first be expressed in terms of *incident* voltages only, because these are the quantities which are known. Before this is done, equations describing scattering into the stubs need to be derived.

3.5.2 Scattering Into Stubs

As mentioned in Sec. 3.3.2, each stub that is introduced to the node couples directly with one particular component of the electric or magnetic field. Therefore, the total voltage on open-circuit ($V_{oi}, i \in \{x, y, z\}$) and electric-loss ($V_{ei}, i \in \{x, y, z\}$) stubs is, by definition, identical to the equivalent total voltage in the center of the node. Taking the stub that couples with the E_x component as a reference, $V_{ox} = V_{ex} = V_x$ and it follows that

$$V_{ox}^r = V_x - V_{ox}^i \quad (3.123)$$

$$V_{ex}^r = V_x \quad (3.124)$$

Note that, as explained in Sect. 3.3.5, there is no incident voltage pulse from the matched electric stub. Similar equations apply to the y - and z -coupled stubs.

In a similar way, the total current flowing through a short-circuit and magnetic-loss stub is, by definition, identical to the equivalent total current in the node. However, in order to maintain consistency with the original matrix derived in Ref. [32], the orientation of the incident voltages on the short-circuit and magnetic loss stubs is chosen in the opposite direction to that of the total current flow. Thus, taking as a reference the stubs that couple with the H_z component, the following equations are

Figure 3.7: Transmission-lines coupling with the E_y field component

obtained

$$V_{sz}^r = V_{sz}^i + I_z Z_{sz} \quad (3.125)$$

$$V_{mz}^r = I_z R_{mz} \quad (3.126)$$

where $(V_{si}, i \in \{x, y, z\})$ and $(V_{mi}, i \in \{x, y, z\})$ represent voltage pulses in the short-circuit and magnetic-loss stubs respectively. Similar equations apply to the x - and y -coupled stubs.

3.5.3 Equivalent Total Node Voltage

The derivation of the equivalent nodal voltage in terms of incident voltage pulses will be done for the y -component. Referring to Fig. 3.4, the link-lines that are coupled with V_y can be isolated as shown in Fig. 3.7. Two observations can readily be made

from the schematic: the center of the node is undetermined and the electric-loss stub, which had not been included in Fig. 3.4, is now present.

The nodal voltage V_y can be found by resorting to balance and conservation of charge. When the principle of charge conservation is invoked to all link-lines contributing to E_y , the following equation results

$$\Delta Q_y = \sum_n \Delta Q_y^n = \sum_n I_y^n = 0 \quad (3.127)$$

where the expression, $\Delta Q^n = I^n \Delta t$, has been used. In Eq. (3.127), ΔQ_y^n is the charge contributed to the node by the current circulating in the n^{th} y -polarized transmission-line. Using the general expression, $I = Y(V^i - V^r)$, the previous equation can be written as

$$Y_{xny}(V_{xny}^i - V_{xny}^r) + Y_{xpy}(V_{xpy}^i - V_{xpy}^r) + Y_{zny}(V_{zny}^i - V_{zny}^r) + \\ Y_{zpy}(V_{zpy}^i - V_{zpy}^r) + Y_{oy}(V_{oy}^i - V_{oy}^r) - G_{ey}V_{ey}^r = 0. \quad (3.128)$$

In addition, using Eq. (3.115), the following expressions can be written, respectively, for the x -directed y -polarized and z -directed y -polarized link-lines as

$$V_y = \frac{Y_{xny}(V_{xny}^i + V_{xny}^r) + Y_{xpy}(V_{xpy}^i + V_{xpy}^r)}{Y_{xny} + Y_{xpy}} \quad (3.129)$$

$$V_y = \frac{Y_{zny}(V_{zny}^i + V_{zny}^r) + Y_{zpy}(V_{zpy}^i + V_{zpy}^r)}{Y_{zny} + Y_{zpy}} \quad (3.130)$$

Inserting Eqs. (3.129) and (3.130) into (3.128) and using Eqs. (3.123) and (3.124),

the equivalent nodal voltage in the y -direction is found in terms of incident voltages

$$V_y = 2 \frac{Y_{xny} V_{xny}^i + Y_{xpy} V_{xpy}^i + Y_{zny} V_{zny}^i + Y_{zpy} V_{zpy}^i + Y_{oy} V_{oy}^i}{Y_{xny} + Y_{xpy} + Y_{zny} + Y_{zpy} + Y_{oy} + G_{ey}} \quad (3.131)$$

Following identical procedures, similar equations can be obtained for the V_x and V_z components. Note that the nodal voltage V_y may also be calculated from the Thevenin equivalent circuit resulting from Fig. 3.7, when the undetermined node is replaced by a “real” node that connects the link-lines in parallel. However, the Thevenin equivalent circuit is misleading as it is not consistent with the pulses scattered into the link-lines [61].

3.5.4 Equivalent Total Node Current

The derivation of the equivalent nodal current will be done for the z -component. Using as a reference Fig. 3.5, the link-lines that are coupled with I_z can be isolated as shown in Fig. 3.8. In this case, the nodal current I_z is found by resorting to balance and conservation of magnetic flux. When the principle of magnetic flux conservation is applied to the n link-lines crossing a closed surface as shown in Fig. 3.8, the following equation results

$$\Delta\Phi_z = \sum_n \Delta\Phi_y^n = \sum_n V_z^n = 0, \quad (3.132)$$

where the expression, $\Delta\Phi^n = V^n \Delta t$, has been used. In Eq. 3.132, $\Delta\Phi_y^n$ is the flux contributed to the node by the voltage in the n^{th} transmission-line contributing to the magnetic field in the z -direction. Using the general expression, $V = (V^i + V^r)$,

Figure 3.8: Transmission-lines coupling with the H_z field component

the previous equation can be written as

$$(V_{xpy}^i + V_{xpy}^r) - (V_{xny}^i + V_{xny}^r) + (V_{ynx}^i + V_{ynx}^r) - (V_{ypx}^i + V_{ypx}^r) - (V_{sz}^i + V_{sz}^r) - V_{mz}^r = 0 \quad (3.133)$$

Using Eq. (3.116), the following expressions can be written, respectively, for the x -directed y -polarized and y -directed x -polarized link-lines

$$I_z = \frac{(V_{xpy}^i - V_{xpy}^r) - (V_{xny}^i - V_{xny}^r)}{Z_{xny} + Z_{xpy}} \quad (3.134)$$

$$I_z = \frac{(V_{ynx}^i - V_{ynx}^r) - (V_{ypx}^i - V_{ypx}^r)}{Z_{ynx} + Z_{ypx}}. \quad (3.135)$$

Inserting Eqs. (3.134) and (3.135) into (3.133) and using Eqs. (3.125) and (3.126), the equivalent nodal current in the z -direction is found in terms of incident voltages

$$I_z = 2 \frac{V_{xpy}^i - V_{xny}^i + V_{ynx}^i - V_{ypx}^i - V_{sz}^i}{Z_{xny} + Z_{xpy} + Z_{ynx} + Z_{ypx} + Z_{sz} + R_{mz}} \quad (3.136)$$

Following identical procedures, similar equations can be obtained for the I_x and I_y components. Note that the nodal current I_z may also be calculated from the Thevenin equivalent circuit resulting from Fig. 3.8 when the undetermined node is replaced by a “real” node that connects the link-lines in series. However, this circuit is not consistent with the pulses scattered into the link-lines as previously indicated.

This concludes the description of the scattering process in TLM. After a scattering event, the resulting set of reflected voltage pulses needs further processing. The reflected pulses from the node travel along the link-lines and become incident again, at the next time step, on the neighboring nodes. The process whereby a new set of incident voltage pulses is determined, based on the reflected voltage pulses at the previous time step, is called *connection*.

3.6 Connection in TLM

The connection process in TLM is illustrated schematically in Fig. 3.9. In the figure, V_{xpy}^r and V_{xny}^r represent, respectively, the reflected voltage pulses from the nodes located at (x_0, y_0, z_0) and $(x_0 + \Delta x, y_0, z_0)$, at an arbitrary time step $(n\Delta t)$. Similarly, V_{xpy}^i and V_{xny}^i represent, respectively, the incident voltage pulses at the nodes located at (x_0, y_0, z_0) and $(x_0 + \Delta x, y_0, z_0)$, at the next time step $(n\Delta t + \Delta t)$. The task of the connection process is to find the latter voltage pulses based on the former ones.

Figure 3.9: Impedance discontinuity at the connection between link-lines pertaining to two adjacent nodes.

Equating the total incident and reflected charge from the impedance discontinuity one gets

$$C_{xpy}V_{xpy}^i + C_{xny}V_{xny}^i = C_{xpy}V_{xpy}^r + C_{xny}V_{xny}^r \quad (3.137)$$

where C_{xpy} and C_{xny} are the capacitances associated with the link-lines. The capacitance of a transmission-line with characteristic impedance Z_{ch} , is given by $C = \Delta t/Z_{ch}$.

Thus, using expressions of this form, Eq. (3.137) becomes

$$\frac{V_{xpy}^i}{Z_{xpy}} + \frac{V_{xny}^i}{Z_{xny}} = \frac{V_{xpy}^r}{Z_{xpy}} + \frac{V_{xny}^r}{Z_{xny}} \quad (3.138)$$

Similarly, the conservation of flux at the impedance discontinuity leads to the following equation

$$L_{xpy} \left(\frac{V_{xpy}^r}{Z_{xpy}} \right) - L_{xny} \left(\frac{V_{xny}^r}{Z_{xny}} \right) = L_{xpy} \left(-\frac{V_{xpy}^i}{Z_{xpy}} \right) - L_{xny} \left(-\frac{V_{xny}^i}{Z_{xny}} \right). \quad (3.139)$$

The negative signs inside the parenthesis on the right hand side arise because the currents due to incident pulses are defined as being negative. Using the expression that relates the characteristic impedance of a transmission line to its inductance ($Z_{ch} = L/\Delta t$), the previous equation reduces to

$$V_{xpy}^r - V_{xny}^r = -V_{xpy}^i + V_{xny}^i \quad (3.140)$$

Solving equations (3.138) and (3.140), the new incident pulses are found in terms of the reflected ones as

$$V_{xpy}^i = \Gamma_{aa} V_{xpy}^r + T_{ab} V_{xny}^r \quad (3.141)$$

$$V_{xny}^i = \Gamma_{bb} V_{xny}^r + T_{ba} V_{xpy}^r \quad (3.142)$$

where

$$\begin{aligned} \Gamma_{aa} &= \frac{Z_{xny} - Z_{xpy}}{Z_{xny} + Z_{xpy}} \\ \Gamma_{bb} &= \frac{Z_{xpy} - Z_{xny}}{Z_{xny} + Z_{xpy}} \\ T_{ab} &= \frac{2Z_{xpy}}{Z_{xny} + Z_{xpy}} \\ T_{ba} &= \frac{2Z_{xny}}{Z_{xny} + Z_{xpy}} \end{aligned} \quad (3.143)$$

note that in the SL-SCN, the characteristic impedance of all transmission-lines is equal such that $\Gamma_{aa} = 0 = \Gamma_{bb}$, $T_{ab} = T_{ba} = 1$ and the connection process is reduced to a simple swapping of the voltage pulses between adjacent nodes. That is, for the present example,

$${}_{n\Delta t+\Delta t}V_{xpy}^i(x_0, y_0, z_0) = {}_{n\Delta t}V_{xny}^r(x_0 + \Delta x, y_0, z_0) \quad (3.144)$$

$${}_{n\Delta t+\Delta t}V_{xny}^i(x_0 + \Delta x, y_0, z_0) = {}_{n\Delta t}V_{xpy}^r(x_0, y_0, z_0). \quad (3.145)$$

Since graded meshes are discretized using the HSCN, the transmission-lines between adjacent nodes may have different characteristic impedances, in which case the equations in (3.143) must be used. Due to the cumbersome notation that results when the time step is implicitly shown, the indices indicating time ($n\Delta t$) will be dropped in subsequent equations. However, it should be kept in mind that whenever incident voltage pulses are computed from reflected ones, there is a one time step difference between the two sets of pulses.

3.6.1 Connection in a Multi-grid Mesh

The connection process in multi-grid meshes, such as the ones used in this thesis, is considerably more involved. For the connection of the fine and coarse meshes, we follow a similar procedure as that presented in Ref. [50], where the nodes are connected by means of matching transformers. The details of the connection between blocks are shown in Fig. 3.10. For this type of connection, the equations relating the reflected to the incident voltage pulses for a block whose position, with respect to

Figure 3.10: Broken open view of a 4:1 block transition at an interface commonly found in quad-tree meshes.

Fig. 3.10, is denoted by the two subscripts, are given by

$$\begin{aligned}
 V_{00}^i &= V_{00}^r + (V - V_0)Y_0f_{00}Z_{00} \\
 V_{11}^i &= V_{11}^r + (V - V_1)Y_1f_{11}Z_{11} \\
 V_{12}^i &= V_{12}^r + (V - V_2)Y_2f_{12}Z_{12} \\
 V_{21}^i &= V_{21}^r + (V - V_1)Y_1f_{21}Z_{21} \\
 V_{22}^i &= V_{22}^r + (V - V_2)Y_2f_{22}Z_{22}
 \end{aligned} \tag{3.146}$$

where V_{ij}^i and V_{ij}^r are incident and reflected pulses, and

$$V_0 = 2[f_{00}V_{00}^r]$$

$$V_1 = 2[f_{11}V_{11}^r + f_{21}V_{21}^r]$$

$$V_2 = 2[f_{12}V_{12}^r + f_{22}V_{22}^r]$$

and

$$Y_0 = \frac{1}{f_{00}^2 Z_{00}}$$

$$Y_1 = \frac{1}{f_{11}^2 Z_{11} + f_{21}^2 Z_{21}}$$

$$Y_2 = \frac{1}{f_{12}^2 Z_{12} + f_{22}^2 Z_{22}}$$

and

$$V = \frac{Y_0 V_0 + Y_1 V_1 + Y_2 V_2}{Y_0 + Y_1 + Y_2}$$

and finally,

$$f_{ij} = \frac{\Delta x_{ij}}{\Delta y_{ij}}.$$

Note that these equations connect the transmission-lines in only one direction and one polarization. However, by careful rotation of Fig. 3.10, similar equations for the other directions and polarizations can be obtained.

3.7 Other Features in TLM

To complete the description of the TLM algorithm, there are a number of issues that remain to be addressed.

3.7.1 Excitation in TLM

In TLM, as well as in other numerical techniques, the simulation process begins by applying a field excitation to the mesh. Given that TLM is a time-domain technique, the most common form of excitation is a Gaussian field with the spectral content of interest. This excitation can be applied at a node or directly on the link-lines. In addition, it can be applied as “incident” or “reflected” voltage pulses. The basic idea behind the excitation process, is to find appropriate initial voltage pulses which are consistent with the field quantities used as the excitation. The details are briefly explained below.

When an electric field is applied at a node, the set of incident voltage pulses that must be applied to the link-lines which are coupled with that particular field, is given by

$$V^i = -\Delta l \left[\frac{4 + \hat{Y}_o + \hat{G}_e}{8} \right] E$$

for the SL-SCN, and

$$V^i = -\Delta l \left[\frac{2(\hat{Y}_1 + \hat{Y}_2) + \hat{Y}_o + \hat{G}_e}{4(\hat{Y}_1 + \hat{Y}_2)} \right] E$$

for the HSCN. In these equations, Δl represents the size of the block in the direction

of the applied field, and $\hat{Y}_o$ and $\hat{G}_e$ represent the admittances of the open and electric-loss stubs, respectively. In addition, $\hat{Y}_1$ and $\hat{Y}_2$ are the admittances of the two pairs of link-lines associated with the electric field. In these equations, the $\hat{\cdot}$ indicates that these quantities have been normalized with respect to the background admittance (Y_0).

Similarly, when a magnetic field is applied at a node, the set of incident voltage pulses that must be applied to the link-lines which are coupled with that particular field, is given by

$$V^i = \Delta l Z_0 \left[\frac{4 + \hat{Z}_s + \hat{R}_m}{8} \right] H$$

for the SL-SCN, and

$$V^i = \Delta l Z_0 \left[\frac{4 + \hat{Y} \hat{R}_m}{8 \hat{Y}} \right] H$$

for the HSCN. In these equations, $\hat{Z}_s$ and $\hat{R}_m$ are the impedances of the open and magnetic-loss stubs, respectively. Contrary to the previous case, these quantities are normalized with respect to the background impedance (Z_0). Finally, $\hat{Y}$ is the normalized admittance of the link-lines associated with the component of the magnetic field being excited.

3.7.2 Output in TLM

After an excitation is applied and carried forward in time by repeatedly applying the scattering and connect procedures, a field distribution develops on the mesh. This

field distribution, or the time signature of a field at a particular point in the mesh, is generally the purpose of the simulation. In TLM, the fields can be computed at every node and time step from the set of incident or scattered pulses. Thus, the output procedure can be viewed as the process of converting voltage pulses, at a node or link-line, into field quantities ($\mathbf{E}$ or $\mathbf{H}$).

The electric field is proportional to the (average) voltage across the node. Thus, the expressions derived in Sec. 3.5.3 can be directly applied. For example, the y -component of the electric field at a node is given by

$$E_y = -\frac{V_y}{\Delta y}, \quad (3.147)$$

where V_y is given by Eq. (3.131). Similarly, the magnetic field is proportional to the equivalent nodal current. For example, the z -component of the magnetic field is given by

$$H_z = \frac{I_z}{\Delta z}, \quad (3.148)$$

where I_z is given by Eq. (3.136).

3.8 Boundary Conditions in TLM

The term “Boundary condition” is very common in computational techniques. In a simple sense, boundary conditions refer to those regions in the mesh (a volume or surface), where the fields must satisfy a particular condition at all times. In TLM, boundary conditions can be internal or external, can be applied at nodes or link-lines, and are generally implemented as part of the connect procedure.

3.8.1 Internal Boundary Conditions in TLM

The most common form of an internal boundary condition occurs when modelling an infinitely thin, perfectly conductive metal sheet. In this case, the tangential electric fields on the metal sheet must be set to zero. This condition can be easily enforced by placing the metal sheet at the mid-point between link lines and by calculating the new incident voltage pulses (reflected from the metal sheet) as the negative of the reflected pulses (from the node). In this sense, a perfect metal behaves as a perfect reflecting surface. This is equivalent to terminating the link-line with a short-circuit.

3.8.2 External Boundary Conditions in TLM

External boundary conditions are commonly used in TLM for two purposes: to imply symmetry in a structurally symmetric problem, and to emulate a perfectly matched medium impedance such that no reflections from the boundaries of the problem space are created.

In numerical modeling, exploiting the symmetry of the structure can considerably reduce the simulation time. An example of symmetry is illustrated in Fig. 3.11. From this figure, it is obvious that the pairs of nodes connected along the symmetry plane will exchange voltage pulses during the connect procedure in the form $V^i(a) = V^r(b)$ and $V^i(b) = V^r(a)$. From symmetry, the reflected voltage pulses will be identical such that one can write $V^i(a) = V^r(a)$ and $V^i(b) = V^r(b)$. It is therefore sufficient to simulate only one half of the structure; the presence of the other half is implied by terminating the link-lines along the symmetry plane with an open-circuit boundary condition. That is, the voltage pulses traveling toward the plane of symmetry, are reflected and become incident in those nodes at the next time step without any

Figure 3.11: Implying symmetry in TLM

modifications.

External boundaries of arbitrary reflection

External boundaries of arbitrary reflection coefficient ρ_w are modelled in TLM by terminating the link-lines on the edge of the computation domain with an appropriate load. For normally incident fields, the reflection coefficient between a block of space of characteristic impedance Z_{int} and a medium of “resistance” R is given by

$$\rho_w = \frac{R - Z_{int}}{R + Z_{int}}. \quad (3.149)$$

From this equation, the resistance needed to terminate this block in order to give reflection coefficient ρ_w is found to be

$$R = Z_{int} \frac{1 + \rho_w}{1 - \rho_w}. \quad (3.150)$$

Similarly, the reflection coefficient of a link-line ρ_l of characteristic impedance Z_l terminated with this same resistance is given by

$$\rho_l = \frac{R - Z_l}{R + Z_l} \quad (3.151)$$

Comparing Eqs. (3.149) and (3.151), it is obvious that if the characteristic impedance of the link-line is different from the intrinsic impedance of the medium, the equivalent link-line reflection coefficient ρ_l , will differ from ρ_w . Substituting (3.150) into (3.151), the reflection coefficient of the link-line required to model a medium-to-medium reflection coefficient of ρ_w , is

$$\rho_l = \frac{Z_{int}(1 + \rho_w) - Z_l(1 + \rho_w)}{Z_{int}(1 + \rho_w) + Z_l(1 + \rho_w)} \quad (3.152)$$

For example, if the external boundary represents an electric wall, $\rho_w = -1$ and it follows from Eq. (3.152) that $\rho_l = -1$. Similarly, for a magnetic wall, $\rho_w = 1$ and $\rho_l = 1$. Therefore, for magnetic or electric walls $\rho_l = \rho_w$. For other values of ρ_w , ρ_l depends on Z_{int} and Z_l . For example, consider a matched boundary, $\rho_w = 0$ used to match the mesh to free space. To find ρ_l , consider an electromagnetic wave propagating in the x -direction with tangential field components E_y and H_z . Note that in TLM notation, these fields are represented by a y -polarized voltage pulse as shown in Fig. 3.12. The total capacitance and inductance of the block seen by such a wave are given by (3.44) and (3.49)

$$C_i^y = \epsilon_y \frac{\Delta x \Delta z}{\Delta y}, \quad L_i^z = \mu_z \frac{\Delta x \Delta y}{\Delta z}.$$

Figure 3.12: External boundaries in TLM

The intrinsic impedance of the medium seen by the fields is defined by

$$Z_{int} = \sqrt{\frac{L_t^z}{C_t^y}} = Z_0 \frac{\Delta y}{\Delta z} \sqrt{\frac{\mu_{rz}}{\epsilon_{ry}}}.$$

For the SL-SCN, $Z_l = Z_0$ and from (3.152),

$$\rho_l = \frac{\sqrt{\mu_{rz}} - \sqrt{\epsilon_{ry}}}{\sqrt{\mu_{rz}} + \sqrt{\epsilon_{ry}}} \quad (3.153)$$

Similarly, for the HSCN, Z_l is given by (3.110)

$$Z_l = Z_0 \frac{\mu_{rz} \Delta x \Delta y}{2c \Delta t \Delta z}, \quad (3.154)$$

and it follows that

$$\rho_l = \frac{2c \Delta t - \Delta x \sqrt{\mu_{rz} \epsilon_{ry}}}{2c \Delta t + \Delta x \sqrt{\mu_{rz} \epsilon_{ry}}}. \quad (3.155)$$

Similar expressions can be found for the other directions and polarizations.

In order to implement a matched boundary ($\rho_w = 0$), ρ_l is, in general, not equal

to zero. It should be mentioned that, although matched boundaries can be used to represent radiation boundaries, they are a first approximation since they only work perfectly for a wave which is normally incident on the boundary.

3.9 A TLM algorithm

To conclude this chapter, pseudo-code for the TLM algorithm is given below.

```

function TLM_Algorithm()
    Initialize_Variables();
    Define_Mesh();
    Set_Node_EM_Parameters();    // define node  $\epsilon_r$ ,  $\mu_r$ , etc.
    Define_Delta_t();            // based on smallest nodal dimension
    Calculate_Node_Impedances(); // impedances (or Admittances) of link-lines
    Define_Store_Nodes();        // where field signatures are to be stored
    Apply_Field_Excitation();    // in the form of incident voltage pulses
    for t = 1 to Num_time_steps
        for N=1 to All_Nodes
            Calculate_Nodal_Voltage_And_Current();
                                                    //from incident pulses
        end for
        for N=1 to All_Nodes
            Calculate_Scattered_Pulses;
        end for
        for N=1 to All_Nodes
            if (N==Output_Node) Store_Field();
        end for
        for N=1 to All_Nodes
            Conversion_And_Connection();
                                                    // new incident pulses from scattered ones
        end for
    end for
    Post_Process_Time_Data();
end function

```

Chapter 4

Time-domain Simulation of PC

4.1 Introduction

In this Chapter, a formulation that allows to compute the dispersion relation of PC by means of the TLM method is presented. To the best of the author's knowledge, a formulation of this type for the TLM method, has not been previously addressed in literature. Nevertheless, the formulation presented in this Chapter can be regarded as an extension (or the counterpart) of the FDTD formulation presented in Ref. [70] for the analysis of microwave periodic structures.

In Sects. 4.4 and 4.4.1 of this Chapter, the implementation and stability aspects of the method are presented in detail. As it will become evident soon, the stability analysis of this so-called complex-valued formulation, plays an important role in solving the stability problems of the real-valued formulation presented in the next Chapter.

In Sect. 4.5, the TLM formulation presented in Sec. 4.4 is expanded to handle PC composed of frequency dependent materials such as metals and semiconductors. In

addition, the extended formulation is made compatible with the type of meshes used in this thesis, by deriving the necessary equations for their application in non-cubic meshes.

Finally, throughout the Chapter, this formulation is applied for the computation of the dispersion relation of PC composed of simple dielectrics and dispersive materials.

4.2 A one-dimensional example

Before the time-domain computational technique for computing the DR is presented in detailed, it is interesting to investigate the validity of the results obtained by assuming an array of infinite extent. In other words, it is intuitive that the dispersion properties of a finite structure will approximate those of an infinite structure provided the number of unit cells in the finite problem, “is large enough”. However, the question arises of how many periods of the unit cells are actually required. In this section, it is shown that depending on the permittivity contrast, the required number of unit cells in the finite problem to obtain a strong confinement of radiation can be as small as two or three.

Consider the one-dimensional PC shown in Fig. 4.1. The reflectivity R (ratio of reflected to transmitted power) for a structure like this can be obtained analytically and is given by

$$R = \left[\frac{1 - (n_H/n_L)^{2m}(n_H^2/n_L)}{1 + (n_H/n_L)^{2m}(n_H^2/n_L)} \right]^2 \quad (4.1)$$

where n_H and n_L are the refractive indices of the alternating layers and m is the number of periods. As this figure shows, depending on the permittivity contrast (of course, $n_H = \sqrt{\epsilon_r}$), the number of periods required to achieve a high reflectivity

Figure 4.1: One-dimensional photonic crystal.

Figure 4.2: Reflectivity of the one-dimensional PC shown in Fig. 4.1 as a function of the number of periods for various permittivity contrasts.

(≈ 1.0) can be as low as three. This is in particular the case for most semiconductor materials, whose refractive indices are ≥ 3.0 . In Ref. [71], a high radiation confinement (leakage below -40 dB) was reported for only two periods of metallic cylinders.

To further pursue this example, Fig. 4.3 (top) shows the dispersion relation of the (infinite) PC shown in Fig. 4.1 predicted by the PWE. The middle figure shows the frequency response (Transmission Coefficient) of the finite structure when it is excited with a Gaussian pulse. As expected, forbidden frequency gaps appear in both cases. Note that the stop bands predicted by the PWE and TLM methods are in very good agreement.

The bottom figure shows the Fourier Amplitude along the structure calculated at two different frequencies: 0.25 GHz, which lies within the stop-band, and 0.38 GHz, which is inside the pass-band. As the figure shows, the second frequency corresponds to a propagating mode and its amplitude does not decay as it traverses the photonic structure. Conversely, the former frequency lies within the stop-band and forms an evanescent mode whose amplitude decays exponentially as it propagates across the structure. Note that by the time the signal has reached the far end of the structure, its amplitude has almost decayed to zero.

To conclude, in this section it has been verified that the results obtained by simulating infinite PC, are appropriate for studying periodic structures of finite size. Thus, the simulation aspects of infinite PC are addressed next.

Figure 4.3: From top to bottom: Dispersion relation, Transmission Coefficient and Fourier Amplitude throughout the structure of Fig. 4.1 at 0.38 and 0.25 GHz.

4.3 Problem Formulation

In this section, a description of the basic mathematical concepts governing the simulation of PC within the formulation of a time-domain method, such as TLM, is provided. Rather than attempting a rigorous mathematical derivation, the necessary equations are reproduced here only for the sake of completeness. For more details see for example Ref. [72].

From solid state theory, one knows that the periodic nature of semiconductors results in electron conduction without scattering being possible only for electrons that have energies within specific ranges called the allowed energy bands. Electromagnetic wave propagation in periodic dielectric media is similar to electron-wave propagation in semiconductor crystals. Thus, some well-known results from solid state theory can be applied directly in the simulation of PC.

From the basic solid state physics theory, one knows that periodic problems have solutions of the form [23],

$$\Psi(\mathbf{r}) = u_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}} \quad (4.2)$$

where the function $u_{\mathbf{k}}$ is periodic in space and $\mathbf{k}$ is a propagation vector. Eq. (4.2) is Bloch's theorem, although it is usually referred to as Floquet's theorem in one-dimensional problems. If $\mathbf{T}$ describes the spatial period of the structure, that is, if it represents a *lattice constant vector*, then

$$u_{\mathbf{k}}(\mathbf{r} + \mathbf{T}) = u_{\mathbf{k}}(\mathbf{r}). \quad (4.3)$$

Note that Eqs. (4.2) and (4.3) imply that

$$\Psi(\mathbf{r} + \mathbf{T}) = e^{-i\mathbf{k} \cdot \mathbf{T}} \Psi(\mathbf{r}), \quad (4.4)$$

thus, the points $\mathbf{r}$ and $\mathbf{r} + \mathbf{T}$ have the same physical properties and the functions differ from each other only by a phase factor. The application of Eq. (4.4) for the simulation of PC within the formulation of the TLM method leads to equations of the form

$$\begin{aligned} V^i(\mathbf{r} + \mathbf{T}) &= V^r(\mathbf{r})e^{-i\mathbf{k} \cdot \mathbf{T}} \\ V^i(\mathbf{r}) &= V^r(\mathbf{r} + \mathbf{T})e^{i\mathbf{k} \cdot \mathbf{T}} \end{aligned} \quad (4.5)$$

relating the incident and reflected pulses from the boundaries of the simulation domain. In Eq. (4.5), V^i and V^r represent the incident and reflected pulses of the nodes on the edge of the simulation domain, respectively. Note that in this equation, the time dependency is not shown but implicit.

4.4 Formulation of a Complex-Valued TLM Algorithm

It is obvious from Eq. (4.4) that the simulation of PC in the time-domain requires a complex-valued network. There are different ways of implementing a complex-valued algorithm. A well known approach is to compute the real and imaginary parts of the complex fields separately using real-valued arithmetic, and to couple them only at the

boundaries [70]. Similarly, in the TLM formulation the fields can be represented by complex voltage pulses traveling in the mesh. The real and imaginary parts can be scattered separately in the usual way throughout the simulation domain, and coupled only at the boundaries in accordance with Eq. (4.5).

After a little algebra, the periodic boundary conditions in Eq. (4.5) can be written in terms of the real and imaginary components of the voltage pulses as:

$$V_{real}^i(\mathbf{r} + \mathbf{T}) = V_{real}^r(\mathbf{r})\cos(\mathbf{k} \cdot \mathbf{T}) - V_{ima}^r(\mathbf{r})\sin(\mathbf{k} \cdot \mathbf{T}) \quad (4.6)$$

$$V_{ima}^i(\mathbf{r} + \mathbf{T}) = V_{real}^r(\mathbf{r})\sin(\mathbf{k} \cdot \mathbf{T}) + V_{ima}^r(\mathbf{r})\cos(\mathbf{k} \cdot \mathbf{T}) \quad (4.7)$$

$$V_{real}^i(\mathbf{r}) = V_{real}^r(\mathbf{r} + \mathbf{T})\cos(\mathbf{k} \cdot \mathbf{T}) + V_{ima}^r(\mathbf{r} + \mathbf{T})\sin(\mathbf{k} \cdot \mathbf{T}) \quad (4.8)$$

$$V_{ima}^i(\mathbf{r}) = -V_{real}^r(\mathbf{r} + \mathbf{T})\sin(\mathbf{k} \cdot \mathbf{T}) + V_{ima}^r(\mathbf{r} + \mathbf{T})\cos(\mathbf{k} \cdot \mathbf{T}) \quad (4.9)$$

The recursive application of these equations to the voltage pulses traveling toward the boundaries of the simulation domain, singles out the physical solutions of the PC under simulation. That is, it filters out the spectral content of the applied excitation such that, after several thousand iterations, it is only comprised of frequency modes satisfying a prescribed Bloch condition. This formulation is what it is referred to in this work, as a complex-valued TLM algorithm.

It must be emphasized at this point that this complex-valued formulation, which originated from the complex-valued nature of the Bloch boundary condition, is *only required when computing the DR* of infinite PC. For all other types of EM problems, the inherently real-valued TLM method described in Sect. 3.3, is perfectly applicable.

To conclude this section, pseudo-code for the complex-valued TLM algorithm is given below.

```

function Compute_Dispersion_Relation()
    Define_Unit_Cell();           // out of the infinite photonic crystal
    for k= $\Gamma$  to G                // k-points along edge of first Brillouin zone
        Apply_Field_Excitation(); // in the form of incident voltage pulses
        Define_Store_Nodes();     // choose random nodes in the unit cell
        for t = 1 to Num_time_steps
            for N=1 to All_Nodes
                TLM_real_Algorithm();
                TLM_complex_Algorithm();
                if (N==Boundary_Node)
                    Apply_Periodic_BC(); // Apply Eqs. (4.6) to (4.9)
                end if
            end for
        end for
        Fourier_Transform_Time_Data();
        Find_Resonant_Modes();
    end for
    plot_k_vs_omega();
end function

```

4.4.1 Stability Analysis of the Complex-Valued TLM Algorithm

Due to its physical realization (a TLM network consists of positive, passive components), it is well known that the TLM method is unconditionally stable. Thus, the total energy stored in lossless passive components must be accounted for at all times and must, therefore, remain constant in time. This in turn implies that the unconditional stability of the complex-valued TLM algorithm described in the previous section, is guaranteed, if the application of Eqs. (4.6-4.9) preserves the energy as a constant in the mesh. Thus, the purpose of this section is to show that the TLM scheme does remain unconditionally stable and to provide some insight into the

Figure 4.4: Scheme used for the calculation of the energy flow across a symmetry plane.

interaction between the real and imaginary grids.

Without loss of generality, we will restrict the following discussion to one polarization and one dimension and will denote the spatial period of the structure as t_x in that particular direction. Consider a single link-line connecting two nodes on opposite sides of the simulation domain as shown in Fig. 4.4. Note that the periodicity of the structure allows one to think of the two nodes as being the last and first nodes of two consecutive unit cells or equivalently, as the last and first nodes of the same unit cell. In the figure, the SCN presented in Sect. 3.3, is being used as a reference to define the voltage pulse notation.

The electric and magnetic fields in the link-line due to the incident pulses to the interface (reflected from the nodes) determine the energy density which leaves the unit cell at every scattering event. Taking as a reference Fig. 4.4, the energy density

can be calculated as follows. Starting with the electric and magnetic fields,

$$\begin{aligned} E &= -\frac{(V_{11}^r + V_3^r)}{\Delta x} \\ H &= \pm \frac{(V_{11}^r - V_3^r)}{Z_o \Delta x} \end{aligned} \quad (4.10)$$

where Z_o is the characteristic impedance of the transmission lines, which, for simplicity, is assumed to be the same for all branches ($Z_3 = Z_{11} \equiv Z_o$).

Thus, the electric and magnetic energy densities ω_e and ω_m are given, respectively, by

$$\begin{aligned} \omega_e &= \frac{\epsilon E^2}{2} = \frac{\epsilon (V_{11}^r + V_3^r)^2}{2 \Delta x^2} \\ \omega_m &= \frac{\mu H^2}{2} = \frac{\mu (V_{11}^r - V_3^r)^2}{2 Z_o^2 \Delta x^2} \end{aligned} \quad (4.11)$$

The total energy density, ω , is given by $\omega = \omega_e + \omega_m$ which, after carrying out the algebra and performing some straightforward substitutions, reduces to

$$\omega = \frac{(V_{11}^r)^2 + (V_3^r)^2}{c Z_o^2 \Delta x^2}. \quad (4.12)$$

where c is the speed of light in a vacuum.

Equation 4.12 indicates that the amount of energy that leaves the unit cell at a given scattering event, is proportional to the sum of the square of the voltage pulses traveling toward the boundaries. Thus, for the energy to be preserved as a constant in the simulation domain, the sum of the square of the voltage pulses reflected from the nodes adjacent to the symmetry planes, must be equal to the sum of the square of the incident voltage pulses calculated from Eqs. (4.6-4.9). Following these ideas,

the proof that the complex-valued TLM algorithm presented in the previous section is unconditionally stable, becomes a trivial matter. Squaring Eqs. (4.6) and (4.7) and adding them, we get,

$$[V_{real}^i(\mathbf{r} + \mathbf{T})]^2 + [V_{ima}^i(\mathbf{r} + \mathbf{T})]^2 = [V_{real}^r(\mathbf{r})]^2 + [V_{ima}^r(\mathbf{r})]^2, \quad (4.13)$$

similarly, squaring Eqs. (4.8) and (4.9) and adding them, we get,

$$[V_{real}^i(\mathbf{r})]^2 + [V_{ima}^i(\mathbf{r})]^2 = [V_{real}^r(\mathbf{r} + \mathbf{T})]^2 + [V_{ima}^r(\mathbf{r} + \mathbf{T})]^2. \quad (4.14)$$

Equations (4.13) and (4.14) show that the energy that enters and leaves the real and imaginary grids through the boundaries of the unit cell is equal. In addition, the equations show how the energy circulates between the two grids while remaining constant in time. This indicates that the application of Eqs. (4.6) to (4.9) to enforce the periodicity condition preserves the unconditional stability of the TLM method.

4.4.2 Simulation Examples

In this section, the use of the previously described TLM algorithm for the simulation of PCs is illustrated. First, a two-dimensional chessboard PC is analyzed. Such a structure is shown in Fig. 4.5. Note that for this structure the unit cell can be defined in different, but equivalent ways. For example, the dashed lines in the figure show two possible equivalent ways of defining the unit cell.

The general procedure used in this Section to calculate the band structure of the PC was described in Section 2.2. For the simulation of the two-dimensional chessboard lattice an air-dielectric composite was chosen. The value of the dielectric material

Figure 4.5: Simulated two-dimensional chessboard structure. The dashed lines illustrate two possible (equivalent) ways of defining the unit cell. The permittivity of the square pillars is $\epsilon_r = 11.7$ and $a = 1$.

was set to $\epsilon_r = 11.7$, which corresponds to square pillars of Si connected by the corners and embedded in air. For the numerical calculations, the lattice constant was normalized such that $a = 1$ and the unit cell was discretized into 32×32 uniformly spaced mesh points.

Given that the simulated photonic structure is two-dimensional, Maxwell's equations decouple into TE and TM modes. For TE modes, the electric $\mathbf{E}$ and magnetic $\mathbf{H}$ fields are $\mathbf{E}(\mathbf{r}) = (E_{x_1}, E_{x_2}, 0)$ and $\mathbf{H}(\mathbf{r}) = (0, 0, H_{x_3})$, respectively. Similarly, for TM modes the fields become $\mathbf{E}(\mathbf{r}) = (0, 0, E_{x_3})$ and $\mathbf{H}(\mathbf{r}) = (H_{x_1}, H_{x_2}, 0)$. In this example only TM modes were considered; that is, the excitation was such that the electric field was kept parallel to the square pillars. Note that these TE and TM mode conventions are in apparent contradiction with those commonly used in most textbooks where the transverse mode is defined with respect to the direction of propagation. However, the convention used in this thesis is consistent with that used in

Figure 4.6: Dispersion relation of the PC shown in Fig. 4.5. Dots: Simulation results. Solid line: PWE method. The inset shows the first Brillouin zone and the symmetry points used for the calculation.

Ref. [1].

The dispersion curves in Fig. 4.6 show the relation between the light frequency and the direction of propagation $\omega(\mathbf{k})$ for the chessboard structure. In this case, only light propagating in the plane containing the array of interconnected square pillars is considered (xy -plane). Thus, the dispersion curves were calculated by letting $\mathbf{k}$ take on values along the edge of the irreducible Brillouin zone as shown in the inset to Fig. 4.6. In this figure, the frequency has been normalized with respect to $2\pi c/a$. The dispersion curves shown in solid lines were obtained by using the PWE method and the dots correspond to the points predicted by the complex-valued TLM formulation. As the figure shows, good agreement was found.

The shaded areas in Fig. 4.6 show two frequency gaps in which no mode, regardless

of k , can exist in the PC. In other words, light of frequency falling within these gaps will create evanescent modes (which decay exponentially) and will not propagate across the structure. This property of PC can be exploited to fabricate a wide range of waveguides, filters, resonators, etc. since the width and position of the gaps can be engineered by changing the air-dielectric permittivity contrast, for example.

The second analyzed structure is a triangular lattice of circular rods of radius $r = 0.38a$ embedded in air as shown in Fig. 4.7. The dashed lines in the figure indicate the area comprising the unit cell. For this example, the dielectric constant of the cylinders was set to $\epsilon_r = 12$ corresponding to GaAs in air. Note that the spatial periodicity of this structure is defined by the lattice constant vectors $\mathbf{T}_1 = a\hat{x}$ and $\mathbf{T}_2 = a\hat{x}/2 + \sqrt{3}a\hat{y}/2$. Thus, the correct enforcement of the periodicity condition in the y direction requires that the voltage pulses between symmetry planes be swapped at an angle. That is, in order to correctly mimic the infinite triangular lattice, the voltage pulses on the horizontal planes have to be exchanged in accordance with $\mathbf{T}_2$. Note that this will guarantee that the fields have the same periodicity as the structure, $field(\mathbf{r} + \mathbf{T}_2) = field(\mathbf{r}) \times PhaseFactor$, as required by the Bloch condition.

Fig. 4.8 shows a comparison of the dispersion relations of the triangular lattice shown in Fig. 4.7. In the figure, the frequency has been normalized as before. The dispersion curves shown in solid lines were obtained by using the PWE method and the dots correspond to the points predicted by the complex-valued TLM formulation. Once more, the figure shows that the results between these two methods are in good agreement. The inset to the figure shows the first Brillouin zone of the triangular lattice and the symmetry points used for the calculation of the dispersion relation. As in the previous example, the dispersion curves show the presence of two frequency

Figure 4.7: Simulated two-dimensional structure. The dashed lines indicate the definition of the unit cell. The permittivity of the cylinders is $\epsilon_r = 12$ and their radii is $r = 0.38a$.

Figure 4.8: Dispersion relation of the PC shown in Fig. 4. Dots: Simulation results. Solid line: PWE method. The inset shows the first Brillouin zone and the symmetry points used for the calculation.

gaps in which no propagation modes can exist. However, the figure indicates that, although the air-dielectric contrast is very similar to that of the previous structure, the resulting band gaps are considerably wider. This is a typical behavior of *TM* modes for which frequency gaps are favored by isolated dielectric pillars [1].

4.5 Simulation of Frequency Dependent Material Properties

In the last few years, the scope of the TLM method has systematically been extended to include frequency-dependent, anisotropic and non-linear materials [15], [73], [74]. However, the development presented in these papers is not compatible with the stan-

dard TLM nodes (i.e., SLN and HSCN) used in this thesis and is only valid for uniform-cubic meshes.

In this section, the TLM method is expanded for the analysis of PC. Specifically, the complex-valued TLM formulation presented in Sect. 4.4 is extended for the analysis of PC composed of frequency dependent materials such as metals and semiconductors. In addition, by expanding the equations presented in Ref. [40] (which are only valid for cubic meshes), the frequency-dependent formulation is generalized and made compatible with the type of meshes used in this thesis. It should be mentioned that the derivation of the necessary equations for their application in non-cubic meshes follows a very similar procedure to that presented in Sect. 3.4.2. For this reason, only the relevant modifications are emphasized in the next sections.

4.5.1 Problem Formulation

In Maxwell's equations, dispersive materials are accounted for by relating the electric field and electric displacement vectors in the frequency domain by a frequency-dependent permittivity $D(\omega) = \epsilon(\omega)E(\omega)$. When converted to the time-domain, this equation becomes a convolution involving the susceptibility function of the material under consideration. In the TLM method, the implementation of dispersive materials is accomplished by mapping TLM equations into a discretized version of the Maxwell's equations incorporating dispersive media. In the HSCN-TLM method, this results in the introduction of one voltage source for each electric field component, at each TLM node. In turn, these new voltage sources require the introduction of three additional ports (16-18) at the center of the node where the sources are to be connected [75].

The explicit form of the voltage sources is given by,

$${}_{n+1}V_{sq} = -{}_nV_{sq} - \frac{\chi_0(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} {}_nV_q - \frac{(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} \sum_{m=0}^{n-1} {}_{n-m}V_q (\chi_{m+1} - \chi_m) \quad (4.15)$$

where $q \in \{x, y, z\}$. This is the update equation for the voltage sources at time $(n + 1)\Delta t$. In Eq. (4.15), V_q is the average voltage at the node, ϵ_∞ is the relative permittivity of the medium at very high frequencies, χ_m is the general susceptibility given by

$$\chi_m = \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau) d\tau, \quad (4.16)$$

χ_0 is the static susceptibility and is obtained by evaluating this integral between 0 and Δt . In addition, $\hat{Y}_o^q$ is the normalized stub admittance of the dispersive material. For example, for a cubic mesh and taking as a reference the z -field component, $\hat{Y}_o^z$ is given by [40], [75]

$$\hat{Y}_o^z = 4(\epsilon_\infty + \chi_0 - 1). \quad (4.17)$$

The extension of this equation for use with general meshes is somewhat straightforward. For the materials presented in this section, one has the following relation between the electric and displacement field vectors

$$\mathbf{D}(\omega) = \epsilon_0(\epsilon_\infty + \chi(\omega))\mathbf{E}(\omega) \quad (4.18)$$

thus, given that the frequency dependency is already accounted for by the voltage source term, one can define a static relative permittivity as

$$\epsilon_r = \epsilon_\infty + \chi_0. \quad (4.19)$$

notice that if the permittivity is independent of frequency, then $\chi(\tau) = 0$ and $\chi_m = 0$ for all m , resulting in $\epsilon_r = \epsilon_\infty$ as required.

Using the definition in Eq. (4.19) and following a similar procedure to that shown in Sect. 3.4.2, the following equation is obtained for $\hat{Y}_o^z$

$$\hat{Y}_o^z = \frac{4(\epsilon_\infty + \chi_0)\Delta x \Delta y}{\Delta L_{min} \Delta z} - \frac{2\Delta L_{min}[(\Delta x)^2 + (\Delta y)^2]}{\mu_r \Delta x \Delta y \Delta z}, \quad (4.20)$$

where ΔL_{min} is the smallest of all nodal dimensions present in the non-uniform mesh and μ_r is the relative permeability of the node. Note that ΔL_{min} has been related to the time step used for the simulations by Eq. (3.112). Note that when modelling non-magnetic media in a uniform mesh $\Delta L_{min} = \Delta x = \Delta y = \Delta z$ and Eq. (4.20) reduces to Eq. (4.17).

4.5.2 Calculation of Equivalent Nodal Voltages and Currents

The calculation of the voltage at the node can be done by using the Thevenin equivalent circuit of the link-lines. In this Section, the calculation is shown for the y -component of the electric field, however, the procedure is identical for the other field components as well. In Fig. 3.7, the link-lines contributing to the y -component of the electric field are shown. Using the Thevenin equivalent circuit for the link-lines and adding a current source to the node, the circuit shown in Fig. 4.9 is obtained. Note that the usual HSCN includes the possibility of adding current sources for each space dimension of the node [76]. In this case, these current sources are transformed into the new needed voltage source elements.

Using the circuit shown in Fig. 4.9, the average voltage across the node can be

Figure 4.9: Norton equivalent circuit of the link-lines contributing to the y -component of the electric field.

found by superposition. Having in mind that for a symmetric node, $Y_{xny} = Y_{xpy} \equiv Y_z$ and $Y_{zpy} = Y_{zny} \equiv Y_x$, the following equation is obtained after a little algebra

$$V_y = \frac{2Y_z(V_{xny}^i + V_{xpy}^i) + 2Y_x(V_{zny}^i + V_{zpy}^i) + 2Y_o^y V_{oy}^i + I_{sy}}{2(Y_x + Y_z) + Y_o^y + G_{ey}} \quad (4.21)$$

one can now normalize the admittances to free-space (Y_0) by multiplying top and bottom by $\frac{1}{Y_0}$, this results in

$$V_y = \frac{2\hat{Y}_z(V_{xny}^i + V_{xpy}^i) + 2\hat{Y}_x(V_{zny}^i + V_{zpy}^i) + 2\hat{Y}_o^y V_{oy}^i + V_{sy}}{2(\hat{Y}_x + \hat{Y}_z) + \hat{Y}_o^y + \hat{G}_{ey}} \quad (4.22)$$

Thus, in this equation, $\hat{Y}_x$ and $\hat{Y}_z$ are the normalized admittances (to Y_0) of the link-lines associated with the x - and z -components of the magnetic field respectively. They are given by Eqs. (3.108) and (3.110). Similarly, $\hat{Y}_o^y$ and $\hat{G}_{ey}$ are the normalized characteristic admittances of the open-circuit and electric loss stubs associated with the y -component of the electric field. They are given by a similar equation to (4.20) and by (3.88) respectively. In addition, V_{sy} is the voltage source term that accounts

for the dispersive properties of the medium for the E_y -component. Finally, it should be noted that in a cubic mesh, Eq. (4.22) reduces to the equation given in Ref. [40]:

$$V_y = \frac{2(V_{xny}^i + V_{xpy}^i + V_{zny}^i + V_{zpy}^i + \hat{Y}_o^y V_{oy}^i + 0.5V_{sy})}{4 + \hat{Y}_o^y + \hat{G}_{ey}}. \quad (4.23)$$

It should also be noted that the new voltage sources only interact with the link-lines associated with the electric fields. Therefore, they have no effect on the nodal current (required for the calculation of the magnetic fields) and the equations found in Sect. 3.5.4 can be used as follows. For example, for the current associated with z -directed magnetic field, the general equation for the nodal current was found to be (Eq. 3.136)

$$I_z = 2 \frac{V_{xpy}^i - V_{xny}^i + V_{ynx}^i - V_{ypx}^i - V_{sz}^i}{Z_{xny} + Z_{xpy} + Z_{ynx} + Z_{ypx} + Z_{sz} + R_{mz}} \quad (4.24)$$

now, given that for the HSCN the characteristic impedances of the link-lines associated with a given magnetic field component are equal (Sect. 3.4.2), it follows that $Z_{xny} = Z_{xpy} = Z_{ynx} = Z_{ypx} \equiv Z_z$. In addition, a HSCN does not have short-circuit stubs, thus $Z_{sz} = V_{sz}^i = 0$ and Eq. (4.24) reduces to

$$I_z = 2 \frac{V_{xpy}^i - V_{xny}^i + V_{ynx}^i - V_{ypx}^i}{4Z_z + R_{mz}} \quad (4.25)$$

To complete the description of the frequency dependent TLM algorithm, the reflected voltage pulses are obtained by performing a standard scattering procedure. Furthermore, the calculation of the incident voltage pulses is done by swapping voltage pulses from adjacent nodes or by connecting the small and big internal faces of the blocks using ideal matching transformers when required. The scattering and connect

procedures were explained in more detail in Sects. 3.5 and 3.6.

4.5.3 Simulation Examples

In this section, the previous method is validated by simulating two PC whose solutions are known in order to facilitate the comparison of results. The calculation of the PBS for an infinite periodic structure composed of frequency-dependent materials follows an identical methodology to that described in Section 4.4. In summary, it requires the enforcement of the periodicity condition at the sidewalls of the simulation domain (unit cell). This is accomplished by enforcing on the fields the Bloch condition $\Psi(\mathbf{r} + \mathbf{T}) = e^{-i\mathbf{k} \cdot \mathbf{T}} \Psi(\mathbf{r})$, where $\mathbf{r}$ and $\mathbf{T}$ are the position and lattice constant vectors respectively, and $\mathbf{k}$ is a prescribed propagation vector. Owing to linearity, this formulation is incorporated into a standard TLM method by breaking it into its real and imaginary parts. The resulting real and imaginary voltage pulses are then treated separately throughout the simulation domain and coupled only at the boundaries as before.

There is an important issue that needs to be addressed during the excitation of the unit cell when simulating frequency dependent materials. Owing to the lossy nature of the PC, the Gaussian pulse previously used as the excitation, needs to be replaced by an oscillating dipole to avoid having the radiation totally absorbed after a few thousand iterations.

For the materials presented in this section, the complex relative permittivity is modelled by a plasma-type equation of the form

$$\epsilon^*(\omega) = \epsilon_\infty \left(1 + \frac{\omega_p^2}{\omega(j\nu_c - \omega)} \right) = \epsilon_\infty (1 + \chi(\omega)) \quad (4.26)$$

where ν_c is the electron collision frequency, ϵ_∞ is the permittivity at very high frequencies and $\chi(\omega)$ is the frequency-dependent susceptibility function. The radian plasma frequency (ω_p) is given by

$$\omega_p = \sqrt{(N_e e^2)/(\epsilon_\infty \epsilon_0 m_e)}, \quad (4.27)$$

where ϵ_0 is the permittivity of free space, N_e the number of electrons per unit volume, e the electronic charge and m_e the effective mass of the electrons. When converted to the time-domain, Eq. (4.26) leads to a time-domain susceptibility function of the form

$$\chi(\tau) = \frac{\omega_p^2}{\nu_c} [1 - e^{-\nu_c \tau}] u(\tau) \quad (4.28)$$

where $u(\tau)$ is the unit step function. The exponential form of this equation allows to write the convolution in Eq. (4.15) in a recursive way such that the values of the electric field at every time step do not need to be stored. For details see Appendix A.

Note that for these types of materials, Eqs. (4.16) and (4.28) lead to the following expression for the static susceptibility χ_0 appearing in Eqs. (4.15) and (4.20)

$$\chi_0 = \int_0^{\Delta t} \chi(\tau) d\tau = \frac{\omega_p^2}{\nu_c} \Delta t - \left(\frac{\omega_p}{\nu_c} \right)^2 [1 - e^{-\nu_c \Delta t}]. \quad (4.29)$$

The first analyzed structure is a two-dimensional square PC composed of metallic cylinders previously analyzed in Ref. [1] by means of the FDTD method. For a pure metal, $\epsilon_\infty = 1.0$ in Eq.(4.26). Following this reference, the radius of the cylinders was set to $r = 0.472a$, with a representing the lattice constant. In addition, the plasma frequency was set to a constant value of $\omega_p = 2\pi c/a$, where c is the speed of light in

Figure 4.10: Comparison of PBS for 2D square PC composed of metallic cylinders. Solid line: FDTD [1]. Filled-squares: TLM method.

a vacuum. Finally, the electron collision frequency was set to $\nu_c = \omega_p/100$.

Figure 4.10 shows a comparison of the PBS corresponding to this PC. For the actual TLM simulations, the unit cell was discretized into 20×20 uniformly spaced mesh points. As in Ref. [1], the numerical simulation was done for the E polarization. The PBS was calculated for the wavevectors in the (1,0) and (1,1) directions in the first Brillouin zone of the two-dimensional square lattice. In Fig. (4.10) a comparison of TLM and FDTD results are presented and are in good agreement.

The second simulated structure was a two-dimensional square PC composed of InSb cylinders. For this case, the permittivity of the cylinders is adequately modelled by Eq. (4.26) provided that the frequencies of interest are well below the far infrared resonance region. This allows the approximation $\epsilon_\infty = \epsilon_r$. For the simulation $\epsilon_r = 17.7$, the radius of the cylinders was set to $0.282a$, $\omega_p = 9.3479 \times 10^{12}$ rad/s and

Figure 4.11: a) Comparison of PBS for a 2D square PC composed of InSb cylinders. Solid line: PWE [2]. Filled-squares TLM method. b) Discretized unit cell used in the simulations. The permittivity of the cylinders is $\epsilon_r = 17.7$ and their radii is $r = 0.282a$.

$$\nu_c = \omega_p/100 [2].$$

Figure 4.11(a) shows a comparison of the PBS corresponding to this PC for PWE and TLM results. The figure shows that, although there is a small discrepancy between the results predicted by the two methods, the agreement is fairly good. The discrepancy can be attributed to the discretization error and to the approximation of Eq. (4.26) in the PWE method [2]. To minimize the first source of error, the unit cell was discretized by using a non-uniform mesh as shown in Fig. 4.10(b). In addition, the permittivity value on the edge of the cylinder was averaged to smooth the air-medium interface.

4.6 Summary

In this Chapter, a so called complex-valued formulation that allows to compute the dispersion relation of PC by means of the TLM method was presented. The implementation and stability aspects of the method were shown in detail. In addition, the formulation was extended for handling PC composed of frequency dependent materials such as metals and semiconductors. By deriving the necessary equations for their application in non-cubic meshes, the extended formulation was made compatible with the types of meshes used in this thesis. Finally, the formulation was validated by computing the DR of PC composed of simple dielectrics and dispersive materials.

Chapter 5

Optimization of the Complex-Valued Formulation

5.1 Introduction

It was mentioned before that one of the main drawbacks of time-domain methods is that they are inherently slow. In particular for the simulation of PC, time-domain methods are even slower because the complex-valued formulation proposed in the previous section can be viewed as two traditional (real-valued) TLM algorithms running simultaneously for the same structure. This obviously increases the demand for computational resources by a factor of two, making large, three dimensional problems, more unwieldy. For this reason, suitable ways for speeding up the algorithm proposed in Sect. 4.4 must be found.

A first natural approach for the optimization of the complex-valued algorithm is to decouple the real and imaginary parts of the voltage pulses and try to compute

the PBS by using only either part. Obviously, such a “real-valued” approach would reduce the computation effort by half.

5.2 Real-Valued Formulation

It was mentioned in Sect. 4.4 that given that the periodicity condition is complex, its implementation in the time-domain requires a complex-valued network. In Sect. 4.4, this issue was dealt with by introducing two electromagnetic fields, each having sinusoidal and cosinusoidal time dependence. These fields can be thought of as the real and imaginary parts of a complex electromagnetic field and constitute two solutions (modes) of the complex-valued network with identical spectral information. As previously explained, the real and imaginary parts are coupled to each other only at the boundaries. As shown in Sect. 4.4.1, this coupling allows for energy to be exchanged between the two fields ensuring the stability of the complex time-domain method.

In a real-valued problem formulation, the real and imaginary fields are decoupled and treated independently. Thus, the real-valued network has two solutions (cosinusoidal and sinusoidal-like) and can potentially produce either one depending on the part of the Bloch condition (real or imaginary) that is applied at the boundaries. It should be noted that both solutions are real and governed by the same scattering principles and represent in reality two standing waves shifted in space by $\lambda/4$ as described in Ref. [27].

In Sect. 2.2, it was mentioned that early attempts to compute the PBS of PC using a real-valued formulation have resulted in unstable algorithms. In Ref. [31], the lack of stability was attributed to numerical noise and a non-perfect excitation.

Further details for these statements were not provided nor, to the best of the author's knowledge, can they be found in the literature.

In this section, a circuit-type formulation for implementing periodic boundary conditions in the real-valued TLM method is presented. This formulation leads to an absolutely stable algorithm that enforces the Bloch boundary conditions at the cell sidewalls while preserving energy. By comparing the performance of this method with that presented in [28], the introduction of numerical energy from the boundaries was identified as the source of the high frequency components. The numerical energy introduced by the boundaries is the result of energy that would otherwise couple to the imaginary network of the complex formulation. In the context of this work, the term “numerical energy” is used to refer to the energy that a) is not coupled to the Bloch modes which constitute the physical solutions of the problem and b) is introduced as a result of the violation of energy conservation when imposing the Bloch condition on the boundaries of the unit cell leading to a physically meaningless divergent solution.

5.2.1 Formulation of a Real-Valued Network

In this section, the methodology of the solution method presented in [57] is briefly reviewed. Following the application of Eq. (4.4) within the framework of the SCN-TLM method yields the following equations relating the fields at the j^{th} set of planes:

$$\psi(x_{j,1}, t) = v_{j,2}\psi(x_{j,2}, t), \quad \text{and} \quad \psi(x_{j,2}, t) = v_{j,1}\psi(x_{j,1}, t), \quad (5.1)$$

where t is time and

$$v_{j,1} = \frac{1}{v_{j,2}} = \frac{\cos(k_j t_j + \sum_j k_j x_{j,1})}{\cos(\sum_j k_j x_{j,1})}. \quad (5.2)$$

Thus, for the SCN shown in Fig. 3.3, equations of the following form apply in the x_1 direction:

$$V_{3,6}^i(x_{1,1}) = v_{1,2} V_{11,10}^r(x_{1,2}), \quad V_{11,10}^i(x_{1,2}) = v_{1,1} V_{3,6}^r(x_{1,1}). \quad (5.3)$$

Similar equations apply in the other directions. Additionally, it was shown in [57] that the use of Eq. (5.2) is not enough to implement periodicity in a real-valued TLM scheme because $v_{j,1}$ is not single-valued and may possibly be associated with more or less arbitrary values of k_j . This can be solved easiest by fixing the phase at $x_{j,1}$ with the aid of a magnetic (or electric) wall. In numerical modelling, magnetic and electric walls are a convenient way of imposing Dirichlet or Neumann boundary conditions [77]. For example, the tangential fields at the walls satisfy the following conditions:

$$\text{On electric walls: } E_t = 0, \quad \frac{\partial H_t}{\partial n} = 0$$

$$\text{On magnetic walls: } H_t = 0, \quad \frac{\partial E_t}{\partial n} = 0$$

where the subscript indicates that the boundary condition applies to the tangential components of the fields and n denotes the normal to the corresponding wall. Thus, by imposing these boundary conditions on the amplitude of the fields at the first interface, their phase also become fixed. This allows one to use the known phase at the first symmetry plane as a reference, to evaluate the phase at the second symmetry plane unambiguously.

When a magnetic wall is used, the condition $\frac{\partial E_t}{\partial n} = 0$ leads to an initial phase of zero ($\sum_j k_j x_{j,1} = 0$) for a cosinusoidal-like field. Therefore, Eqs. (5.2) and (5.3) reduce to,

$$v_{j,1} = \frac{1}{v_{j,2}} = \cos(k_j t_j) \quad (5.4)$$

and (see Sect. 3.8.2),

$$V_{3,6}^i(x_{1,1}) = V_{3,6}^r(x_{1,1}) \quad (5.5)$$

$$V_{11,10}^i(x_{1,2}) = 2.0v_{1,1}V_{3,6}^r(x_{1,1}) - V_{11,10}^r(x_{1,2}), \quad (5.6)$$

respectively. In these equations, the superscript r stands for the voltage pulse scattered from the node and traveling toward the periodic boundary. Similarly, i stands for the voltage pulse scattered at the boundary that becomes incident on the node at the next time step.

The one-dimensional forms of Eqs. (5.4), (5.5) and (5.6) were used in [57] to simulate a periodic capacitively loaded rectangular waveguide and high frequency numerical noise was detected. We also found this to be true, the application of these equations to simulate a two-dimensional PC led to similar problems. Specifically, high frequency components, which could not be controlled by varying the excitation, appeared. In addition, the numerical noise was quickly amplified rendering the simulation unstable after a few thousand iterations.

Figure 5.1 shows a typical spectral intensity of one of our simulations using Eqs. (5.5) and (5.6) to simulate the periodicity of the PC. The structure will be described in more detail later on. The high frequency component that the figure shows was introduced by the exchange algorithm imposing the periodic boundaries (Eqs. (5.5) and (5.6)) and could not be controlled by the spectral width of the excitation (also shown

Figure 5.1: Typical computed spectral intensity indicating the presence of a parasitic frequency component introduced by the periodic boundaries (solid line). The spectral information in the region of interest has been completely overshadowed by this frequency component. The dashed line shows the spectral content of the excitation.

in the figure in dashed line). As can be seen, the algorithm has introduced a high frequency parasitic component well above the spectral content of the excitation. In the time-domain, this high frequency component manifested itself by the field intensities growing in time that eventually led to unstable simulations. The position of such frequency components was random for different k_j values. However, the overall effect was to shadow the spectral information in the region of interest ($\sim 0-1$ units of normalized frequency). Note that in Fig. 5.1 the excitation and computed spectral intensity are not plotted in the same scale since the amplitude of the parasitic component was many orders of magnitude larger at the time that the simulation was stopped.

5.2.2 Circuit-type Implementation of Periodic Boundaries

It has already been mentioned that the TLM method is unconditionally stable because the transmission line network consists of positive, passive components. Thus, it is evident that the stability problems described in the previous section have their origin at the boundaries. Physically speaking, a stable time-domain simulation can be related to conservation of energy, since the total energy stored in lossless passive components must be accounted for at all times. It is obvious from Eq. (5.6) that this exchange algorithm for the periodic boundaries does not preserve energy (which, as shown in Sect. 4.4.1, is proportional to the square of the voltage pulses), since in general, the energy carried by the pulses traveling toward the boundaries will be different from that carried by the pulses reflected back into the node. Note that Eqs. (5.5) and (5.6) will preserve energy if $V_{1,10}^r(x_{1,2}) = v_{1,1} V_{3,6}^i(x_{1,1})$, which will occur when a magnetic wall is used such that $v_{1,1}$ is calculated from Eq. (5.4). This condition then represents the Bloch theorem written for the standing cosinusoidal-like mode. This indicates that the implementation of the Bloch condition using this formulation will maintain the amplitude of the cosinusoidal-like mode stable. However, the amplitude relations of the sinusoidal-like mode are still indeterminate and once this solution is excited from numerical noise or the applied excitation, its amplitude will, in general, increase in time. Thus, the fact that numerical energy is being added as time progresses has no physical counterpart for the simulated problem. This energy appears as a high frequency noise and renders the simulation unstable.

Additionally, Eq. (5.6) indicates that the amount of energy that is reflected back into the node (and into the simulation domain) is k_j dependent. Thus, the algorithm behaves differently for different k_j values and this makes its general application quite

difficult. It should be emphasized that if the nature of the solution is known (e.g. standing waves) the passivity of the boundaries is not an indispensable condition for stable simulations to occur. If the excitation is carefully implemented in the simulation domain (as suggested by [31]), the numerical energy does not increase with time but is eventually filtered out as the standing wave patterns of both solutions are established. This method requires some expertise and is problematic for a general excitation.

Proposed solution

The solution to these problems is to proceed in such a way that conservation of energy is intrinsically guaranteed. This is the case for example of circuit-based techniques. Any alteration of the TLM network at the boundaries, based on passive linear circuit models, is guaranteed to preserve energy and produce an unconditionally stable scheme. This is the motivation behind the circuit-type implementation of periodic boundaries shown in Fig. 5.2. By using matching transformers to connect the transmission link-lines between the $x_{j,1}$ and $x_{j,2}$ planes, energy conservation is enforced. A similar technique was previously used in [50] to preserve energy at the interfaces between multi-grid meshes. Whereas the ideal matching transformers account for conservation of energy, the phase condition is implemented by calculating the transformers turn ratios (X,Y) such that Eq. (5.3) is satisfied. Although Fig. 5.2 shows the circuit representation for only one direction and polarization, similar circuits apply for the remaining directions and polarizations.

Thus, the problem comes down to solving the circuit network of Fig. 5.2 subject to Eq. (5.3). To get the circuit equations, one resorts to the Norton equivalent circuit of the network (see Appendix B). After some algebra, the following circuit equations

Figure 5.2: Circuit-type implementation of the periodic boundary conditions.

are obtained

$$V_{11}^i(x_{1,2}) = V_{11}^r(x_{1,2}) + \left(\frac{2[XV_{11}^r(x_{1,2}) + YV_3^r(x_{1,1})]}{X^2 + Y^2} - \frac{2.0V_{11}^r(x_{1,2})}{X} \right) X \quad (5.7)$$

$$V_3^i(x_{1,1}) = V_3^r(x_{1,1}) + \left(\frac{2[XV_{11}^r(x_{1,2}) + YV_3^r(x_{1,1})]}{X^2 + Y^2} - \frac{2.0V_3^r(x_{1,1})}{Y} \right) Y \quad (5.8)$$

In addition, from Eq. (5.3) one gets the following relation for the voltage pulses of interest

$$V_{11}^i(x_{1,2}) + V_{11}^r(x_{1,2}) = v_{1,1} [V_3^i(x_{1,1}) + V_3^r(x_{1,1})] \quad (5.9)$$

Equations (5.7), (5.8) and (5.9) comprise the set of equations to solve. Note that in these equations, there are four unknowns ($V_{11}^i(x_{1,2})$, $V_3^i(x_{1,1})$, X and Y) and only three equations. To go around this problem, it is assumed that the turn ratio of one of the transformers is known (e.g. Y). This allows to solve the set of equations for the three remaining unknowns.

The solution to this problem leads to the following equations for the reflected pulses

from the interfaces:

$$V_3^i(x_{1,1}) = \frac{2.0v_{1,1}V_{11}^r(x_{1,2}) + V_3^r(x_{1,1}) - (v_{1,1})^2V_3^r(x_{1,1})}{(v_{1,1})^2 + 1} \quad (5.10)$$

$$V_{11}^i(x_{1,2}) = \frac{(v_{1,1})^2V_{11}^r(x_{1,2}) - V_{11}^r(x_{1,2}) + 2.0v_{1,1}V_3^r(x_{1,1})}{(v_{1,1})^2 + 1} \quad (5.11)$$

and to the following equation for the unknown transformer's turn ratio

$$X = Yv_{1,1} \quad (5.12)$$

Note that Eqs. (5.10) and (5.11) have i as superscript because the reflected pulses from the boundaries are in reality the incident pulses on the nodes at the next time step. By using these equations to calculate the reflected pulses, the energy of both solutions is conserved and the Bloch phase condition satisfied at the boundaries for any k_1 value.

There is still one unresolved problem. Specifically, the phase at one of the symmetry planes needs to be fixed or calculated in such a way that $v_{j,1}$ is a single-valued function of k_j . In the new formulation, the use of a magnetic (or electric) wall is not an option since this would imply losing one degree of freedom (the reflected pulse would have to be equal to the incident one) and the simultaneous enforcement of Bloch condition and energy conservation would not be possible for both solutions.

This problem has been overcome by using the following expression to calculate the initial phase,

$$\sum_j k_j x_{j,1} = \frac{\pi}{4} - \frac{k_j t_j}{2}. \quad (5.13)$$

By using Eq. (5.13) to calculate the phase at the first symmetry plane, $v_{j,1}$ becomes

Figure 5.3: Plot of the phase factor versus the propagation vector. solid line: multi-valued phase factor, dashed line: uni-valued phase factor. The rectangle shows the phase shift of interest between symmetry planes.

a single-valued function of k_j in Eq. (5.2). This is illustrated in Fig. 5.3, where the phase factor is plotted for both cases. In this figure, the rectangle shows the phase shift of interest between symmetry planes (0 to π). It is interesting to note that when Eq. (5.13) is used, the phase factor increases asymptotically to $+\infty$ and $-\infty$ for values outside the phase shift of interest. However, it must be noted that this does not disrupt the unconditional stability of this method. While it is true that using a value of phase factor outside the region of interest will lead to finding incorrect resonances in the unit cell, the method still remains stable. This was verified by plotting Eqs. (5.10) and (5.11) for large values of $v_{1,1}$. The results are shown in Fig. 5.4. As this figure shows, as the phase factor takes large positive or negative

Figure 5.4: Incident voltage pulses as a function of the phase factor. solid line: $V_3^i(x_{1,1})$, dashed line: $V_{11}^i(x_{1,2})$. For the calculations $V_3^r(x_{1,1}) = 2.0$ and $V_{11}^r(x_{1,2}) = 1.0$.

values, the incident voltage pulses predicted by Eqs. (5.10) and (5.11) remain finite and asymptotically approach constant values. This demonstrates the claim that this formulation remains unconditionally stable even for large values of the phase factor.

In summary, in the new model, Eqs. (5.2) and (5.13) are used to implement the Bloch condition, and Eqs. (5.10) and (5.11) replace Eqs. (5.5) and (5.6) of the previous model and are used to calculate the incident pulses of the link-lines connected to the boundaries. Pseudo-code for the real-valued TLM algorithm is given below.

```

function Compute.Dispersion.Relation()
    Define_Unit_Cell();           // out of the infinite photonic crystal
    for k=Γ to G                  // k-points along edge of first Brillouin zone
        Apply_Field_Excitation(); // in the form of incident voltage pulses
        Define_Store_Nodes();     // choose random nodes in the unit cell
        for t = 1 to Num.time.steps
            for N=1 to All.Nodes
                TLM_real_Algorithm();
                if(N==Boundary.Node)
                    Apply_Periodic_BC(); // Apply Eqs. of the form (5.9)
                end if
            end for
        end for
        Fourier.Transform.Time.Data();
        Find_Resonant_Modes();
    end for
    plot_k_vs_ω();
end function

```

Figure 5.5 shows a comparison of the evolution of the total instantaneous energy in the cell calculated by using the previously discussed models. It can be clearly seen that the model based on [57] is unstable as the total energy is not conserved, thus violating the physicality of the simulated problem. As the figure also indicates, the real-valued TLM method based on the new formulation maintains the time-averaged

Figure 5.5: Comparison of the evolution of the instantaneous energy. The energy has been normalized with respect to the time averaged value.

energy as a constant and thus captures the physics of the complex-valued networks with half the computational effort. The predictions of the complex-valued TLM method are also shown for the sake of comparison. It should be pointed out that in the new method (the same is true for the complex version) there is, in general, an instantaneous flow of energy across the boundaries. This happens because the incident and reflected energies at a given interface are not equal at all times. However, the matching transformers balance the inflow and outflow such that the net flow of energy is null.

Figure 5.6: Black box replacing the circuit-type implementation of the periodic boundary conditions. The inflow and outflow of energy from the black box must be balanced to keep energy as a constant.

5.2.3 Derivation from Energy Considerations

In the previous section, the stability problems of the real-valued formulation originally reported in Ref. [57] were identified as a lack of energy conservation. As already shown, this problem was solved by using a circuit type implementation (a network of matching transformers) of the periodicity condition which preserved the energy as a constant. Following these ideas, one can think that if the overall effect of the matching transformers is to keep the energy as a constant, it should be possible to replace them with an element which also keeps the energy as a constant. This idea is illustrated in Fig. 5.6, where the replacing element has not been defined and is represented by a black box.

Based on the analysis of the stability properties of the complex-valued formulation presented in Sect. 4.4, one can expect the energy to be preserved as a constant if the inflow and outflow of energy from the black box, is balanced. Thus, based on Eq. (4.12) and restricting our attention to one polarization and one dimension as

before, this requirement translates into,

$$[V_{11}^r(x_{1,2})]^2 + [V_3^r(x_{1,1})]^2 = [V_{11}^i(x_{1,2})]^2 + [V_3^i(x_{1,1})]^2 \quad (5.14)$$

That is, the sum of the square of the voltage pulses flowing into (reflected) and out of the black box (incident), must be equal.

Note that the periodicity condition (Eq. (5.9)) and Eq. (5.14) form a set of two equations with two unknowns. The solution of this set of equations is precisely Eqs. (5.10) and (5.11). Thus, the conservation of energy condition achieved by using circuit-based techniques and directly from energy considerations are equivalent. However, the latter formulation is more transparent and the resulting set of equations to be solved, simpler.

Although it is not the intention of this thesis to compare the performance of the FDTD and TLM methods, it should be noted at this point that the complex-valued formulation of both methods follows a very close resemblance. As a matter of fact, the FDTD counterpart of Eqs. (4.6-4.9) can be obtained simply by replacing voltage pulses by electric and magnetic fields in those equations. While it can be shown that the energy is a conserved quantity on the lattice of a complex-valued FDTD algorithm [26], initial results indicate that such is not the case for a real-valued formulation. Thus, the real-valued TLM algorithm presented in this section proves advantageous since it has no straightforward counterpart within the formulation of the FDTD method.

5.2.4 Limitations of the Real-valued Formulation

In the previous section the real-valued TLM algorithm was made unconditionally stable by satisfying the energy conservation condition. Thus, the resulting algorithm has not only overcome the initial stability problems, but has also reduced the computational effort required to calculate the dispersion relation by half. However, this advantage is achieved at the expense of introducing some limitations in the definition of the unit cell under simulation.

Consider the one-dimensional form of the phase factor plotted as a function of wave vector value (k_1) shown in Fig. 5.3. Note that the normalization condition of the unit cell ($t_x = a = 1$), makes the propagation vector numerically equal to the phase difference between symmetry planes. In addition, the first Brillouin zone indicates that this phase difference can only take values between 0 and π .

Now consider what happens when $v_{1,1}$ is substituted in Eqs. (5.10) and (5.11) for three different phase values. For a phase difference of zero we can see from Fig. 5.3 that $v_{1,1} = 1$. Thus Eqs. (5.10) and (5.11) reduce to $V_3^i(\mathbf{r}_1) = V_{11}^r(\mathbf{r}_2)$ and $V_{11}^i(\mathbf{r}_2) = V_3^r(\mathbf{r}_1)$ so that the voltage pulses are just wrapped around the cell without any alterations. Similarly, when the phase difference is equal to π , Fig. 5.3 indicates that $v_{1,1} = -1$ and Eqs. (5.10) and (5.11) reduce to $V_3^i(\mathbf{r}_1) = -V_{11}^r(\mathbf{r}_2)$ and $V_{11}^i(\mathbf{r}_2) = -V_3^r(\mathbf{r}_1)$ such that the voltage pulses are now wrapped around but with opposite signs. These results are somewhat intuitive and pose no difficulty to our simulation method. Consider however what happens when the phase difference varies between these two extreme values. When the phase difference is equal to $\pi/2$, $v_{1,1} = 0$ and Eqs. (5.10) and (5.11) reduce to $V_3^i(\mathbf{r}_1) = V_3^r(\mathbf{r}_1)$ and $V_{11}^i(\mathbf{r}_2) = -V_{11}^r(\mathbf{r}_2)$.

The fact that the reflected and incident voltage pulses at one end of the simulation

domain become equal, implies a *mirror* symmetry plane (or magnetic wall) at that end. Note that this condition holds true regardless of how the unit cell has been defined. In other words, for the results of the simulation to be valid, the unit cell cannot be defined arbitrarily, but it has to be defined such that it is bounded by planes of mirror symmetry.

For example, from solid state physics theory, one knows that it is possible to define the unit cell of a given infinite structure in different but equivalent ways. However, based on the analysis of this section, the flexibility of defining the unit cell in different ways in our TLM formulations, is only true for the complex-valued formulation. In the real-valued formulation, different unit cell definitions are, in general, not equivalent. This is illustrated in Fig. 5.7. The fact that the equations imposing the periodicity condition intrinsically contain the assumption that a perfectly symmetric scattering problem (with respect to the edge of the simulation domain) exists on “adjacent” cells, is in agreement only with the unit cell definition shown on the right hand side of Fig. 5.7. Note that this constraint makes the real-valued TLM algorithm not applicable to some PC. However, the number of structures satisfying the symmetry conditions to be well posed within its formulation is very wide.

5.2.5 Simulation Examples

In this section, the accuracy of the previously described methodology is illustrated by simulating the two-dimensional PC shown in Fig. 5.8. To facilitate the comparison of results, a photonic structure previously studied in Ref. [1] was chosen. The structure consists of dielectric cylinders embedded in air in a square lattice. The dielectric constant of the cylinders (ϵ_a) was set to 9.0 and their radius to $0.38a$, with a representing

Figure 5.7: Unit cell definitions in the complex and real-valued formulations. a) Alternative definitions are equivalent in a complex-valued formulation. b) The definition of the unit cell is restricted to be bounded by mirror symmetry planes in the real-valued formulation.

the lattice constant.

Figure 5.9(a) shows the simulation domain that the photonic structure is reduced to by applying symmetry. For convenience, the lattice constant was normalized such that $t_j = a = 1$. Fig. 5.9(b) shows the first Brillouin zone of the square lattice indicating the irreducible zone and some of the high symmetry points customarily used in the calculation of the dispersion relation of the structure. In the TLM simulations, the cell was divided into 32×32 uniformly spaced mesh points. Instead of using a stair case approach for the cylinder, the transition between the two media was smoothed by calculating an average dielectric value based on the filling ratio of each cell.

In the following discussion, only TM modes are considered; that is, the excitation is such that the electric field is kept parallel to the cylinders.

To determine a set of ω points for a particular k_j value the cell was excited with

Figure 5.8: Simulated two-dimensional PC. For the cylinders, $\epsilon_a = 9.0$ and $r_a = 0.38a$.

Figure 5.9: Reduced simulation domain a), and b) First Brillouin zone of the square lattice.

Figure 5.10: Spectral intensity at the X point produced by sampling 128 randomly selected points in the simulation domain (single cell).

a Gaussian pulse and the time-domain data stored at 128 randomly selected points. Each simulation was run for 2^{14} iterations at a maximum time step determined by the stability of the TLM method. The time-domain data for each point were then fast Fourier transformed and the spectra added. The position of the peaks in the frequency-domain indicated the frequency of the allowed modes. As a way of example, Fig. 5.10 shows the frequency domain data that was obtained by using this procedure to evaluate the allowed frequency points at the $k = X$ point (see Fig. 5.9(b)).

Figure 5.11 shows a comparison of the dispersion relations of the photonic structure shown in Fig. 5.9(a) obtained by two different methods. In the figure, the frequency has been normalized with respect to $2\pi c/a$. The dispersion curves shown in solid lines were obtained by using the PWE method and the dots correspond to the points predicted by a SCN-TLM scheme using our method to implement the periodic bound-

Figure 5.11: Dispersion relation of the PC shown in Fig. 3. Dots: Simulation results. Solid line: PWE method.

aries. As the figure shows, good agreement was found.

During the simulations, the presence of high-frequency components was not detected. In addition, the stability of the method was tested by running longer simulations (2^{16}) without problems being found. These results indicate that previously detected high frequency components leading to stability problems have been introduced by the non-passivity of the periodic boundaries.

5.3 Multi-grid Approach

In the previous section, the real-valued TLM method was presented as an alternative for reducing the computational effort when computing the dispersion relation of PC. However, from the analysis of the equations enforcing the periodicity condition, it

was shown that such an approach can only be applied to unit cells satisfying certain symmetry conditions. Thus, a more general way to proceed toward an efficient computation of the dispersion relation of PC, is to reduce the number of blocks used for the discretization of the simulation domain. There are two basic ways of accomplishing this; a) to increase the discretization step while maintaining a uniform mesh, and b) to combine regions with different discretization steps in a multi-grid fashion.

The choice of a) or b) depends on several factors. While increasing the discretization step results in fewer blocks and therefore faster simulations, it decreases the cut-off frequency of the mesh and increases node dispersion. In addition, the resolution of the mesh is decreased and fine structural details of the cell, cannot be properly represented. In a multi-grid mesh, the cut-off frequency is still limited by the biggest block present in the simulation domain, however, it provides the flexibility to properly represent localized structural details where required. This approach is particularly important for the simulation of three-dimensional unit cells of arbitrary shape and large complex structures, where the use of a uniform mesh is computationally prohibited.

5.3.1 Multi-grid Technique

The multi-grid mesh for the simulation of PC was implemented using an in-house computer program (Atar). The engineering principles of this simulation program were presented in detail in Ref. [78]. The basic idea behind the model building process is to create a complex mesh geometry using rectangular blocks of varying sizes. The model is created such that a block and its neighbors form a relatively simple topology. Each block in the mesh can have either two or four blocks on any side in what is

called a *quad tree mesh*. The mesh is automatically generated based on a set of input parameters such as the minimum and maximum block size, number of levels and location of refinements, etc. A constraint that is imposed during the building process for a periodic structure, is that there is a one-to-one correspondence between blocks on opposite sides of the simulation domain. This facilitates the connection of these blocks when enforcing the periodicity condition. In terms of the TLM method, the small and big internal faces of the blocks are connected using ideal matching transformers as in Ref. [50].

5.3.2 Simulation Examples

To illustrate the advantages and disadvantages of a multi-grid approach for simulating PC, a square lattice of circular rods embedded in air is used next as an example. The dielectric constant of the cylinders was set to $\epsilon_r = 9.0$ which corresponds to alumina rods embedded in air. The radius of the rods was set to $0.38a$, with a representing the lattice constant. The corresponding unit cell and first Brillouin zone are the same as those previously shown in Fig. 5.9.

The multi-grid mesh utilized for discretizing the unit cell is shown in Fig. 5.12. Note that an averaging procedure was applied at the interface between the air and dielectric rods to smooth the transition between the two media. The criterion applied for the discretization of the simulation domain was to limit the refinement to no more than two levels. That is, the multi-grid mesh consisted of rectangular blocks formed by the combination of three basic lengths: ΔL , $2 * \Delta L$, and $4 * \Delta L$. Where ΔL is the step size used for the discretization of the cell using a uniform mesh.

Figure 5.13 shows a comparison of the dispersion relations of the square lattice of

Figure 5.12: Multi-grid mesh used for the discretization of the unit cell. For the cylinders, $\epsilon_r = 9.0$ and $r = 0.38a$.

circular pillars obtained by applying three different methods. The dots correspond to the frequency points predicted by the complex-valued formulation using a uniform mesh. In addition, the filled-squares represent the frequency points predicted by the complex-valued formulation using the multi-grid mesh of Fig. 5.12. In the figure, the frequency has been normalized as before. As a way of comparison, the solid lines show the results predicted by the PWE.

As Fig. 5.13 shows, the overall agreement between the three different approaches is fairly good. However, the introduction of a coarser mesh has slightly degraded the accuracy of the TLM method as expected. The accuracy of the results were mainly affected by two sources of error: node dispersion and meshing error. Node dispersion relates to the fact that short wavelengths (compared with the block size) are not properly represented by the mesh. As a result, the wave velocity becomes dispersive

and dependent on the direction of the propagation vector. Meshing error refers to the degree of accuracy with which structural details of the unit cell and dense fields are represented in the mesh. Naturally, the multi-grid mesh can be devised so that the structural details of the cell are properly represented in the mesh. However, there is no guarantee that the resulting mesh will properly represent the field modes in all regions. As a consequence, field meshing error is still present in the multi-grid mesh.

While it is generally true that in a multi-grid mesh the maximum error occurs at higher frequencies, the present example shows that this is not necessarily the case. For the present dispersion relation, the worst discrepancy between frequency modes predicted by the uniform and multi-grid meshes occurred near the ends of the sixth band, with an error of approximately 2.7%. Also note that the predictions of the multi-grid mesh are in good agreement for frequencies well above the theoretical cut-off frequency of the mesh (~ 0.26 units of normalized frequency). For this example, the discretized structure consisted of 220 blocks; when compared with a 32×32 uniform mesh, the computational efficiency is increased by a factor of 4.65.

The efficiency of time-domain methods is directly related to the number of blocks used to build the model. A multi-grid mesh is therefore a natural approach to reduce the number of blocks and hence the computational effort. However, there is a large number of ways in which a multi-grid mesh can be defined to discretize a given PC. Thus, while it is not possible to characterize all the different multi-grid meshes individually, they can be characterized collectively by the minimum and maximum block size present in the mesh. The minimum block size determines the spatial resolution and the maximum block size determines the cut-off frequency of the mesh.

The real advantage of a multi-grid mesh is better appreciated in larger problems. To

Figure 5.13: Dispersion relation of the PC shown in Fig. 3. Dots: Simulation results using the R-V formulation in a uniform mesh. Filled-squares: Simulation results using a C-V formulation in a multi-grid mesh. Solid line: PWE method.

illustrate this point, the next example that is simulated is a three-dimensional one. For this case, a structure consisting of dielectric spheres embedded in air was chosen. The dielectric constant of the spheres was set to 12.0 and their radius to $0.3125a$. To also illustrate the trade-offs that come into play when multi-gridding is used, two different meshes were looked at. Figure 5.14 shows the multi-grid meshes that were used for the discretization of the unit cell. In Figs. 5.14(a) and 5.14(b), one and two levels of refinement were allowed, respectively, during the generation of the mesh. While the spatial resolution is the same for both meshes (equal to $1/32$), the cut-off frequency of the mesh in Fig. 5.14(b) is half that of the mesh in Fig. 5.14(a). In what follows, these meshes are denoted as “Multi-grid(1/16)” and “Multi-grid(1/8)” respectively, where the number in parentheses denotes the maximum block size (remember that the lattice constant has been normalized to $a = 1$). Similar to the previous example, an averaging procedure was applied to smooth the transition between the dielectric spheres and the air. Figs. 5.14(a) and 5.14(b) also show that three-dimensional structures favor the formation of cubic, rather than rectangular blocks during the building process.

Figure 5.15(a) shows the dispersion relation of the cubic lattice of dielectric spheres. The corresponding first Brillouin zone and symmetry points used as a reference for the computation of the band structure are shown in Fig. 5.15(b). The solid lines were obtained by using a computer program based on the PWE method in a uniform mesh [79]. The open circles represent the frequency points predicted by the complex-valued TLM formulation using the Multi-grid(1/16) for discretizing the unit cell. Similarly, the filled-squares represent the frequency points predicted by the complex-valued TLM formulation when the Multi-grid(1/8) is used. For the Multi-grid(1/16), the simulation domain consisted of 5776 blocks. This indicates that the computational

Figure 5.14: Multi-grid meshes used for the discretization of the unit cell. The maximum block has been limited to: a) (1/16) and b) (1/8). For the spheres, $\epsilon_r = 12.0$ and $r = 0.3125a$.

efficiency is increased by a factor of 5.7 when compared with a $(32 \times 32 \times 32)$ uniform mesh. In terms of accuracy, Fig. 5.15(a) shows that the agreement between the uniform and multi-grid meshes is fairly good up to the frequency shown. This is true despite the fact that, strictly speaking, the cut-off frequency of the Multi-grid-(1/16) is only ~ 0.46 units of normalized frequency. In calculating this frequency, a minimum of ten nodes per wavelength has been used as a reference. In addition, it has been calculated with respect to the dielectric sphere, where the shorter wavelengths (for a fixed frequency) are expected.

When the Multi-grid-(1/8) was used to discretize the unit cell, the resulting structure consisted of 3928 blocks. In this case, the computational efficiency is increased by a factor of 8.3 when compared with a $(32 \times 32 \times 32)$ uniform mesh. Note that this corresponds to computational savings of over 80%. As expected, the addition of bigger blocks in the simulation domain has further degraded the accuracy of the results. However, one can see from Fig. 5.15(a) that although the cut-off frequency of

Figure 5.15: a) Dispersion relation of the simple cubic lattice. Filled-squares: Multi-grid-(1/16) mesh. Open circles: Multi-grid-(1/8). Solid lines: PWE method using a uniform mesh and b) First Brillouin zone of the simple cubic lattice.

this mesh is only ~ 0.23 units of normalized frequency, the results are in good agreement up to at least two times this value. One can also see that the worst discrepancy between the uniform and multi-grid methods occurred near the ends of the upper most bands. That is, when one (or more) of the components of the propagation vector is equal to zero. This is again, an expected result, since it is known that block dispersion is worst under this scenario [61]. It should be pointed out that these results were obtained by using a stub-loaded node and are expected to improve, due to the superior dispersion properties of hybrid or super condense nodes [66].

Figure 5.16 shows the computational time associated with the various methods presented in this section as a function of the spatial resolution of the mesh (minimum block size). In the figure, the computational time has been normalized with respect to the complex-valued TLM method applied in a uniform mesh, which is the slowest, but most accurate scenario. This method is indicated by the dashed line in the figure. Similarly, the dot-dashed line represents the computational time of the real-valued TLM method also applied in a uniform mesh. As it was explained before, this method can reduce the computational effort by half as compared with the complex-valued formulation while retaining the same accuracy. The two remaining lines in the figure show the results of the multi-grid approach. As the figure indicates, two cases were considered. The solid and dotted lines correspond to multi-grid meshes where the resolution is varied while the maximum block size is limited to $(1/16)$ and $(1/8)$ respectively. In the figure, the corresponding locations of the multi-grid meshes shown in Fig. 5.14 are also indicated.

Figure 5.16 shows that the computational efficiency of a multi-grid approach is enhanced toward higher resolutions (smaller block size). This is particularly impor-

Figure 5.16: Computational time as a function of minimum block size for the various methods. Dashed (dot-dashed) line: Complex (real)-valued formulation in a uniform mesh. Solid and dashed lines: Complex-valued formulation in a multi-grid mesh, the maximum block size is limited to (1/16) and (1/8) respectively.

tant for the simulation of PC because it is in this region where the cut-off frequency of a uniform mesh is unnecessarily high (>1 unit of normalized frequency). This translates into the possibility of finding a good compromise between computational time and accuracy. On the contrary, the semi-flat portion of the solid line indicates that the effectiveness of the multi-grid approach decreases as the minimum block size approaches the maximum block size. This is so because as the resolution increases, it becomes increasingly difficult to accommodate more than one block at each connecting interface. Finally, it should be noted that the computational time associated with the multi-grid method could further be reduced by half, if the geometry of the unit cell allowed for the real-valued formulation to be used.

The results presented in this section indicate that a multi-grid approach can considerably reduce the simulation time that is required for computing the photonic band structure of PCs while maintaining a good accuracy.

5.4 Summary

In this Chapter, two methodologies for the optimization of the complex-valued formulation presented in Chapter 4 were presented. The optimizations were based on a real-valued formulation and multi-gridding techniques. The advantages and disadvantages of each approach were discussed and a comparison between these formulations was made from the points of view of computational expense and accuracy.

It was shown that an important property of the TLM method is its ability to simulate PC using a real-valued formulation. In this respect, the exchange algorithm relating voltage pulses between symmetry planes was derived by using a network of

matching transformers and from energy considerations. Although this formulation reduces the computational effort by half, it poses some limitations. Specifically, it was shown that in order to correctly model an infinite periodic structure, the unit cell needs to be defined such that it is bounded by planes of mirror symmetry.

In terms of computational efficiency, it was found that a combination of a real-valued method in a multi-grid mesh results in the most efficient algorithm. However, unlike the complex-valued formulation, its applicability is limited to unit cells satisfying certain geometrical details as already discussed. Finally, it was shown that a multi-grid approach can considerably reduce the computational effort required for simulating PCs. In this respect, our results indicate that a good compromise between execution time and accuracy can be found when using this approach. In addition, it was observed that the multi-grid meshes presented in this Chapter had good performance, well above the typical theoretical cut-off frequency of the mesh.

Chapter 6

Dispersion Analysis of Quad-tree Meshes

6.1 Introduction

In this Chapter, the mesh conditions that produce the least numerical dispersion error in complex meshes are determined. Specifically, a detailed analysis of how geometrical factors influence node dispersion is performed in order to obtain guidelines for use with Atar (meshing tool). These guidelines will ensure the optimum use of the various degrees of freedom offered by this meshing tool. These degrees of freedom are briefly discussed below.

The meshing tool for the TLM method that has been used for work in this thesis, is, to the best of the author's knowledge, superior to the more commonly used meshing techniques in TLM. More specifically, the majority TLM publications rely on *a*) a uniform mesh, *b*) a multi-grid mesh with one or two levels of refinement and fixed

block aspect ratios, and c) a variable or graded mesh.

The meshing tool presented in this work has the potential of taking advantage of the best features of a), b) and c) and producing a more accurate and efficient mesh. On the other hand, the great flexibility offered by the combination of these meshing techniques, can also have a negative effect. For example, it might be tempting to use “excessively” small or large block aspect ratios to represent thin layers or to minimize the number of blocks in the discretization. Thus, it is necessary to investigate the limitations that such general meshes must be subject to, in order to obtain optimum performance.

In what follows, the meshes produced by our simulation tool are referred to as *quad-tree meshes*. The reason for this choice can be found in Ref. [78].

6.2 Numerical Dispersion

In simple words, numerical dispersion can be defined as the dependence that the velocity of the propagating wave has on frequency. This is an undesired non-physical effect that occurs in most numerical methods as a result of space discretization. The reason for this is that for a given frequency and discretization step (Δl), there is a relation of the form

$$N = \frac{\lambda}{\Delta l} \quad (6.1)$$

between the wavelength of the propagating wave (λ) and the discretization step. In Eq. (6.1), N is the number of nodes that can fit in one spatial period. As the frequency increases, the wavelength decreases ($\lambda \propto 1/f$) and N does too. Consequently, there are less nodes per spatial period, and the wavelength cannot be properly repre-

sented by the mesh. As a rule of thumb, there should be no less than ten nodes per spatial period corresponding to the maximum frequency of interest. The frequency corresponding to this discretization condition is referred to as the *cut-off frequency of the mesh*.

In qualitative terms, numerical dispersion causes distortion of waveforms since the frequency dependence makes the high-frequency content of a wave lag (or lead). In the frequency-domain, numerical dispersion appears as a mislocation of the resonant frequencies.

In quantitative terms, the deviation in the wave velocity from its theoretical value due to numerical dispersion can be studied as follows. A wave of a given frequency f_0 which is excited in a discrete mesh propagates with a wavelength λ , different from the theoretical value $\lambda_0 = v/f_0$. The deviation of the wave velocity can be analysed through the difference between the magnitude of the modelled propagation vector k given by $k = 2\pi/\lambda$ and the theoretical propagation constant defined by $k_m = 2\pi f_0 \sqrt{\epsilon\mu}$. In this way, the propagation error, given as $[(|k| - k_m)/k_m]$, is used as a figure of merit to evaluate dispersion.

The major problem associated with numerical dispersion is that it causes cumulative phase error. Thus, even a small numerical dispersion error like 0.3% can lead to substantial phase error in propagating waves. For example, assuming a discretization of 20 nodes per wavelength, after a wave has propagated over a distance of 200 grid cells, the difference between the physical and numerical phases is

$$\begin{aligned}\Delta\phi &= \beta l|_{\text{physical}} - \beta l|_{\text{numerical}} = \frac{\omega}{c_0} \left(200 \frac{\lambda_0}{20} \right) - \frac{\omega}{0.997c_0} \left(200 \frac{\lambda_0}{20} \right) \\ \Delta\phi &= -10.83^\circ\end{aligned}\tag{6.2}$$

Thus, a cumulative propagation error of 10.83° is introduced by numerical dispersion over a distance of $10\lambda_0$. This phase error would be totally unacceptable if the performance of the device under simulation was based on phase cancellation (e.g. a Mach-Zehnder interferometer).

In some cases, it is possible to pre-estimate the effect of dispersion error and compensate it by using proper spatial resolution for the discretization. However, this compensation process is rarely possible since it relies on the assumption that the wave propagates in only one direction. Obviously, this assumption is rarely true in general three-dimensional problems.

6.3 Numerical Dispersion in TLM

In the TLM method, there are many factors that influence numerical dispersion. For example, in addition to frequency, dispersion is also a function of

1. Node type used in the TLM simulations.
2. The cell shape or, equivalently, the cell aspect ratio.
3. The medium relative permittivity and permeability.
4. The direction of propagation of the wave in the mesh.
5. The time step used for the simulations.

Given the many factors that influence numerical dispersion in TLM, the estimation and compensation in quad-tree meshes, is a very difficult task. An additional factor that makes prediction difficult in these meshes, is that some combinations of node

Figure 6.1: Loaded microwave waveguide used to evaluate the mesh error of the TLM and FDTD methods.

types and block aspect ratios produce bilateral dispersion. That is, for a given direction of propagation, a wave can experience phase lead or lag, as it traverses different regions of the mesh. Thus, the overall dispersion error of a mesh exhibiting bilateral dispersion, is difficult to predict and compensate for.

6.3.1 Comparison between TLM and FDTD

In Ref. [80], it was found that the TLM method can potentially be more accurate than the FDTD method because it exhibits less dispersion error. Thus, before deriving a semi-analytical expression for evaluating the dispersion error in TLM, a numerical experiment is carried out to verify the claim made in the above reference. The simulated structure is shown in Fig. 6.1. It corresponds to a two-dimensional loaded microwave waveguide.

The six lowest *TM* resonant frequencies of the resonator obtained by the FDTD and TLM methods are shown in Table 6.1 for three different levels of discretization.

Since an analytical solution is not available for this problem, the results predicted by the fine mesh are used as a reference to evaluate the error obtained by the coarse meshes. Clearly, the differences in the resonant frequencies predicted by the three meshes are due to the dispersion errors.

Frequency [GHz]	$\Delta l = 1$ mm		$\Delta l = 5$ mm		$\Delta l = 10$ mm	
	TLM	FDTD	TLM	FDTD	TLM	FDTD
f1	1.2521	1.2650	+0.002%	+3.99%	+0.004%	+9.01%
f2	1.8798	1.8982	+0.06%	+3.78%	+0.22%	+7.87%
f3	2.3175	2.3404	+0.28%	+3.59%	+0.85%	+6.90%
f4	2.5584	2.5831	+0.20%	+3.17%	+0.77%	+5.68%
f5	2.8094	2.8370	+0.16%	+3.34%	+0.59%	+5.74%
f6	3.2312	3.2627	+0.28%	+3.45%	+0.94%	+5.69%

Table 6.1: Comparison of lowest resonant modes computed by the FDTD and the TLM methods using three different meshes.

A comparison between the results obtained by the FDTD and TLM methods shows that the TLM method is potentially more accurate than the FDTD method. As a matter of fact, the results obtained by the TLM method using a discretization step of $\Delta l = 10$ mm are more accurate than those obtained by the FDTD method using a better discretization ($\Delta l = 5$ mm). Thus, these results are in agreement with those presented in Ref. [80] and corroborate the fact that TLM exhibits less node dispersion error and is therefore a more accurate method than FDTD (for the same level of spatial discretization). It should be kept in mind, however, that this example constitutes a very small sample and therefore the conclusion that TLM is more accurate than FDTD can not be considered an absolute one. Such an assessment would require an extensive comparison between the two methods which is beyond the scope of this thesis.

Figure 6.2: Coordinate system used as a reference for the dispersion analysis.

Before proceeding to the next section, the coordinate system shown in Fig. 6.2 is introduced. This coordinate system is as a reference for the analyses of dispersion error presented in the remaining of this Chapter.

6.4 The Dispersion Relation in TLM

The general procedure to compute the dispersion relation in a discrete mesh is based on evaluating the voltage at a particular node, in relation to the voltages of the six (identical) adjacent nodes. Assuming that the solution is a spatially harmonic voltage, after a little algebra, the following determinantal equation is obtained [67], [81]

$$|PQ - W| = 0 \quad (6.3)$$

where $Q = (I + S_n)T$ and $W = I + TS_nT$. In these equations, $[I]$ is the identity matrix and S_n is the frequency domain scattering matrix of the type of TLM node

used to create the mesh.

The matrix T is a propagation matrix representing the connection between nodes. Typical non-zero elements of this matrix have the form $e^{-j\beta_{ij}\Delta_i}$, where the propagation constants β_{ij} , are associated with the link-lines and thus depend on TLM parameters. The subscripts ij indicate the direction of propagation and polarization, respectively, of the associated voltage wave (see Fig. 3.3).

The matrix P represents Bloch's theorem. It relates the total voltages at one node, to the total voltages at the adjacent nodes in the periodic network of transmission lines. It contains the Cartesian components of the propagation vector $k = (k_x, k_y, k_z)$ describing phase shifts along the three coordinate directions. Thus, typical non-zero elements of this matrix are similar to those of the T matrix, except that the propagation constants are associated with the medium, rather than with the link-lines of the TLM node. Depending on the node type, the size of these matrices can range from (12×12) to (18×18) .

The dispersion of the mesh is obtained by solving numerically (or analytically when possible) Eq. (6.3) for the medium propagation constant of a plane wave of arbitrary orientation. For example, the dispersion relation of a mesh composed of cubic ($\Delta x = \Delta y = \Delta z = \Delta l$), stub-less SCN (for simulating free space) was obtained analytically in Ref. [10] as

$$\cos^2(\omega_0 \Delta t) = \frac{1}{4} [\cos(k_x \Delta l) \cos(k_y \Delta l) + \cos(k_x \Delta l) \cos(k_z \Delta l) + \cos(k_y \Delta l) \cos(k_z \Delta l) + 1] \quad (6.4)$$

where the term $\omega_0 \Delta t$ represents the phase shift per node and k_x , k_y and k_z are the components of the propagation vector. Note that equation (6.4) is the discrete

Figure 6.3: Percentage error due to dispersion for different angles of propagation and levels of discretization.

counterpart of the well-known dispersion relation of free space given by

$$\left(\frac{\omega}{c}\right)^2 = (k_x)^2 + (k_y)^2 + (k_z)^2, \quad (6.5)$$

where ω is the angular frequency and c the speed of light.

To illustrate the effect that the level of discretization has on the dispersion error, Fig. 6.3 shows the propagation error for different directions of propagation and levels of discretization obtained by solving Eq. (6.4). The details of the computations are explained later on. It is possible to extract some useful information from Fig. 6.3. For example, a TLM mesh composed of cubic, stub-less nodes does not exhibit dispersion

along the axial directions. This corresponds to the point where $\theta = 0^\circ$ in the figure. One can also see that a discretization of 20 nodes per wavelength results in a “small” percentage error of less than 0.14%. However, such a choice of discretization results in a very large number of nodes in realistic three-dimensional problems. In turn, this would lead to high memory requirements and slow simulations.

The figure also indicates that the rule of thumb discretization of 10 nodes per wavelength, results in a range of percentage error of approximately 0.5%. Based on the experience of research groups working on the TLM method, this level of discretization is considered adequate because it has been found to provide a good compromise between computational expense and accuracy. However, for large three-dimensional problems, even this degree of discretization can easily become unwieldy for modern personal computers. Thus, it is often required to minimize the number of nodes in a given discretization by using blocks whose dimensions do not satisfy the $\frac{\lambda}{10}$ condition. Note that these blocks can be strategically placed in regions of space where the fields are weak or have small spatial variations. Such is the purpose of a quad-tree mesh.

It must be emphasized that operating a mesh at frequencies above cut-off, may result in large errors. For example, according to Fig. 6.3, operating the mesh at twice its cut-off frequency (5 nodes per wavelength) would result in a propagation error of over 2.5% (an increase of over 5 times compared with the acceptable discretization condition).

6.4.1 Numerical Solution of the Dispersion Relation

Due to its complexity, the dispersion relation Eq. (6.3) must, in general, be solved numerically. As it was implied in the previous section, when solving the dispersion

relation, it is customary to relate the operating wavelength to one of the physical dimensions of the nodes comprising the mesh (ΔL). For this purpose, the operating wavelength is introduced into the dispersion relation as follows.

In the TLM method, it is a well known fact that the velocity of voltage pulses travelling along the link-lines, v_l , is twice the velocity of waves propagating in the medium with background parameters ϵ_0 and μ_0 and is given by

$$v_l = 2c = \frac{2}{\sqrt{\epsilon_0\mu_0}} \quad (6.6)$$

On the other hand, in a medium with parameters ϵ_r and μ_r , the velocity of waves propagating in the medium v_m , is given by

$$v_m = \frac{c}{\sqrt{\epsilon_r\mu_r}} \quad (6.7)$$

thus, from these equations, it follows that

$$v_m = \frac{v_l}{2\sqrt{\epsilon_r\mu_r}} \quad (6.8)$$

In addition, given that the medium propagation constant k_m , is given by $k_m = \frac{\omega_0}{v_m}$, the anticipated phase shift ϕ_s along the TLM link-lines would be

$$\phi_s = \omega_0\Delta t = k_mv_m\Delta t = k_m\frac{v_l\Delta t}{2\sqrt{\epsilon_r\mu_r}} = k_m\frac{\Delta L}{2\sqrt{\epsilon_r\mu_r}} \quad (6.9)$$

Thus, the level of spatial discretization can be described by the factor $k_m\Delta L$ appearing

in the phase shift as follows

$$k_m \Delta L = 2\pi \frac{\Delta L}{\lambda_0}. \quad (6.10)$$

For the acceptable discretization of ten nodes per wavelength, $k_m = 0.2\pi$. In this way, in solving the dispersion relation, the value of phase shift is set such that it satisfies the discretization level of interest. The amplitude of the modelled propagation constant k , is then computed from the dispersion relation for different directions of propagation, and compared to the chosen propagation constant k_m .

6.5 Numerical Dispersion of Uniform Meshes

Due to the difficulties involved in predicting dispersion error in general quad-tree meshes discussed in Sect. 6.3, a simplified approach is taken here. Initially, the analysis is done assuming a uniformly graded mesh. By uniform grading, one refers to a mesh in which the spatial discretizations in the x -, y - and z -directions ($\Delta x, \Delta y, \Delta z$) can differ, but do not change throughout the problem space resulting in non-cubic cells of equal dimensions. In addition, the mesh is assumed to be of infinite extent and the relative permittivity and relative permeability of the medium can be changed arbitrarily.

The analysis of the dispersion error as a function of the block aspect ratio presented in this section requires the repetitive solution of the dispersion relation of a TLM node. In this respect, the SSCN has been selected because a closed algebraic expression is

available for this node. The dispersion relation for the SCCN is given by [82]

$$\begin{aligned} & \cos^2 \theta - \cos \theta [\cos x(b_z - b_y) + \cos y(b_x - b_z) + \cos z(b_y - b_x)] \\ & + s_x(\cos y \cos z - 1) + s_y(\cos z \cos x - 1) + s_z(\cos x \cos y - 1) - 1 = 0 \end{aligned} \quad (6.11)$$

where $\theta = \omega \Delta t$, $x = k_x \Delta x$, $y = k_y \Delta y$, $z = k_z \Delta z$,

$$b_i = \frac{Z_{ki}}{Z_{ki} + Z_{ji}} \quad (6.12)$$

$$s_i = s_0 - 2b_j b_k - b_i \quad (6.13)$$

with indices $(i, j, k) \in \{(x, y, z), (y, z, x), (z, x, y)\}$ and

$$s_0 = b_x b_y + b_y b_z + b_z b_x. \quad (6.14)$$

Finally, Z_{ij} are the characteristic impedances of the transmission lines [66]. By solving Eq. (6.11) for various directions of propagation and block aspect ratios, the contour plots presented in the next sections are obtained.

6.5.1 Investigation of the Dispersion Error as a Function of the Block Aspect Ratio

In the simulation of large problems, it is usually advantageous to resort to non-cubic blocks for space discretization. For example, structures whose dimensions vary by various orders of magnitude in the x -, y - and z -directions, can be more conveniently discretized using non-cubic nodes ($\Delta x \neq \Delta y \neq \Delta z$). However, due to the many

degrees of freedom that exist in the way in which a non-cubic node can be formed, it is necessary to determine the shape of the nodes that result in the least dispersion. This is the purpose of this section.

However, before attempting to determine the shape of the block that introduces the least dispersion error, a systematic way to evaluate the error must be found. Given that dispersion error is a function of the direction of propagation, it would be very computationally intensive to find the propagation error for all possible combinations of directions and block aspect ratios. For this reason, one must first determine the directions of propagation for which the maximum dispersion error occurs, and limit future analyses to only those directions. Finding the directions of propagation for which the dispersion error is maximum is the purpose of the next section.

Dispersion as a function of direction of propagation

In the following analysis, the propagation error is investigated for four aspect ratios: a cubic node and three different non-cubic nodes. The aspect ratios of the non-cubic nodes are selected based on the most commonly found scenarios in quad-tree meshes. In all cases, the frequency is selected such that the condition $\frac{\lambda}{\Delta x} = 10$ is satisfied.

a) Cubic block ($\Delta x = \Delta y = \Delta z$)

As an initial approach, the dispersion error is investigated as a function of direction for a mesh composed of cubic blocks. Figure 6.4 shows the results in a contour plot for all possible directions. In the figure, the indices in square brackets represent the main directions. As the figure indicates, the propagation error due to dispersion is minimum along the axial directions $\langle 100 \rangle$, it increases as the propagation vector moves to the $\langle 110 \rangle$ directions, and reaches a maximum along the main space diagonal

Figure 6.4: Percentage error due to dispersion for different angles of propagation in a cubic mesh.

Figure 6.5: Percentage error due to dispersion for different angles of propagation in a mesh composed of non-cubic blocks ($\Delta x = \Delta y = 2\Delta z$).

[111].

b) Non-cubic block ($\Delta x = \Delta y = 2\Delta z$)

In this case, the mesh is composed of blocks which have a square face and are shorter in the third dimension. The corresponding dispersion error for this mesh is shown in Fig. 6.5. As the figure shows, for a mesh of this type, there is positive and negative dispersion. This simply indicates that the computed propagation constant can either be an overestimation or underestimation of the physical propagation constant.

For this mesh, the contour plot indicates that the maximum dispersion error occurs in the direction [110]. That is, it occurs along the diagonal of the plane formed by

Figure 6.6: Percentage error due to dispersion for different angles of propagation in a cuboid block ($2\Delta x = 2\Delta y = \Delta z$).

the two larger dimensions (Δx and Δy). In addition, the figure indicates that the minimum (absolute) error does not occur along any of the axial directions as it occurs in the cubic mesh. In this case, the minimum error occurs at some arbitrary angles.

c) Non-cubic block ($2\Delta x = 2\Delta y = \Delta z$)

In this case, the mesh is formed by blocks which have a square face as before, but are now longer in the third dimension. The corresponding dispersion error for this mesh is shown in Fig. 6.6. As the contour plot indicates, the maximum (absolute) error for this mesh occurs along the direction of the maximum block dimension (Δz). An interesting feature that can be deduced from the quasi-vertical lines is that, for

Figure 6.7: Percentage error due to dispersion for different angles of propagation in a cuboid block ($2\Delta x = \Delta y = 4\Delta z$).

this type of mesh, the dispersion error is a very weak function of ϕ . That is, the error is dominated by propagation along the largest block dimension.

d) Non-cubic block ($2\Delta x = \Delta y = 4\Delta z$)

In this case, the mesh is formed by blocks whose dimensions are all different. The corresponding dispersion error for this mesh is shown in Fig. 6.7. As the figure indicates, the maximum (absolute) error occurs along the direction of the maximum block dimension as before (note that in this case the maximum dimension is Δy). Thus, the propagation error is again dominated by propagation along the largest dimension of the block.

Figure 6.8: Reference planes used to calculate the dispersion error.

From these results, one can conclude that depending on the block aspect ratio, the maximum dispersion error can occur along an axis, along the diagonal formed by two axes, or along the main space diagonal. Thus, the analysis of the next section is restricted to those directions of propagation contained within two planes. The plane that contains the main space diagonal, formed by the angles $[\theta = 0 \dots 90^\circ, \phi = \text{atan}(\Delta y / \Delta x)]$, which is denoted as plane ONE, and the plane formed by the angles $[\theta = 90^\circ, \phi = 0 \dots 90^\circ]$, which is denoted as plane TWO. These two planes are shown by the shaded areas in Fig. 6.8.

By restricting the directions of propagation to within these planes, the error is analyzed for the main directions of propagation in the mesh. At the same time, all the directions where the maximum dispersion error is likely to occur are taken into consideration.

Determination of the optimum block aspect ratio

We are finally in a position to investigate, in a more general way, the effect that the block aspect ratio has on the dispersion error. Recall that one of the purposes

of graded and quad-tree meshes is to minimize the number of nodes used in the discretization of a problem. Two scenarios commonly used in quad-tree meshes during the discretization process are investigated here. In the first case, two of the dimensions of the blocks are increased, while keeping the third dimension constant and satisfying the acceptable discretization condition. This is similar to the way in which a variable mesh is formed.

In the second case, all the dimensions of the blocks are allowed to increase to a larger value than the dimension satisfying the acceptable discretization condition. This is similar to the way in which a multi-grid mesh is formed. These two cases of practical interest are investigated next.

a) Optimum block aspect ratio around the acceptable discretization condition

First, the effect of distorting the blocks around the acceptable discretization condition is investigated. That is, the investigation focuses on non-cubic nodes where, for example, the Δz dimension satisfies two conditions: *a)* It is kept constant (e.g. $\Delta z = 1$) while Δx and Δy are allowed to change, and *b)* it satisfies the acceptable discretization condition ($\frac{\lambda}{\Delta z} = 10$). In addition, based on the previous discussion, it is obvious that the main interest is in those cases where $\Delta x > \Delta z$ and $\Delta y > \Delta z$.

The procedure for calculating the dispersion error is to sweep the propagation vector along planes ONE and TWO (c.f. Fig. 6.8), and to obtain the *error range* for each block aspect ratio. That is, for a block of given dimensions, the propagation vector is swept for each plane and the error range calculated as the difference between the (absolute) minimum and maximum errors. The results are shown in Figs. 6.9(a) and 6.9(b) as contour plots for planes ONE and TWO, respectively.

Useful information can be extracted from Figs. 6.9(a) and 6.9(b). For example, it

a)

b)

Figure 6.9: Range of propagation error due to dispersion for different block aspect ratios. The direction of the propagation vector is along: a) plane ONE and b) plane TWO.

can be seen from both figures that the contours are more closely spaced in the vertical and horizontal directions. In terms of block shapes, this means that the dispersion error increases more sharply for “needle” type blocks. That is, blocks where one of the dimensions is increased while the other two stay constant. In this respect, it is interesting to note that a block with dimensions $\Delta x = 1, \Delta y = 4, \Delta z = 1$ has almost as much as twice the dispersion error of a block of space with dimensions $\Delta x = 4, \Delta y = 4, \Delta z = 1$. This is indeed an unexpected result considering that in the former case, two of the dimensions satisfy the acceptable discretization condition (Δx and Δz) while in the latter, only one dimension does (Δz).

Another important observation that can be made from Figs. 6.9(a) and 6.9(b) is that the contours are further apart in the direction along one of the diagonals. This corresponds to blocks of space where two of the dimensions are equal and increased at the same ratio while the other one stays constant. In other words, blocks of space with an increasing square face and fixed longitudinal dimension are less prone to dispersion error. It should be noted that, in this case, the longitudinal dimension (Δz) is shorter than that of the square face (Δx and Δy).

b) Optimum block aspect ratio away from the acceptable discretization condition

In this section, the optimum shape that blocks must have when they are distorted away from the acceptable discretization condition is investigated. That is, we look for an answer to the question: When blocks whose all dimensions exceed the acceptable discretization condition are admitted in the mesh, what is the shape of the block introducing the least dispersion error?

To answer this question, one must proceed in a similar way as in the previous section. The main difference is that for this particular case, the frequency of interest

Figure 6.10: Propagation error due to dispersion for a block of arbitrary aspect ratio and longitudinal dimension twice that satisfying the acceptable discretization condition.

is chosen such that Δz satisfies the discretization condition $\frac{\lambda}{\Delta z} = 5$. That is, the search is now for the shape of the block that introduces the minimum dispersion error for a block of space whose longitudinal dimension is twice that satisfying the acceptable discretization condition. Proceeding as in part a), first the error range for planes ONE and TWO is found. This produces similar plots to those shown in Figs. 6.9(a) and 6.9(b). Next, the two resulting contour plots are merged into one by comparing them point to point and selecting the bigger dispersion error. The result is shown in Fig. 6.10 as a contour plot.

Figure 6.10 provides the answer to our original question. Once blocks whose dimen-

sions do not satisfy the acceptable discretization condition are permitted in the mesh, their ideal shape should be *cubic* for minimum dispersion error to be introduced.

From the results obtained in this section one can extract the following guidelines to be applied during the creation of quad-tree meshes:

1. Keep blocks which do not satisfy the acceptable discretization condition as cubic as much as possible in the mesh.
2. When non-cubic blocks are part of the mesh, avoid the introduction of elongated (needle type) blocks as much as possible. These blocks introduce a large dispersion error, particularly in the direction of the largest dimension.
3. Preferably, introduce non-cubic blocks with a large cross-section area, they introduce less dispersion error than elongated ones.

It should be kept in mind that these guidelines describing the optimum block aspect ratio have been obtained by analyzing the dispersion error of blocks of varying shapes. However, as the shape of the block changes, so does the discretization condition (number of nodes per wavelength) associated with the dimensions of the block which are not held constant at the acceptable discretization condition. As a result, the dispersion error computed in this way, has also the intrinsic contribution made by this change of discretization condition. In order to eliminate the contribution made by the discretization condition to the dispersion error, and isolate that made by the block's shape, it would be necessary to use blocks where the contribution of discretization is minimized by $\frac{\Delta l}{\lambda} \rightarrow 0$. In our analysis, we ignored this effect because we were only interested in realistic blocks which are likely to have dimensions comparable to that related to the acceptable discretization condition.

It should also be kept in mind that these guidelines were obtained by assuming a mesh of infinite extent and hence contain the intrinsic assumption that a block of given aspect ratio and material parameters would exhibit similar dispersion properties regardless of the properties of the blocks adjacent to it. In other words, by extrapolating these results to more general meshes, it is assumed that any given block would produce the same dispersion error when present in a uniform, variable, or quad-tree mesh.

By considering a unit cell composed of an agglomerate of five blocks, a more fundamental analysis of the dispersion properties of quad-tree meshes is performed in the next section.

6.6 Dispersion Relation of Quad-tree Meshes

In this section, the dispersion properties of quad-tree meshes are investigated taking a more realistic approach. That is, following a similar procedure to that described in Sect. 6.4, a matrix formulation of the dispersion relation of an infinite quad-tree mesh is first derived, and then solved numerically by minimizing a determinantal equation.

6.6.1 Derivation of the Dispersion Relation of a Quad-tree Mesh

Consider an array of blocks as that shown in Fig. 6.11, which is denoted as array a . This array is some arbitrary agglomerate of five blocks in an infinite TLM mesh composed of identical arrays of this type. Each node in the array has, in general, 12 transmission-lines and six stubs. The scattered voltages at node a are related to the

Figure 6.11: Basic block array for the analysis of dispersion in a quad-tree mesh.

incident voltages by

$$[V_a]^r = [S][V_a]^i \quad (6.15)$$

where $[V_a]^r$ and $[V_a]^i$ are 60-element column vectors of incident and reflected voltage pulses respectively, and $[S]$ is a 60×60 scattering matrix given by

$$[S] = \begin{bmatrix} [S_1] & [0] & [0] & [0] & [0] \\ [0] & [S_2] & [0] & [0] & [0] \\ [0] & [0] & [S_3] & [0] & [0] \\ [0] & [0] & [0] & [S_4] & [0] \\ [0] & [0] & [0] & [0] & [S_5] \end{bmatrix} \quad (6.16)$$

where $[0]$ is a 12×12 null matrix and $[S_i]$, $i \in \{1 \cdots 5\}$, is a 12×12 scattering matrix of the i^{th} block. Note that even in the presence of stubs, the size of $[S_i]$ is determined by the twelve link-lines composing each node. This is so because the stubs are only

connected internally to the node they belong to, and do not exchange voltage pulses with the adjacent blocks. The elements of $[S_i]$ can be found from the general matrix given in Ref. [83] and by using a procedure similar to that described in Ref. [81] to reduce the 18×18 original matrix to a 12×12 matrix.

To proceed with the derivation of the dispersion relation, let b denote some hypothetical array which is formed by the transmission-lines of the nodes surrounding array a that can be reached at time $n\Delta t + \Delta t$ by the pulses scattered from the external link-lines of the nodes in a at time $n\Delta t$. Assuming a monochromatic plane wave, one can define a 60×60 matrix $[P]$ which establishes a relationship between the scattered pulses from a , to those scattered from b , as follows

$$[V_b]^r = [P][V_a]^r \quad (6.17)$$

by inserting (6.15) into (6.17) gives

$$[V_b]^r = [P][S][V_a]^i \quad (6.18)$$

To proceed, let us define two new 60×60 matrices which relate the incident voltage pulses at a , to the reflected voltage pulses from a and b such that

$$[V_a]^i = [T_1][V_a]^r + [T_2][V_b]^r \quad (6.19)$$

In this equation, $[T_1]$ is a matrix containing information about the internal connection of the blocks in array a , and T_2 is a similar matrix containing information about the (external) connection between the link-lines of array a with those of array b . Inserting

(6.19) into (6.18) gives,

$$[V_b]^r = [P][S][T_1][V_a]^r + [P][S][T_2][V_b]^r. \quad (6.20)$$

Finally, one can relate the reflected pulses in a to those in b by utilizing Eq. (6.17), in this way, Eq. (6.20) reduces to

$$[V_b]^r = [P][S][T_1][P]^{-1}[V_b]^r + [P][S][T_2][V_b]^r \quad (6.21)$$

where $[P]^{-1}$ is the inverse matrix of $[P]$. This equation has a non-trivial solution only if the determinant vanishes, that is, only if

$$\det[A] = 0 \quad (6.22)$$

where

$$A = ([P][S][T_1][P]^{-1} + [P][S][T_2]) - [I] \quad (6.23)$$

and $[I]$ is a 60×60 identity matrix. The above condition is the dispersion relation for a quad-tree mesh which, to the best of the author's knowledge, had not been derived previously.

Note that the elements of matrices $[P]$, $[T_1]$ and $[T_2]$ still remain to be found. However, before the explicit elements of these matrices can be determined, a scattering matrix formulation of the connecting interface between the five nodes comprising array a must be obtained.

6.6.2 Derivation of the Scattering Matrix at a Quad-tree Mesh Interface

In Sect. 3.6.1, the equations relating the incident and reflected pulses at the interface formed between two regions of space with different spatial resolutions were shown. However, in order to be consistent with the matrix formulation of the dispersion relation presented in the previous section, the scattering matrix that describes the connection between blocks must be expressed in terms of its S -parameters. Taking as a reference Fig. 6.11, the connection of matching transformers can be seen as a five port network as shown in Fig. 6.12.

Note that the S -parameter formulation of the connecting interface is totally compatible with the TLM method. For example, the voltage pulses reflected from their respective nodes travel across the link-lines to become incident upon the connecting interface where they undergo scattering according to the S -matrix of the network. The resulting scattered pulses into each port, become incident on the respective node at the next time step. As shown in Fig. 6.12, the impedances of the transmission lines at each port have been labelled with two subscripts as originally shown in Fig. 6.11.

The calculation of the S -parameters follows a standard procedure [84]. For example, port 1 is coupled to itself and to the other ports by the S_{n1} parameters, where $n = 1...5$. Note that S_{11} is the reflection coefficient at port 1 and is given by

$$S_{11} = \frac{Z_{T1} - Z_{00}^*}{Z_{T1} + Z_{00}} \quad (6.24)$$

where Z_{T1} is the input impedance to the network at port 1 as shown schematically in Fig. 6.12 and Z_{00}^* is the complex conjugate of the Z_{00} impedance. The remaining S_{n1} -

Figure 6.12: Equivalent five port network at the connection interface.

parameters represent the forward transmission coefficients from port 1 to all others. These can be calculated from:

$$S_{n1} = \frac{b_{pn}}{a_{p1}} \quad (6.25)$$

where $n=2$ to 5 . The terms a_{p1} and b_{pn} represent incident and reflected power waves respectively. They are defined such that the quantity $\frac{1}{2}|a_{p1}|^2$ is equal to the power available from the source connected at the input of port 1, and b_{pn} is a reflected power wave on the impedance at the n -th port ($n=2$ to 5). These terms can be calculated from

$$a_{p1} = \frac{1}{2\sqrt{R_1}}(V_1 + Z_{00}) \quad (6.26)$$

$$b_{pn} = \frac{1}{2\sqrt{R_n}}(V_n - Z_n^* I_n). \quad (6.27)$$

where $R_n = \text{Re}[Z_n^*]$ and V_n is the voltage drop on the impedance associated with the n -th port. To illustrate the S -parameter calculation process more clearly, consider for example the computation of S_{21} . From Eq. (6.25) we have $S_{21} = b_{p2}/a_{p1}$, where

Figure 6.13: Electrical circuit illustrating the voltages and currents required for the calculation of S_{21} .

a_{p1} is as given by Eq. (6.26) with $R_1 = \text{Re}[Z_{00}]$. From Eq. (6.27), it follows that,

$$b_{p2} = \frac{1}{2\sqrt{R_2}}(V_2 - Z_{12}^* I_2), \quad (6.28)$$

where $R_2 = \text{Re}[Z_{12}]$ and V_1 , V_2 , I_1 and I_2 would be as calculated from the circuit shown in Fig. 6.13. Note that in this circuit, the voltage source connected at the input of port 1, is given by twice the scattered (reflected) pulse from the (0,0) node, as predicted by transmission line theory [61]. After some straightforward but tedious algebra, the S_{21} parameter is found to be

$$S_{21} = \frac{2\sqrt{Z_{12}}\sqrt{Z_{00}}\Delta x_0\Delta y_0\Delta x_1\Delta y_2 [Z_{21}(\Delta x_2)^2 + Z_{11}(\Delta x_1)^2]}{A + B + C + D}, \quad (6.29)$$

where

$$\begin{aligned}
A &= (\Delta y_0)^2 (\Delta x_1)^2 Z_{12} [(\Delta x_2)^2 Z_{21} + (\Delta x_1)^2 Z_{11}], \\
B &= (\Delta y_0)^2 (\Delta x_2)^2 Z_{22} [(\Delta x_2)^2 Z_{21} + (\Delta x_1)^2 Z_{11}], \\
C &= (\Delta x_0)^2 (\Delta y_1)^2 Z_{00} [(\Delta x_2)^2 Z_{22} + (\Delta x_1)^2 Z_{12}], \\
D &= (\Delta x_0)^2 (\Delta y_2)^2 Z_{00} [(\Delta x_2)^2 Z_{21} + (\Delta x_1)^2 Z_{11}].
\end{aligned}$$

Equation (6.29) is a general equation that allows the calculation of the S_{21} parameter for an interface consisting of different block sizes. The remaining S -parameters are calculated in a similar way. After the 25 entries of the scattering matrix are calculated, the reflected power waves into each port can be calculated as a function of the input power waves using $b_p = [S_v]a_p$, where a_p and b_p are column vectors containing the incident and reflected power waves at each port. For incorporation into the TLM method, the power waves must be written in terms of the incident and reflected voltage pulses as follows

$$V^r = \frac{Z_n^*}{\sqrt{R_n}} a_{pn}, \quad V^i = \frac{Z_n}{\sqrt{R_n}} b_{pn}. \quad (6.30)$$

Note that in these equations, the *scattered* voltage pulses from the nodes become the *incident* power waves at the interface, and that the *reflected* power waves from the interface, become the *incident* voltage pulse at the node at the next time step.

The 5×5 scattering matrix obtained in this section is denoted as $[S_v]$, where the subscript indicates that the matrix corresponds to the vertical polarization. Following a similar procedure, a matrix $[S_h]$ must be obtained for the horizontal polarization

across the interface.

6.6.3 Filling the Matrices

For the following analysis, the blocks in array a are numbered according to Fig. 6.14(a), and the link-lines at each node are numbered according to Fig. 6.14(b).

Let us begin by finding the elements of matrix $[P]$. This matrix was introduced in Eq. (6.17). It was defined as a matrix which, under monochromatic conditions, relates the reflected pulses between the a and b arrays. Thus, for a plane wave with arbitrary propagation constant ($k^2 = k_x^2 + k_y^2 + k_z^2$), there must be a fixed phase relationship between the pulses in a to those in b . For example, taken as a reference

a)

b)

Figure 6.14: Numbering of a) nodes and b) link-lines used as a reference in the derivation of the dispersion relation.

node number 2, the elements in the $[P]$ matrix related to this node are as follow

$$\begin{aligned}
P(V_3^{B_2}, V_{11}^{B_3}) &= e^{ik_x(\Delta x_1 + \Delta x_2)} & P(V_6^{B_2}, V_{10}^{B_3}) &= e^{ik_x(\Delta x_1 + \Delta x_2)} \\
P(V_{11}^{B_2}, V_3^{B_3}) &= e^{-ik_x(\Delta x_1 + \Delta x_2)} & P(V_{10}^{B_2}, V_6^{B_3}) &= e^{-ik_x(\Delta x_1 + \Delta x_2)} \\
P(V_1^{B_2}, V_{12}^{B_3}) &= e^{ik_y(\Delta y_1 + \Delta y_2)} & P(V_{12}^{B_2}, V_1^{B_3}) &= e^{-ik_y(\Delta y_1 + \Delta y_2)} \\
P(V_5^{B_2}, V_7^{B_3}) &= e^{ik_y(\Delta y_1 + \Delta y_2)} & P(V_7^{B_2}, V_5^{B_3}) &= e^{-ik_y(\Delta y_1 + \Delta y_2)} \\
P(V_2^{B_2}, V_9^{B_1}) &= S_h(1, 2)e^{ik_z(\Delta Z + \delta z)} & P(V_9^{B_2}, V_2^{B_1}) &= S_h(1, 2)e^{-ik_z(\Delta Z + \delta z)} \\
P(V_4^{B_2}, V_8^{B_1}) &= S_v(1, 2)e^{ik_z(\Delta Z + \delta z)} & P(V_8^{B_2}, V_4^{B_1}) &= S_v(1, 2)e^{-ik_z(\Delta Z + \delta z)} \\
P(V_2^{B_2}, V_2^{B_2}) &= S_h(2, 2) & P(V_2^{B_2}, V_2^{B_3}) &= S_h(3, 2) \\
P(V_2^{B_2}, V_2^{B_4}) &= S_h(4, 2) & P(V_2^{B_2}, V_2^{B_5}) &= S_h(5, 2) \\
P(V_9^{B_2}, V_9^{B_2}) &= S_h(2, 2) & P(V_9^{B_2}, V_9^{B_3}) &= S_h(3, 2) \\
P(V_9^{B_2}, V_9^{B_4}) &= S_h(4, 2) & P(V_9^{B_2}, V_9^{B_5}) &= S_h(5, 2) \\
P(V_4^{B_2}, V_4^{B_2}) &= S_v(2, 2) & P(V_4^{B_2}, V_4^{B_3}) &= S_v(3, 2) \\
P(V_4^{B_2}, V_4^{B_4}) &= S_v(4, 2) & P(V_4^{B_2}, V_4^{B_5}) &= S_v(5, 2) \\
P(V_8^{B_2}, V_8^{B_2}) &= S_v(2, 2) & P(V_8^{B_2}, V_8^{B_3}) &= S_v(3, 2) \\
P(V_8^{B_2}, V_8^{B_4}) &= S_v(4, 2) & P(V_8^{B_2}, V_8^{B_5}) &= S_v(5, 2).
\end{aligned}$$

The elements inside the parenthesis of P indicate the connection between the link-lines of the various blocks. For example, $P(V_8^{B_2}, V_4^{B_1})$ refers to the element of the matrix connecting the link-line number 8 of block 2, to the link-line number 4 of block 1. S_v and S_h are the scattering matrices of the vertical and horizontal polarizations derived in Sect. 6.6.2. The numbers inside the parenthesis indicate the S -parameter between ports. For example, $S_v(4, 2)$ is the S_{42} parameter of the vertical polarization between ports (nodes) 2 and 4.

To complete the elements of matrix $[P]$, similar entries are required for the four

remaining nodes. A useful property of this matrix is that because one is dealing with a lossless network, the total reflected power from array a must be equal to the total reflected power in array b (see Eq. (6.17)). This results in the unitary condition for the matrix $[P]$ such that $[P] \cdot [P]^\dagger = [I]$, where $(\dagger)$ denotes the conjugate transpose of $[P]$. This property is useful to verify that the elements of the matrix have been determined correctly.

Now we proceed to determine the elements of $[T_1]$. Recall that this matrix was introduced in Eq. (6.19) to define a relationship between the reflected and incident voltage pulses in array a . Thus, this matrix contains information about the internal connection between the link-lines of the nodes in array a . As before, using as an example the matrix elements corresponding to node number 2, the required elements are as follows

$$\begin{aligned}
T_1(V_1^{B_2}, V_{12}^{B_4}) &= e^{-i\phi_s} & T_1(V_5^{B_2}, V_7^{B_4}) &= e^{-i\phi_s} \\
T_1(V_3^{B_2}, V_{11}^{B_3}) &= e^{-i\phi_s} & T_1(V_6^{B_2}, V_{10}^{B_3}) &= e^{-i\phi_s} \\
T_1(V_8^{B_2}, V_4^{B_1}) &= S_v(2, 1)e^{-i\phi_s} & T_1(V_8^{B_2}, V_8^{B_2}) &= S_v(2, 2)e^{-i\phi_s} \\
T_1(V_8^{B_2}, V_8^{B_3}) &= S_v(2, 3)e^{-i\phi_s} & T_1(V_8^{B_2}, V_8^{B_4}) &= S_v(2, 4)e^{-i\phi_s} \\
T_1(V_8^{B_2}, V_8^{B_5}) &= S_v(2, 5)e^{-i\phi_s} & T_1(V_9^{B_2}, V_2^{B_1}) &= S_h(2, 1)e^{-i\phi_s} \\
T_1(V_9^{B_2}, V_9^{B_2}) &= S_h(2, 2)e^{-i\phi_s} & T_1(V_9^{B_2}, V_9^{B_3}) &= S_h(2, 3)e^{-i\phi_s} \\
T_1(V_9^{B_2}, V_9^{B_4}) &= S_h(2, 4)e^{-i\phi_s} & T_1(V_9^{B_2}, V_9^{B_5}) &= S_h(3, 5)e^{-i\phi_s}
\end{aligned}$$

where the notation and numbering scheme are the same as previously described. In these matrix elements, ϕ_s is the phase shift that the voltage pulses undergo in one time step and is given by $\phi_s = \omega\Delta t$, where ω is the angular frequency of the plane wave. By considering the relative position of the other blocks in the array, similar entries

corresponding to the internal connections of blocks 1, 3, 4 and 5 can be obtained.

Finally, we now proceed to find the elements of matrix $[T_2]$. Similarly to $[T_1]$, matrix $[T_2]$ was introduced in Eq. (6.19). The elements of this matrix were defined such that they connect the reflected pulses from b , to those incident in a . That is, it connects the external link-lines of array a , to those of b . To define the elements of $[T_2]$, recall that the infinite mesh is composed of a periodic repetition of array a . In addition, also recall that array b was defined as being composed of those link-lines which can be reached by the pulses scattered from a in one time step. These two facts imply that the reflected and incident pulses in arrays a and b can be related by the phase shift that the pulses undergo in one time step. This allows to define $[T_2]$ as a diagonal matrix of the for

$$[T_2] = [I]e^{-i\phi_s} \quad (6.31)$$

where $[I]$ is a 60×60 identity matrix. However, given that the internal link-lines of the nodes in a have already been connected by $[T_1]$, one must remove the appropriate entries from $[T_2]$. For example, taking once again node 2 as a reference, the following elements of $[T_2]$ must be set to zero

$$\begin{aligned} T_2(V_8^{B_2}, V_8^{B_2}) &= 0 & T_2(V_9^{B_2}, V_9^{B_2}) &= 0 \\ T_2(V_3^{B_2}, V_3^{B_2}) &= 0 & T_2(V_6^{B_2}, V_5^{B_2}) &= 0 \\ T_2(V_5^{B_2}, V_6^{B_2}) &= 0 & T_2(V_1^{B_2}, V_1^{B_2}) &= 0 \end{aligned}$$

similarly, by using Figs. 6.14 as a reference, the zero elements corresponding to the internal connections of the link-lines of nodes 1, 3, 4 and 5 can be found. This

completes the description of the matrices appearing in the dispersion relation, we now proceed to solve them.

6.6.4 Numerical Solution of the Quad-tree Mesh Dispersion Relation

Due to its complexity, the dispersion relation Eq. (6.22) can only be solved numerically. As seen from the matrices derived in the previous section, the dispersion relation is an implicit function of the mesh propagation constant in the three directions (k_x, k_y, k_z) , the dimensions of the small $(\Delta x_1, \Delta x_2, \Delta y_1, \Delta y_2, \delta z)$ and big blocks $(\Delta X, \Delta Y, \Delta Z)$, the frequency and time step the mesh is operated at $(\phi_s = \omega \Delta t)$ and the constitutive parameters of the medium ϵ_r and μ_r (through $[S]$).

In the next sections, the dispersion of a quad-tree mesh is obtained by solving numerically the determinantal equation (6.22) for the mesh propagation constant of an arbitrary plane wave. This is done by finding the values of k_x , k_y and k_z that minimize the absolute value of the determinant in (6.22) for a given wave orientation. More specifically, after the operating wavelength is defined by the discretization condition (6.10), the wave orientation is chosen by varying θ and ϕ in Fig. 6.2. The components of the wave vector for a particular orientation thus obtained, are used as an initial guess for the minimization problem. For the actual minimization of the determinant, the built-in function *fminunc()* in MATLAB is used. After the minimization problem is solved, the dispersion error is found as the error between the mesh propagation constant found by the minimization process and the actual propagation constant as explained Sect. 6.2.

6.6.5 Dispersion Analysis of Quad-tree Meshes

In this section, the performance of quad-tree meshes is analysed. As it was pointed out in the previous section, there are many factors which influence dispersion error in quad-tree meshes. For this reason, we will restrict our efforts to study some typical scenarios that appear in practical quad-tree meshes. Unless otherwise stated, the same time step is used for all simulations presented in this section. It was determined as the maximum time step which guarantees unconditional stability for all the meshes that are presented. In addition, all calculations have been done for free-space ($\mu_r = \epsilon_r = 1$) and satisfying the discretization condition $\frac{\Delta X}{\lambda} = \frac{1}{10}$.

The first case of interest is to investigate the performance of a quad-tree mesh as such. That is, for a quad-tree mesh composed of blocks of different sizes, it is of interest to find the optimum combination of blocks which results in the least dispersion error. This is the purpose of the next section.

a) Determination of the optimum quad-tree mesh configuration

To determine the combination of blocks that determine the minimum node dispersion in a multi-grid mesh, the following approach is taken. In previous sections it was found that cubic blocks result in the minimum dispersion. Thus, the approach that is taken here consists of using square shapes for the faces of the small and big blocks that are connected at the interface, and to only vary their longitudinal dimensions (ΔZ and δz). In addition, the variations in the z -direction are done at half or integer multiples of the ΔX (or ΔY)-dimension because this would favor the formation of cubic blocks in other parts of the mesh. In this way, three scenarios of interest result. In the three cases, the following parameters are used: $\Delta X = \Delta Y$, $\Delta x_1 = \Delta x_2 = \Delta X/2$, $\Delta y_1 = \Delta y_2 = \Delta Y/2$. The longitudinal dimensions of the blocks are set as follows:

- a) The cells span a distance equal to ΔX in the z -direction ($\Delta Z = \delta z = \Delta X/2$).
- b) The cells span a distance equal to $\frac{3}{2}\Delta X$ in the z -direction ($\Delta Z = 2\delta z = \Delta X$).
- c) The cells span a distance equal to $2\Delta X$ in the z -direction ($\Delta Z = \delta z = \Delta X$).

These configurations are shown schematically in Fig. 6.15.

The dispersion error as a function of the direction of propagation corresponding to each case is shown from top to bottom in Fig. 6.16. This figure shows some interesting results. First of all, one can see that the configuration which produces the minimum dispersion is the one in which the longitudinal dimension of the blocks is the same (case a). This is an expected result since, from the results in Sect. 6.5, we know that the shape of the blocks involved in this configuration are ideal for minimum dispersion. However, somewhat surprisingly is the fact that the combined dispersion errors of the blocks results in zero dispersion along the z -direction (perpendicular to the interface).

In case b), the absolute dispersion error increases in all directions, particularly in the z -direction. Again, this is an expected result because the dimension of the big blocks was increased in this direction. However, it is interesting to note that in this configuration, the propagation error is still not predominant in this direction. As a matter of fact, the figure shows that the propagation error is approximately the same in the directions parallel and perpendicular to the connecting interface. This is an indication that adding smaller blocks in an otherwise uniform mesh composed of blocks satisfying the acceptable discretization condition, does reduce dispersion error. This result will be verified for other scenarios later.

Finally, the figure shows that the configuration presented in c) leads to considerably larger errors compared with the previous cases. In addition, it shows that the error

Figure 6.15: Basic quad-tree mesh configurations studied. In all cases $\Delta X = \Delta Y$, $\Delta x_1 = \Delta x_2 = \Delta X/2$, $\Delta y_1 = \Delta y_2 = \Delta Y/2$, and the longitudinal dimensions of the blocks are set as follows: a) $\Delta Z = \delta z = \Delta X/2$, b) $\Delta Z = 2\delta z = \Delta X$, c) $\Delta Z = \delta z = \Delta X$.

Figure 6.16: Comparison of the dispersion error between three different configurations of a quad-tree mesh. See text for details.

is predominant in the z -direction. This is of course, a result of having increased the dimensions of the small blocks in the z -direction, which resulted in needle type blocks. Thus, the advantage of using this configuration to span more computational volume (and thus reduce the number of nodes) is diminished by the resulting higher dispersion error in the z -direction.

While it is obvious that the choice of configuration depends on the desired accuracy of the particular simulation, based on these results one can conclude that the configurations presented in a) and b) offer a better discretization alternative, from the point of view of dispersion error, than that presented in c). However, case a) only spans the same distance in the z -direction than it does in the x and y -directions. Thus, it is not very justifiable from the point of view that one of the reasons behind quad-tree meshing, is to use less blocks to discretize a given computational volume. Therefore, the configuration presented in b) can be regarded as the optimum one because it offers a good compromise between dispersion error and spanned computational volume. As previously mentioned, an important additional advantage of this configuration is that it favors the formation of cubic blocks in other parts of the mesh, which as found in Sect. 6.5, are ideal from the view point of dispersion. In what follows, we will focus on this configuration.

b) Comparison of quad-tree meshes with uniform cubic meshes

It is a common practice to state that for meshes composed of blocks of different sizes, the cut-off frequency of the mesh is simply determined by the biggest block present in the mesh. Although this is somewhat intuitive, a verification for this statement has not been provided. Furthermore, in the previous section, it was shown that the effect of adding smaller blocks to an otherwise uniform mesh of blocks satisfy-

ing the acceptable discretization condition, was to decrease the dispersion error. In this section, this effect is investigated in more detail by comparing the dispersion properties of quad-tree meshes with those of uniform cubic meshes.

The uniform meshes that the quad-tree mesh is compared to are those which would be obtained from the cubic blocks comprising the quad-tree mesh (case b in the previous section). In addition, the mesh is analyzed for two spatial resolutions. In the first case, the cut-off frequency of the mesh is determined by the coarse mesh such that $\frac{\Delta X}{\lambda} = \frac{1}{10}$. In the second case, the cut-off frequency of the mesh is assumed to be determined by the small blocks by setting $\frac{\Delta X}{\lambda} = \frac{1}{5}$. Note that the second condition is equivalent to $\frac{\Delta x_1}{\lambda} = \frac{1}{10}$. In this way, the performance of the quad-tree mesh can easily be compared with that of the uniform meshes resulting from the small and big blocks it is composed of.

The propagation error as a function of the direction of propagation for the case when the propagation vector is contained on a plane parallel to the connecting interface is shown in Fig. 6.17. This figure shows some interesting results. For the $\frac{\Delta X}{\lambda} = \frac{1}{5}$ discretization, we can see that the small blocks in the quad-tree meshes do help to decrease the overall dispersion error. The results for the finer resolution ($\frac{\Delta X}{\lambda} = \frac{1}{10}$) show the same tendency. The results are summarized in Table 6.2.

Mesh	Resolution	min. error %	max. error %	range %	ave. error %
quad-tree	$\frac{\Delta X}{\lambda} = \frac{1}{5}$	0.54	-3.03	3.57	1.36
uniform	$\frac{\Delta X}{\lambda} = \frac{1}{5}$	-0.78	-4.4	3.62	2.70
quad-tree	$\frac{\Delta X}{\lambda} = \frac{1}{10}$	0.11	-0.81	0.92	0.37
uniform	$\frac{\Delta X}{\lambda} = \frac{1}{10}$	-0.20	-1.2	1.0	0.72

Table 6.2: Summary of results corresponding to Fig. 6.17.

Figure 6.17: a) Comparison of the dispersion error between a quad-tree mesh and the uniform meshes resulting from the blocks it is composed of. b) Top view of a quad-tree mesh illustrating the direction of propagation ($\phi = 0 \dots 90^\circ$ and $\theta = 0^\circ$).

Figure 6.18: a) Comparison of the dispersion error between a quad-tree mesh and the uniform meshes resulting from the blocks it is composed of. b) Top view of a quad-tree mesh illustrating the direction of propagation, ($\theta = 0 \dots 90^\circ$ and $\phi = 0^\circ$).

By comparing the entries of Table 6.2, it is obvious that the dispersion error is smaller in the quad-tree meshes than in the uniform meshes. For example, in the present scenario, the presence of the small blocks in the quad-tree mesh reduce approximately by half the average error that would be present in a uniform mesh composed of big blocks only.

Figure 6.18 shows the dispersion error as a function of the direction of propagation for the case when the propagation vector is varied on a plane perpendicular to the connecting interface. The results corresponding to this figure are summarized in Table 6.3.

Note that due to the rotational symmetry of the structure, the results for the uniform mesh must be symmetric (and identical to those presented in Fig. 6.17).

Mesh	Resolution	min. error %	max. error %	range %	ave. error %
quad-tree	$\frac{\Delta x}{\lambda} = \frac{1}{5}$	0.07	-3.03	3.1	1.55
uniform	$\frac{\Delta x}{\lambda} = \frac{1}{5}$	-0.78	-4.4	3.62	2.70
quad-tree	$\frac{\Delta x}{\lambda} = \frac{1}{10}$	0.01	-0.8	0.81	0.41
uniform	$\frac{\Delta x}{\lambda} = \frac{1}{10}$	-0.20	-1.2	1.0	0.72

Table 6.3: Summary of results corresponding to Fig. 6.18.

However, this is not necessarily the case for the quad-tree mesh because the structure is only symmetric in the x - and y -directions.

In spite of this, the symmetry in the figure indicates that for this particular set of parameters, the contribution to the dispersion error by the small blocks (and the matching transformers) is very similar in the directions parallel ($\theta = 90^\circ, \phi = 0^\circ$) and perpendicular ($\theta = \phi = 0^\circ$) to the connecting interface. Nevertheless, Table 6.3 shows that the average error for this case is slightly higher than in the previous case. This is so because the dispersion error has shifted towards more negative values with respect to the previous case.

Finally, Fig. 6.19 shows the propagation error as a function of the direction of propagation for the case when the propagation vector is varied on a plane which contains the main space diagonal of the big blocks comprising the quad-tree mesh.

The results corresponding to this figure are summarized in Table 6.4.

Figure 6.19 and Table 6.4 show some interesting results. For example, the average error for the quad-tree mesh is very small for both mesh resolutions. However, it can be noted that the absolute propagation error in the quad-tree mesh for the direction of propagation along the main space diagonal of the big block ($\theta = 54.73^\circ, \phi = 45^\circ$) is actually larger than in the uniform mesh. This is contrary to the results presented

Figure 6.19: a) Comparison of the dispersion error between a quad-tree mesh and the uniform meshes resulting from the blocks it is composed of. b) Front view of a quad-tree mesh illustrating the direction of propagation. $\theta = 0 \dots 90^\circ$ and $\phi = 45^\circ$.

Mesh	Resolution	min. error %	max. error %	range %	ave. error %
quad-tree	$\frac{\Delta X}{\lambda} = \frac{1}{5}$	1.49	-2.93	4.42	0.117
uniform	$\frac{\Delta X}{\lambda} = \frac{1}{5}$	0.65	-4.4	5.05	1.24
quad-tree	$\frac{\Delta X}{\lambda} = \frac{1}{10}$	0.33	-0.80	1.13	0.06
uniform	$\frac{\Delta X}{\lambda} = \frac{1}{10}$	0.14	-1.2	1.34	0.34

Table 6.4: Summary of results corresponding to Fig. 6.19.

in the previous figures where the absolute propagation error was always smaller in the quad-tree mesh for all directions of propagation.

Although the results presented so far constitute a very small sample of the many possible combinations of the parameters affecting dispersion error, our results allow to make the following conclusions. The intuitive assumption which regards the cut-off frequency of the mesh as being determined by the biggest block in the simulation domain is a conservative and safe one. That is, our results indicate that the presence of smaller blocks in an otherwise uniform mesh will, in general, decrease the overall dispersion error of the mesh. For the examples presented in this section, the dispersion error was reduced by up to 20%. Note that this observation applies to almost all the directions of propagation analyzed in this section. The only exception is for propagation along the main space diagonal of the big blocks. In this case, the presence of the small blocks has a negative effect and increases the dispersion error as compared with a uniform mesh. This suggests that a quad-tree mesh should be used with care, because under certain circumstances (such as for propagation along the main space diagonal), its performance is poor.

c) Comparison of a quad-tree mesh with a graded mesh

There is one more case of interest which is investigated next. Specifically, we investigate the effect of agglomerating the four small blocks into one. This is a situation which is likely to occur in graded meshes. Thus, for the next simulation the following parameters are used: $\Delta X = \Delta Y = \Delta Z = \Delta x_1 = \Delta y_1$, $\Delta x_2 = \Delta y_2 = 0$ and $\delta z = \Delta Z/2$. This configuration is shown schematically in Fig. 6.20.

The propagation error as a function of the direction of propagation for this case, is shown in Fig. 6.21. The direction of propagation has been chosen along the main

Figure 6.20: Basic graded mesh configuration studied.

Mesh	Resolution	min. error %	max. error %	range %	ave. error %
quad-tree	$\frac{\Delta x}{\lambda} = \frac{1}{10}$	0.33	-0.80	1.13	0.06
uniform	$\frac{\Delta x}{\lambda} = \frac{1}{10}$	0.14	-1.2	1.34	0.33
graded	$\frac{\Delta x}{\lambda} = \frac{1}{10}$	0.14	-0.80	0.94	0.19

Table 6.5: Summary of results corresponding to Fig. 6.21.

space diagonal as in the previous example.

The results corresponding to this figure are summarized in Table 6.5.

Figure 6.21 shows that the dispersion properties of the graded and quad-tree meshes are equal for propagation perpendicular to the connecting interface (z -direction). In addition, both exhibit less dispersion than the uniform mesh in this direction. It is also interesting to see that the absolute dispersion error of the quad-tree mesh is less than that of the graded mesh in the range of propagation given by approximately $\theta = 0 \dots 40^\circ$, $\phi = 45^\circ$. However, as the direction of propagation approaches the main space diagonal, the dispersion error of the graded mesh becomes smaller. The fact

Figure 6.21: a) Comparison of the dispersion error between a quad-tree, a uniform and a graded mesh. b) Front view of a quad-tree mesh illustrating the direction of propagation, $\theta = 0 \dots 90^\circ$ and $\phi = 45^\circ$.

that the absolute error is smaller for the graded mesh along the main space diagonal indicates that it is actually convenient to merge small blocks into larger ones under these propagation conditions.

6.6.6 Numerical Dispersion of Practical Meshes

In the previous section, it was shown that a quad-tree mesh can actually reduce the dispersion properties of a mesh such that its cut-off frequency is not limited by the biggest block present in the mesh. However, the analysis was performed under the assumption that the mesh was composed of an infinite repetition of a given pattern. In addition, the results thus obtained, were only valid for a single frequency (determined by the wavelength in the discretization condition). While this approach was found useful in providing guidelines, it is obvious that it does not represent the reality of practical meshes. Thus, the purpose of this section is to investigate the dispersion properties of realistic meshes, likely to be generated by our meshing tool. For the analysis presented in this section, the HSCN is used.

As it has already been pointed out, strict adherence to the idea of operating a mesh only at lower frequencies than its theoretical cut-off frequency, is not practical from the viewpoint of computational expense. Furthermore, a quad-tree mesh would not be very useful in this sense. On the other hand, this constraint cannot be relaxed without a careful investigation of the effect that it would have on accuracy. In this section, we estimate by how much a quad-tree mesh can be operated at frequencies above cut-off, while maintaining good accuracy. It is expected that by following the guidelines found in the previous sections, the operational limits of a quad-tree mesh can be maximized.

Figure 6.22: Slices of practical quad-tree meshes used to investigate the numerical dispersion error with: a) a small transition region and b) a large transition region between levels.

For the investigation, the accuracy of practical meshes operating at frequencies above the cut-off frequency is numerically evaluated. Figs. 6.22(a) and 6.22(b) show two of the practical meshes used for the initial numerical evaluations. The quad-tree mesh shown in Fig. 6.22(a) is composed of 980 blocks and that shown in Fig. 6.22(b) is composed of 1666 blocks. Note that in order to show the internal details of the mesh, the figures only show one half of the actual simulated structures. In both meshes, the blocks are distributed among three levels of refinement. The levels of refinement have been chosen such that there is a factor of two between the dimensions of blocks belonging to two consecutive levels. These meshes have been built based on the assumption that there is a region of space, which needs to be finely meshed, embedded in a coarsely meshed region. This is a commonly found scenario in practical problems.

where for example, the fine mesh is needed to resolve fields of large gradients or small structural details.

There are a number of commonalities between the two meshes. Firstly, they span the same volume of space (in this case, vacuum). Secondly, the maximum and minimum block dimensions are the same in each case. This means that both meshes have the same spatial resolution and the same theoretical cut-off frequency. This also results in the same maximum allowed time step for both meshes.

For the simulations, a similar approach to that taken for determining the dispersion relation of photonic crystals is used. That is, the boundary conditions of the mesh are such that they represent in reality, an infinitely large array of (empty) unit cells. This methodology has various advantages. Firstly, the dispersion relation of such structure can be computed analytically. Secondly, this formulation allows to test the mesh for any direction of propagation. Thirdly, basically all the resonant modes (up to a certain frequency) that the mesh can support, can be excited in a single simulation. Finally, this choice of boundary conditions prevents the simulation results from being affected by numerical reflections. Note that in theory, it would be possible to study the accuracy of these meshes by using a similar approach to that developed in Sect. 6.6. However, the resulting determinantal equation would be composed of square matrices of size 12 times the number of nodes. Obviously, the minimization of such a problem would be a very difficult task.

Figures 6.23(a) and 6.23(b) show the computed band structures of the meshes. For the computation of the dispersion relation, the symmetry points of the first Brillouin zone shown in Fig. 5.15(b) have been used as a reference. In the figures, the circles correspond to the predictions of the TLM method and the solid lines correspond

to the exact solutions. As the figures show, the agreement between the TLM and exact results is very good in both meshes, even for frequencies above the theoretical cut-off frequency of the mesh. In this respect, strict adherence to the acceptable discretization condition would require to operate the meshes only up to 0.1 units of normalized frequency. However, it is clearly seen from the figures that it is safe to operate either mesh at frequencies 50% above their cut-off frequency and obtain errors less than 1.5%. It should be noted that these results can be considered as a worst case scenario because the frequency modes are not restricted to be localized in the finer mesh as would be the case in practical applications. By carefully comparing Figs. 6.23(a) and 6.23(b), it can be seen that the performance of both meshes is very similar for frequencies below cut-off. However, the mesh shown in Fig. 6.23(b) is more dense and therefore shows less dispersion error at frequencies above cut-off.

A second alternative for simulating a finely meshed region of space embedded in a coarsely meshed one, is by means of a graded mesh as shown in Fig. 6.24. This mesh consists of 2744 cuboid blocks and spans the same volume of space as the meshes shown in Fig. 6.22. In addition, the maximum and minimum block dimensions are the same as before, thus allowing for a straightforward comparison of results. The corresponding dispersion curves for this mesh are shown in Fig. 6.25.

The first observation to make is that this mesh can also be operated at frequencies 50% higher than its theoretical cut-off frequency. In addition, by carefully comparing Figs. 6.23 and 6.25, it is noticeable that above the cut-off frequency of the mesh, the graded mesh exhibits less dispersion error than the quad-tree meshes. This result is in apparent contradiction based on the results obtained in Sect. 6.4, which suggest that cubic blocks are more accurate than non-cubic ones. However, it is supported

a)

b)

Figure 6.23: Band structures corresponding to a) the quad-tree mesh of Fig. 6.22(a) and b) the quad-tree mesh of Fig. 6.22(b). The circles are the predictions of the TLM method and the solid lines are the exact solutions.

Figure 6.24: Practical graded mesh used to investigate numerical dispersion error. The minimum and maximum block dimensions of this mesh are the same as those in Figs. 6.22(a) and 6.22(b).

by the results obtained in Sect. 6.6.5 which indicated that under certain conditions, a variable mesh can perform better than a quad-tree mesh. In this case, the better performance of the variable mesh can be explained from the fact that it is denser throughout the unit cell, and because it contains less blocks of the maximum size than the quad-tree meshes. As a result, the variable mesh captures better the spatial variation of the resonant modes leading to more accurate results. It must be kept in mind, however, that the improvement in accuracy provided by the graded mesh comes at the expense of simulation time because it contains more blocks.

There is one more important observation to make based on Figs. 6.23 and 6.25. As the figures show, mode splitting occurs at high frequencies. That is, the TLM method predicts two resonant frequencies for some branches, while the analytical

Figure 6.25: Dispersion curves of the graded mesh shown in Fig. 6.24.

Figure 6.26: Uniform meshes used to investigate numerical dispersion error: a) fine-uniform mesh and b) coarse-uniform mesh.

results indicate that there should be only one resonant frequency. Mode splitting is a result of the anisotropy of the mesh reported in Refs. [85] and [81]. It has its origins from the fact that the nodes are, in general, not symmetrically loaded by the stubs. An alternative that could potentially increase the operational limits of these meshes by suppressing node anisotropy is reported in Ref. [86].

As a way of comparison, the dispersion curves of the uniform meshes that can be formed from the smaller and bigger blocks present in these meshes were also computed. In this case, the fine-uniform mesh was composed of 21952 blocks and the coarse-uniform mesh was composed of 343 blocks. A section of the uniform and coarse meshes is shown in Figs. 6.26(a) and 6.26(b) respectively.

The dispersion curves corresponding to these meshes are shown in Figs. 6.27(a) and

6.27(b). As these figures show, the results predicted by the fine-uniform mesh are in excellent agreement with the results computed analytically. Of course, this accuracy is achieved at the expense of very long simulation times (≈ 10 times longer than the time required by the quad-tree and graded meshes).

Figure 6.27(b) shows the dispersion diagram computed by using the coarse-uniform mesh. At first sight, this figure shows that the results predicted by this mesh are, in general, at least as accurate as those predicted by the quad-tree and graded meshes for the frequency range shown in the figure. However, it must be noted that several problems arose while computing the dispersion curves of this mesh. To begin with, the dispersion curves could only be computed using a time-step four times larger than that used in all the previous simulations. When the same time-step was used, the resonant frequencies that were detected from the frequency spectrum, were totally offset and a band structure could not be obtained. In addition, even when the four-times larger time-step was used, the frequency modes lying above the cut-off frequency of the mesh were not easily detected. In general, much longer simulations were required to be able to detect these modes. Even then, their amplitudes were so small that it would be very difficult to detect them if one did not know that they were there in the first place. As a conclusion, the dispersion curves shown in Fig. 6.27(b) are misleading in the sense that they cannot be directly compared with those obtained by the previous meshes because they were obtained under very different conditions.

In summary, the results obtained in this section indicate that both quad-tree and graded meshes can safely be operated at frequencies above 50% higher than their theoretical cut-off frequency. The resulting dispersion error in this frequency range is less than 1.5% and this can be considered a worst case scenario.

Figure 6.27: Dispersion curves corresponding to a) fine-uniform mesh and b) coarse-uniform mesh.

6.7 Summary

In this Chapter, the mesh conditions that produce the least numerical dispersion error in quad-tree meshes, were determined. After analyzing in detail how geometrical factors influence node dispersion, the following guidelines for use with our meshing tool were obtained.

1. Keep blocks which do not satisfy the acceptable discretization condition as cubic as possible in the mesh.
2. When non-cubic blocks are part of the mesh, avoid the introduction of elongated (needle type) blocks as much as possible. These blocks introduce a large dispersion error, particularly in the direction of the largest dimension.
3. Preferably, introduce non-cubic blocks with a large cross-section area, they introduce less dispersion error than elongated ones.

In addition, it was found that the presence of smaller blocks in an otherwise uniform mesh does, in general, decrease the overall dispersion error of the mesh. For the examples presented in this chapter, the dispersion error was reduced by up to 20%. Note that this observation applies to almost all the directions of propagation in the mesh. The only exception is for propagation along the main space diagonal of the big blocks. In this case, the presence of the small blocks has a negative effect and increases the dispersion error as compared with a uniform mesh. This suggests that a quad-tree mesh should be used with care, because under these propagation conditions, it exhibits a poor performance.

Finally, it was found that both quad-tree and graded meshes can safely be operated at frequencies above 50% higher than their theoretical cut-off frequency. The resulting

dispersion error in this frequency range is less than 1.5% and this can be considered a worst case scenario.

Chapter 7

Application of Quad-tree Meshes to Non-periodic Problems

7.1 Introduction

The results presented in Chapters 4 and 5 of this thesis were mainly concerned with the simulation of infinite periodic structures. In Chapter 6, the accuracy of different quad-tree meshes was evaluated by analyzing their dispersion relation. The results were summarized in a set of guidelines that the mesh must be subject to, during the discretization process. In this Chapter, the ideas developed in the previous chapters are validated by simulating real-world problems such as microwave and photonic structures. Given that the purpose behind the development of quad-tree meshes is to obtain good accuracy with less nodes in the discretized volume, these ideas are emphasized here. After validation, we concentrate on the analysis of electromagnetic band-gap structures.

The extension of the modelling capability that has been developed so far to the simulation aspects of the problems to be analyzed in this Chapter, is somewhat straightforward. The most important feature to be addressed, is the fact that these structures are no longer of infinite extent. Thus, the periodic boundary conditions need to be modified to reflect the finiteness of these problems. This leads to the introduction of perfectly matched layers.

7.2 Perfectly Matched Layers (PML) in TLM

An important feature in the simulation of finite, unbound structures is to avoid spurious reflections of the otherwise perfectly radiated field. The reflections are caused by the boundaries of the computational volume. For this purpose, absorbing boundary conditions (ABCs) and perfectly matched layers (PMLs) have been developed.

Absorbing boundary conditions were described in Sect. 3.8.2. This type of boundary condition offers two important advantages. First of all, they are very easy to implement within the formulation of the TLM method and, secondly, the implementation of this type of boundary condition does not increase the size of the computational volume. On the negative side, this type of boundary condition is a first order approximation because it works perfectly only for normally incident waves. Despite this, there is numerical evidence that they can work quite effectively, especially when located away from the region of the problem of interest.

PMLs were first introduced for the FDTD method [87], [88] and later extended to the TLM method [89], [90]. PMLs are more effective than ABCs because they can absorb the electromagnetic radiation at any angle of incidence. However, the imple-

mentation of PMLs requires the addition of extra layers surrounding the computational volume. Thus, their implementation is more demanding and can considerably increase the size of the computational volume.

For the purpose of this work, a straightforward implementation of the PMLs presented in Ref. [90] has been carried out. After numerical testing, the implementation of these PMLs has been found to produce numerical reflections of less than -50 dB. For the actual implementation, ten PMLs and a parabolic profile of conductivity are used as in Ref. [35].

It must be noted that PMLs are a mathematical artifact and do not constitute a “real” EM medium¹. Therefore, they are known to be a potential source of stability problems. For the type of PMLs that were implemented in our numerical experiments, no stability problems were detected. However, when dealing with layered structures, it is important that the PMLs between layers satisfy the condition described in Ref. [91] to avoid stability problems.

For the structures studied in this section, both types of boundary conditions have been implemented. However, after comparing the results obtained with either boundary condition and noticing minor differences, it was determined that an absorbing boundary condition was appropriate for most structures. Thus, unless otherwise stated, a first order absorbing boundary is used to terminate the computational volume of the structures analyzed in the next sections.

¹In this sense, a real EM medium is defined as one which obeys Maxwell’s equations.

7.3 Validation of Quad-tree Meshes: General EM Problems

In this section, the accuracy of the quad-tree meshes produced by our meshing technique is analyzed by simulating various EM problems. Given the lack of measurements, our TLM results are compared with those obtained by the FDTD method.

7.3.1 Simulation of a Patch Antenna

The first structure that is simulated is a microstrip patch antenna. The antenna consists of a rectangular patch and a uniform microstrip feed line on a substrate of relative permittivity $\epsilon_r = 2.2$. Its schematic representation and dimensions are shown in Fig. 7.1(a). In addition, the corresponding TLM model is shown in Fig. 7.1(b).

The details of the quad-tree mesh used to discretize the patch antenna are shown in Figs. 7.2(a) and 7.2(b). There are a few interesting observations to make based on these figures. In Fig. 7.2(a), the entire structure is shown. Note that in the discrete model, the air layer plays an important role. As a matter of fact, this layer is 4.5 times thicker than the substrate itself. The reason for this is as follows. For the results of the simulation to be accurate, the electromagnetic field radiated from the rectangular patch must not find its way back into the substrate (as it would normally occur in a real antenna). Thus, an absorbing boundary condition is required on top of the air layer. However, in order to minimize the interaction between the fields and the absorbing boundary, the air layer must be thick enough to propagate the radiated field away from the rectangular patch before being absorbed. As mentioned in the previous section, this maximizes the efficiency of the absorbing boundary.

Figure 7.1: Simulated Patch Antenna: a) Schematic representation and dimensions, b) TLM model (the air layer is not shown in this figure, but present in the simulations).

Figure 7.2: Quad-tree mesh of the patch antenna a) Complete model showing the air layer, b) Detail view of the mesh near the metal patch.

Based on our simulations, a thickness of at least four times that of the substrate is required. Note that if the air layer was discretized using the same spatial resolution as in the metal patch, the computational time would increase considerably (at least by a factor of 4).

Figure 7.2(b) shows a detailed view of the mesh in the region of the metal patch. As the figure shows, a fine mesh has been used to discretize the feed line and the rectangular patch. The fine mesh in these areas is required for two reasons: to properly capture the field resonances in the rectangular patch and to capture the large field gradients around the feed line and the rectangular patch. As is, the computational volume consists of 70992 nodes, the minimum spatial resolution is 0.2 mm and the

cut-off frequency of the mesh is 50 GHz. As a way of comparison, the same resolution would be achieved with 352000 blocks using a uniform mesh and approximately 150000 using a graded mesh. This represents computational efficiencies of 4.95 and 2.11, respectively.

An important feature of time-domain methods such as TLM that has not been discussed in this thesis is that they allow for visualization of EM fields as they propagate in the simulated structure. This feature has been incorporated in our TLM-based numerical tool. For example, Fig. 7.3(a) and 7.3(b) show snapshots of field distributions on the antenna for two different excitations. In Fig. 7.3(a), the antenna was excited with a Gaussian pulse. The figure shows the initial reflection that the pulse undergoes after it has encountered the transmission line discontinuity. In Fig. 7.3(b), the antenna was excited with a frequency corresponding to a (resonant) radiated mode (see Fig. 7.4). The figure shows the steady state resonance of the mode that sets in the metal patch as it is radiated.

Figure 7.4 shows the reflection coefficient (S_{11}) of the microstrip patch antenna at the input of the feeding line. It was computed by

$$S_{11}(\omega) = 20 \cdot \log_{10} \left(\frac{E_{out}(\omega)}{E_{in}(\omega)} \right) \quad [dB] \quad (7.1)$$

In the figure, the results were compared with those obtained by the FDTD method [92] and good agreement was found.

Figure 7.3: Field distribution on the patch antenna for: a) Gaussian excitation, b) Single frequency excitation (radiated mode).

7.3.2 Simulation of a Microwave Low-pass Filter

The second example that was simulated is a low-pass filter built on the same substrate as the patch antenna. Its schematic representation and dimensions are shown in Fig. 7.5(a). In addition, the corresponding TLM model is shown in Fig. 7.5(b).

The details of the quad-tree mesh used for discretizing the low-pass filter are shown in Figs. 7.6(a) and 7.6(b). In Fig. 7.6(a), the entire structure is shown. Similarly to the previous case, the air layer is 4.5 times thicker than the substrate. However, as this figure shows, two levels of refinement were used for discretizing the air layer in this structure. This is another alternative offered by a quad-tree mesh which can further reduce the total number of nodes used in the discretization.

The justification behind this discretization condition is that as the fields propagate

Figure 7.4: Return loss of the rectangular patch antenna.

Figure 7.5: Simulated low-pass filter: a) Schematic representation and dimensions, b) TLM model (the air layer is not shown in this figure, but present in the simulations).

Figure 7.6: Quad-tree mesh of the low-pass filter a) Complete model showing the air layer, b) Detail view of the mesh near the metal patch.

away from the region of interest, their actual spatial resolution becomes less important². Thus, the size of the blocks can be gradually increased as one moves away from the region of interest. It must be noted that this is very useful in modelling problems where the absorbing boundaries must be placed far away from the region of interest, or for discretizing the computational volume in regions where the actual spatial distribution of the fields is not important (for example, deep into the substrate in a rib waveguide). These are typical situations where the advantage of a quad-tree mesh becomes clearly evident.

²At least for these particular problems where the actual radiated field pattern is not the purpose of the simulations.

Figure 7.6(b) shows a detailed view of the mesh in the region of the microstrips comprising the filter. As the figure shows, a fine mesh has been used to discretize the line ports and the rectangular patch. The fine mesh in these areas is required for the same reasons as before: to properly capture the field resonances in the rectangular patch and to capture the large field gradients around the port lines and the rectangular patch. In this case, the computational volume consists of 87298 nodes, the minimum spatial resolution is 0.2 mm and the cut-off frequency of the mesh is 25 GHz. For this structure, the same resolution would be achieved with 794640 blocks using a uniform mesh and approximately 196400 using a graded mesh. This represents computational efficiencies of 9.1 and 2.25, respectively.

Figure 7.7 shows the field distribution on the filter for a Gaussian excitation. The figure shows the reflection of the pulse after it encounters the transmission line discontinuity.

Figure 7.8 shows the reflection coefficient (S_{11}) of the low-pass filter at port 1. It was computed by using Eq. (7.1). In the figure, the results were compared with those obtained by the FDTD method and good agreement was found once more.

In summary, the discretization of these problems illustrates the most important ideas behind quad-tree meshes. A quad-tree mesh makes possible 1) small spatial resolutions only in regions where required, 2) the option to use a coarse mesh to move the PMLs away from the region of interest and 3) the ability to discretize regions of the computational volume where the actual spatial distribution of the fields is not important. The combination of these conditions results in a discretization of the computational volume that offers a good compromise between computational expense and accuracy.

Figure 7.7: Field distribution on the microwave filter after being excited with a Gaussian impulse.

Figure 7.8: Return loss of the low-pass filter.

7.4 Simulation of EBG Structures

In this section, the previous ideas are combined to analyze EM problems that include some sort of periodicity as part of their design. Such structures were defined in Chapter 1 as electromagnetic band gap (EBG) materials.

7.4.1 Temperature Tuned In-line Filter

It is a well known fact that the relative permittivity of semiconductors can be a strong function of temperature [2]. This gives rise to the possibility of manipulating the photonic band structure by means of temperature. In semiconductor composites with a narrow band-gap such as InSb, the temperature dependence of the permittivity is brought about by the temperature dependence of the plasma frequency. Thus, the incorporation of thermal effects in the TLM frequency dependent formulation developed in Sect. 4.5 is straightforward. Considering the relation between the plasma frequency and the complex permittivity given by Eq. (4.26),

$$\epsilon^*(\omega) = \epsilon_\infty \left(1 + \frac{\omega_p^2}{\omega(j\nu_c - \omega)} \right)$$

it is obvious that in order to simulate the temperature dependence of the permittivity, it is only required to find the explicit temperature dependence of the plasma frequency. The plasma frequency was introduced in Sect. 4.5 and is given by Eq. (4.27)

$$\omega_p = \sqrt{(N_e e^2)/(\epsilon_\infty \epsilon_0 m_e)},$$

Figure 7.9: Schematic representation of the in-line filter.

in addition, for InSb the electron density depends on temperature according to the expression [28],

$$N_e(T) = 5.76 \times 10^{14} T^{3/2} e^{-0.13/k_B T} \quad (7.2)$$

thus, by using equation (7.2) in the plasma-type permittivity equation, an expression for the temperature dependence of the permittivity of InSb is found.

To illustrate these ideas, the next example that is simulated is a tunable in-line filter fabricated in InSb. Following [2], an effective mass of $m_e = 0.015 \times m$, where m is the mass of a free electron, and $\epsilon_\infty = 17.7$, were used for the simulations. The in-line filter is shown in Fig. 7.9. The structure consists of 30 rows by 19 columns of square pillars of InSb embedded in air and surrounded by a perfectly matched layer. One of the columns in the structure was removed to form the defect in-line filter.

Various quad-tree meshes were tested for the discretization of the structure. A typical mesh is shown in Fig. 7.10. In this figure, only one section of the structure is

Figure 7.10: Typical discretization of the in-line filter.

shown. As the figure shows, the general idea was to use a fine mesh for discretizing the rods adjacent to the waveguide (where the fields have large spatial gradients), and gradually coarser ones for rods located away from it. In addition, the convergence of the mesh was tested by comparing the results obtained with this mesh, with those obtained with better discretizations. Since the comparison of results did not show considerable differences, this mesh was deemed to be appropriate.

The temperature dependence of the electromagnetic behavior of the filter was characterized by a transmission coefficient. The transmission coefficient is a measure (ratio) of the energy that propagates between the input and output planes shown in Fig. 7.9. It was calculated by recording the fields at those planes at every time step. These fields were then fast Fourier transformed and integrated over the surfaces to

Figure 7.11: Transmission coefficient of the in-line filter: Solid line T=260 K. Dashed line T=300 K.

obtain the total time-averaged Poynting's vectors at every frequency point.

Figure 7.11 shows the transmission coefficient of the waveguide calculated at temperatures of 260 K and 300 K. As the figure shows, the electromagnetic responses of the structure at each temperature, differ considerably from each other. Firstly, it can be seen that there is a low-frequency stopband for both cases. In order to understand this result, it is necessary to analyze in detail the nature of the frequency dependent permittivity used to model the InSb rods. Fig. 7.12 shows the refractive index as a function of frequency for the plasma-type equation used in this model. Obviously, $n^* = \sqrt{\epsilon^*(\omega)} = n_r + in_i$. As the figure shows, for frequencies below the plasma frequency, the imaginary component of the index of refraction of the InSb rods is large, and the radiation is absorbed as it is scattered by the inner rods of the waveguide.

Figure 7.12: Refractive index as a function of frequency for the plasma-type permittivity.

This accounts for the low-frequency stopbands shown in Fig. 7.11.

It can also be seen from Fig. 7.11 that the range of transmitted frequencies is shifted as a result of the increase in temperature. This is a clear indication that a filter of this type can be tuned externally by means of temperature variations. Finally, Fig. 7.11 indicates that as the temperature increases, the width and magnitude of the passbands decrease. These results are consistent with those obtained in [28] and can be explained from the fact that as the temperature increases, the photonic band gaps decrease, owing to the reduced permittivity contrast between the InSb rods and the background.

7.4.2 EBG-based High Speed Interconnect

The next example that is simulated is a single-defect waveguide for a potential application as an on-board high speed interconnect. The motivation behind the analysis of this structure is that currently used metallic interconnects to transfer data between processors are reaching their technological limits. That is, it is expected that future clock speeds of above 3 GHz will create electromagnetic compatibility and electromagnetic interference problems that might render current interconnects impractical. Thus, as clock rates continue to increase, new emerging technologies are being studied to overcome these problems. In this section, we show that these are the types of problems for which the quad-tree modelling technique developed in this thesis, has its greatest potential.

The possibility of making wireless high-speed interconnects based on electromagnetic band gap structures has already been explored in Ref. [71]. However, the analysis of these structures is a highly repetitive process and demands large computational

resources. More specifically, the analysis of realistic interconnects composed of several unit cells long, leads to a large number of nodes in the computational volume when standard discretization techniques are used. In addition, during the analysis process, it is very common to repeat the simulations after varying one or more parameters in the structure.

In summary, the analysis of these types of problems requires a large memory for variable storage and a fast computer for processing. Thus, it is not surprising that most of the analyses of these problems carried out so far, have been done using parallel computing or some sort of super computer. In what follows, we show that a quad-tree mesh can considerably reduce the computational requirements associated with these problems and make analyses amenable to personal computers.

Figure 7.13 shows a schematic representation of the simulated structure. The entire structure consists of 5 rows by 21 columns of metallic cylinders embedded in a dielectric material. As the figure shows, the center row of metallic cylinders is removed forming a single-defect waveguide. Figure 7.13 shows the actual TLM quad-tree model of the simulated structure. The computational volume consists of 222600 nodes, the minimum spatial resolution is 0.2 mm and the cut-off frequency of the mesh is 18 GHz.

The radius and spacing of the metallic cylinders are $r = 0.83$ mm and $a = 4.6$ mm respectively. In order to represent these cylinders as accurately as possible in a rectangular grid, a fine mesh has been used around the cylinders to minimize the stair-case error. A detailed view of the mesh used to discretize the cylinders is shown in Fig. 7.15.

For the simulations, a relative permittivity of $\epsilon_r = 4.3$ has been used for the host

Figure 7.13: Schematic representation of the single-defect waveguide.

medium. The thickness between the lower and upper ground planes is 3.2 mm. This corresponds to FR4 circuit board. In addition, the metallic cylinders have been assumed as perfect electric conductors.

Figure 7.16 shows a contour plot of the field distribution on the waveguide after a Gaussian pulse has propagated for 2000 time steps. The figure shows two interesting features: (a) the fact that the guided pulse is fairly well confined within the waveguide region and (b) the fact that the pulse undergoes strong dispersion as it propagates down the guide.

Discussion

The transmission coefficient for the waveguide is shown in Fig. 7.17. These results correspond to the E -polarization, that is, the electric field is polarized in the direction parallel to the metallic cylinders.

Figure 7.14: TLM quad-tree model of the single-defect waveguide shown in Fig. 7.13.

Figure 7.15: Detailed view of the mesh used to discretize the metallic cylinders.

Figure 7.16: Field distribution on the defect waveguide after a Gaussian pulse has propagated for 2000 time steps.

Figure 7.17: The transmission coefficient of the single-defect waveguide.

These results can be explained as follows. The analysis of an infinite photonic crystal composed of metallic cylinders presented in Sect. 4.5, showed the presence of a low-frequency stopband (see Fig. 4.10). Such is a characteristic behavior of the E mode if the dielectric constant of the cylinders is sufficiently negative [28]. Thus, when a line defect is introduced in the array of metallic cylinders, a waveguide is formed because the electromagnetic waves whose frequencies fall within the stopband of the metallic array, will be guided along the line defect without appreciable losses. It must be noted that although the results presented in Sect. 4.5 involved an infinite array of metallic cylinders, the results presented in Ref. [71] indicate that even a two-row waveguide can provide leakage below -40 dB for the frequency range of interest.

Based on the results presented in Fig. 7.17, the low-frequency stopband of the metallic cylinders extends from approximately 0-16 GHz. Within this range of frequencies, the figure shows the presence of a stopband (for the guided modes in the waveguide) between approximately 0-8 GHz. This corresponds to the inherent stopband in a conventional parallel plate waveguide.

Defining the usable transmission bandwidth as the frequency span over which the transmission magnitude is relatively flat (± 1.5 dB), the transmission bandwidth for the present waveguide is approximately 6 GHz and centered at about 12 GHz. Thus, these preliminary results show the theoretical possibility of obtaining EBG-based high speed interconnects operating at 10+ GHz.

As it has already been mentioned, the analysis of these structures generally requires numerous numerical experiments. For the present structure, the simulation time is approximately 3 hours using a personal computer operating at 2.3 GHz. Although this run time can be considered relatively long under certain circumstances, it would

easily increase by a factor of 5 without the quad-tree meshing techniques developed in this thesis. As a way of comparison, the same resolution would be achieved with 999936 blocks using a uniform mesh and approximately 623200 using a graded mesh. This represents computational efficiencies of 4.5 and 2.8 respectively. It should be noted that this particular waveguide is quasi two-dimensional in nature. For more general and complex three-dimensional problems, it is estimated that the computational efficiency can be increased by factors larger than 20.

7.5 Summary

In this Chapter, the accuracy and efficiency of quad-tree meshes were validated by simulating real-world problems. Specifically, the discretization of the studied problems illustrated the most important applications of quad-tree meshes. These applications are:

1. to obtain small spatial resolutions only in regions where required,
2. to move the PMLs away from the region of interest using a coarse mesh and
3. to discretize regions of the computational volume where the actual spatial distribution of the fields is not important.

It was shown that the combination of these conditions results in a discretization of the computational volume that offers a good compromise between computational expense and accuracy.

Finally, the quad-tree meshing technique was used to show the possibility of tuning an in-line photonic filter by means of temperature and the theoretical possibility of

obtaining EBG-based high speed interconnects operating at 10+ GHz.

Chapter 8

Conclusions and Future Work

8.1 Summary

In this thesis, numerical techniques for simulating electromagnetic band-gap structures were developed. The numerical techniques were based on the TLM method which was found to provide the required flexibility to address the key simulation aspects of these structures.

After building the theoretical foundations in Chapters 2 and 3, in Chapter 4, this work described important aspects for the computation of the dispersion relation of infinitely large PC within the formulation of the TLM method. Given that the general implementation of the Bloch condition requires complex-valued arithmetic, a complex-valued formulation was presented. According to this formulation, the real and imaginary parts of the voltage pulses (fields) are computed separately throughout the simulation domain and coupled only at the boundaries. The analysis of the energy exchange mechanism between the real and imaginary grids, allowed us to look

into the stability properties of the complex-valued formulation. It was shown this formulation remains unconditionally stable because the equations enforcing the periodicity condition at the sidewalls of the simulation domain, retain the energy as a constant.

The complex-valued formulation was extended for handling PC composed of frequency dependent materials such as metals and semiconductors. By deriving the necessary equations for their application in non-cubic meshes, the frequency-dependent formulation was made compatible with the type of meshes used in this thesis.

In Chapter 5, two optimization techniques for reducing the computational effort involved in the simulations of electromagnetic band-gap structures were proposed. The advantages and limitations of each techniques were described.

The first technique was based on a real-valued implementation of the periodicity condition. It relied on a circuit representation such that ideal matching transformers were used to implement the periodicity conditions. This approach led to an unconditionally stable TLM scheme free of high-frequency noise. The stability was a result of an exchange algorithm that did not introduce energy from the sidewalls of the simulation domain as previous formulations did. It was shown that, depending on the physical geometry of the crystal, computational savings of over 50% could be easily achieved with this formulation.

The second optimization technique was based on multi-grid meshing and it was implemented using an in-house computer program (Atar). It was shown that using a multi-gridding approach, computational savings of over 80% could be achieved. In addition, it was shown that this approach retains good accuracy, well above the theoretical cut-off frequency of the mesh.

We validated our numerical technique by simulating various PC composed of dielectric, metallic, and semiconducting materials, using uniform and multi-grid meshes. The results were compared with those predicted by alternative methods such as the PWE method and good agreement was found.

In Chapter 6, the mesh conditions that produce the least numerical dispersion error in quad-tree meshes, were determined. After analyzing in detail how geometrical factors influence node dispersion, the following guidelines for use with our meshing tool were obtained:

1. Keep blocks which do not satisfy the ideal discretization condition as cubic as possible in the mesh.
2. When non-cubic blocks are part of the mesh, avoid the introduction of elongated (needle type) blocks as much as possible. These blocks introduce a large dispersion error, particularly in the direction of the largest dimension.
3. Preferably, introduce non-cubic blocks with a large cross-section area, they introduce less dispersion error than elongated ones.

In addition, it was found that the presence of small blocks in an otherwise uniform mesh does, in general, decrease the overall dispersion error of the mesh. For the examples presented in this chapter, the dispersion error was reduced by up to 20%. Note that this observation applies to almost all the directions of propagation in the mesh. The only exception is for propagation along the main space diagonal of the big blocks comprising a multi-grid mesh. In this case, the presence of small blocks has a negative effect and increases the dispersion error as compared with a uniform mesh.

This suggests that a quad-tree mesh should be used with care, because under these propagation conditions, it exhibits a poor performance.

Furthermore, it was found that both quad-tree and graded meshes can safely be operated at frequencies above 50% higher than their theoretical cut-off frequency. The resulting dispersion error in this frequency range is less than 1.5%, which can be considered a worst case scenario.

In Chapter 7, the accuracy and efficiency of quad-tree meshes were validated by simulating real-world problems. The analysis of the studied problems demonstrated the main advantages of these meshes. In this respect, it was shown that quad-tree meshes are particularly advantageous in the following situations:

1. to obtain small spatial resolutions only in regions where required,
2. to move the PMLs away from the region of interest without increasing considerably the computational effort and
3. to discretize regions of the computational volume where the actual spatial distribution of the fields is not important.

It was shown that the combination of these conditions results in a discretization of the computational volume that offers a good compromise between computational expense and accuracy. For the studied structures, computational efficiencies in the range of 10 and 3.0 were obtained when compared, respectively, with uniform and graded meshes. Furthermore, given the relative simplicity of the studied structures, these computational efficiencies are expected to increase considerably (by factors larger than 20) in structurally more complex three-dimensional problems.

Finally, the quad-tree meshing technique was used to show the possibility of tuning an in-line photonic filter by means of temperature and the theoretical possibility of obtaining EBG-based high speed interconnects operating at 10+ GHz.

8.2 Future Work

In light of the work presented in this thesis, the future work that can be undertaken can be divided into two groups. In the first chapter of this thesis it was pointed out that one of the motivations behind this work, was the lack of commercial software for the simulation of EBG structures. From this perspective, it might be advantageous to further increase the modelling capabilities of the simulation tool that has been developed so far. In this way, the first group refers to those activities which can be undertaken for this purpose:

1. The development of dispersion compensation techniques would greatly increase the potential of quad-tree meshes.
2. Incorporation of self-consistent capability would allow the analysis of problems with strong electrical-optical-thermal coupling.
3. The investigation of the stability problems of PMLs from the point of view of energy conservation condition might shine light on the origin of these problems.
4. The development of special meshing techniques would allow a more accurate representation of circular features without resorting to staircase approximations.
5. The incorporation of new modelling capabilities that allowed the simulation of non-linear materials.

The second group refers to the applications of the work presented in this thesis in the fields of photonics and microwaves. Up until now, the large demand of computational resources imposed by the discretization of large EBG structures using time-domain techniques, has limited the investigation of these structures to those scientific groups which possess large computational resources. Thus, the computational techniques developed in this thesis offer an alternative for the analysis of a wide variety of novel EBG structures with limited computational resources.

Appendix A

Recursive evaluation of the susceptibility in a plasma type equation

In this appendix, the recursive evaluation of the convolution appearing in equation (4.15) is shown in more detail. We begin with Eq. (4.15),

$${}_{n+1}V_{sq} = -{}_nV_{sq} - \frac{\chi_0(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} {}_nV_q + \frac{(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} \sum_{m=0}^{n-1} {}_{n-m}V_q (\chi_m - \chi_{m+1})$$

then, by making the next definition

$$\Phi^n = \sum_{m=0}^{n-1} {}_{n-m}V_q (\chi_m - \chi_{m+1}) \quad (\text{A.1})$$

and evaluating Φ^n for the first few steps, we have:

-for $n = 1$

$$\Phi^1 = \sum_{m=0}^{1-1} {}_{1-0}V_q \Delta\chi_0 = {}_1V_q \Delta\chi_0 \quad (\text{A.2})$$

where $\Delta\chi_0 = (\chi_0 - \chi_1)$.

-for $n = 2$

$$\Phi^2 = \sum_{m=0}^{2-1} {}_{2-m}V_q \Delta\chi_m = {}_2V_q \Delta\chi_0 + {}_1V_q \Delta\chi_1 \quad (\text{A.3})$$

where $\Delta\chi_1 = (\chi_1 - \chi_2)$. From the definition of general susceptibility given by

$$\chi_m = \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau) d\tau, \quad (\text{A.4})$$

and having in mind that $\chi(\tau)$ is given by Eq. (4.28), after evaluating the integrals we get

$$\Delta\chi_m = \chi_m - \chi_{m+1} = -\frac{\omega_p^2}{\nu_c} e^{-m\nu_c \Delta t} [1 - e^{-\nu_c \Delta t}]^2, \quad (\text{A.5})$$

from this equation it follows that $\Delta\chi_{m+1} = \Delta\chi_m e^{-\nu_c \Delta t}$. Using this expression in Eq. (A.3), we get

$$\Phi^2 = {}_2V_q \Delta\chi_0 + {}_1V_q \Delta\chi_0 e^{-\nu_c \Delta t} \quad (\text{A.6})$$

and noting that, from Eq. (A.2) $\Phi^1 = {}_1V_q \Delta\chi_0$, then

$$\Phi^2 = {}_2V_q \Delta\chi_0 + \Phi^1 e^{-\nu_c \Delta t} \quad (\text{A.7})$$

this equation can be generalized to the following recursive expression

$$\Phi^n = {}_nV_q \Delta\chi_0 + \Phi^{n-1} e^{-\nu_c \Delta t} \quad (\text{A.8})$$

and the equation for the voltage source becomes

$${}_{n+1}V_{sq} = -{}_nV_{sq} - \frac{\chi_0(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} {}_nV_q + \frac{(4 + \hat{Y}_o^q)}{\epsilon_\infty + \chi_0} \Phi^n.$$

Note that the evaluation of this equation does not require the storage of the fields at every time step as it is generally required in regular convolution problems.

Appendix B

Solution of the circuit implementing periodic BCs

The solution of the network of matching transformers shown in Fig. 5.2 is rather straightforward. To begin with, the computation of the voltage drop between points V_{AB} in Fig. B.1 is required. Note that in this figure, only the link-lines and volt-

Figure B.1: Link-lines and voltages of interest of the circuit-type implementation.

age pulses of interest are shown. To find V_{AB} , the Norton equivalent circuits of the transmission lines are found. For example, replacing the left link-line by its equivalent Norton circuit leads to the circuit shown in Fig. B.2. In this figure, Z_0 is the characteristic impedance of the link-lines. After doing the same for the link-line on

Figure B.2: Norton equivalent circuit of the left link-line.

the right side and solving the resulting circuit for V_{AB} , one gets

$$V_{AB} = \frac{2[XV_{11}^r(x_{1,2}) + YV_3^r(x_{1,1})]}{X^2 + Y^2} \quad (\text{B.1})$$

After finding V_{AB} , the voltage on either side of the transformers (c.f. Fig. B.1) can easily be found from the transformers turn ratios. For example, the voltage on the right side of the transformers (V_R) would be $V_R = V_{AB}Y$. Finally, having in mind that the total voltage on a link-line is $V_R = V^i + V^r$ and rearranging terms, Eqs. (5.10) and (5.11) are obtained.

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