Efficient PML Boundaries
for
Anisotropic Waveguide Simulations
using the Finite Element Method

A dissertation submitted for the requirements of
Doctor of Philosophy

by
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Declaration

The candidate hereby declares that the work contained in this thesis is his own and that all sources of information have been duly acknowledged. Also, this work has not been submitted previously, in whole or part, with respect of any other award and the work has been carried out since the official date of commencement of the programme.

Arnan Mitchell.
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Abstract

The application of integrated optics has broadened from well established areas, such as high-speed modulators for communication over optical fibre, to such diverse areas as radio frequency (RF) signal processing and antenna beam forming. Simulation tools that are general enough to model a wide range of RF and photonic devices, yet efficient enough to be used trivially are required.

The aim of this thesis is to investigate the use of the perfectly matched layer (PML) boundary condition as a means of improving the efficiency of eigenvalue simulations, and to extend their range of applicability to radiating waveguides. This work focuses in particular on the simulation of waveguides using the biaxial material Lithium Niobate.

Major contributions made by this work include the derivation of a generalised PML suitable for matching biaxial materials, extension of analysis of numerical dispersion and reflection in the finite element method to biaxial media and derivation of closed form expressions for the numerical reflection from a PML interface. These expressions are used to investigate the major contributions to numerical errors in the implementation of the PML boundary and hence a significantly more efficient technique for enhancing the PML’s performance with a minimal increase in unknowns is suggested and demonstrated in a practical simulation. Finally, the generalised PML is applied to three eigenvalue simulations, including a radiating waveguide bend, with greatly improved efficiency and accurate simulation of propagation loss.

In summary, the PML has been extended to biaxial materials and the sources of numerical errors in its implementation have been identified and an efficient means of reducing them devised. The new PML and implementation technique have been demonstrated in eigenvalue simulations of both lossless and lossy waveguides with accurate and efficient results being achieved.
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Chapter 1

Introduction

Radio frequency (RF) photonic technologies are increasingly finding application in modern communication and signal processing systems. The use of optical intensity modulators to transmit broadband RF information across great lengths of optical fiber is now standard, however integrated optics is finding use in such diverse areas as RF phase shifting and filtering. As the system requirements on integrated optic devices increases, and the range of application for integrated optic devices broadens, more rigorous and general tools are required for integrated optic device design. In particular, to effectively design the RF and photonic components required by this range of systems, general numerical electromagnetic models are essential.

General numerical models used in the design of integrated optic and RF components include finite element and finite difference frequency domain, time domain and beam propagation methods. Although extremely general in their application, these methods can prove expensive, limiting their use as a design tool. More efficient but less general models, such as those based on the moment method, can be useful in integrated optic device design, however these methods can be limited, being better suited to predefined sets of geometries.

The majority of integrated optic devices rely on interactions between guided modes of various waveguide structures. Hence a great deal of device modeling can be achieved with a two dimensional mode solver. Although less general in application than the finite methods mentioned above, two dimensional eigenvalue simulations are far more rapid than those in three dimensions. Even so, these simulations can still be cumbersome in certain circumstances and thus further improvement in the efficiency of these eigenvalue models will allow them to be more intimately integrated into the device design methodology. If general models, such as the finite element method (FEM), could be employed trivially, the device design process would be greatly enhanced.

A particular aspect that limits both the efficiency and the accuracy of numerical sim-
ulations is the imposition of external boundaries. Traditional boundary conditions must be placed a significant distance from the features of the problem to ensure an accurate solution. Further, simulation of radiation through this boundary can be troublesome and ineffective with accurate implementations being very computationally expensive. A recently developed boundary condition, the so called perfectly matched layer PML \[1\], has been demonstrated to solve many of these problems in both time domain and frequency domain problems. It is proposed that this boundary condition can be applied to eigenvalue simulations.

This thesis aims to investigate the PML as a means of improving the efficiency and effectiveness of electromagnetic eigenvalue simulations using FEM. In particular, the investigation will focus on simulations involving the uniaxial, electro-optic material LiNbO\(_3\). The major areas of research in this work are the development of a more general PML formulation capable of matching biaxial materials, analysis of the nature of numerical errors in the FEM and their effect on the efficiency and accuracy of PML implementations, investigation of more efficient PML implementation and demonstration of this PML as an effective means of improving the efficiency of eigenvalues simulations involving anisotropic material. This thesis is divided into six Chapters and four Appendices. A preview, highlighting the novel contributions made in each Chapter follows.

A literature survey tracing the development of the PML boundary is presented in Chapter 2. Available PMLs that are applicable to FEM analysis are found to be valid only when using isotropic materials. Thus the remainder of Chapter 2 is dedicated to the derivation of a new generalised PML for use with anisotropic media. The derived PML is verified using an FEM simulation and discrepancies with the expected results are observed.

The discrepancies between simulated results and closed form predictions observed in Chapter 2 are attributed to numerical errors in the FEM simulation caused by an insufficient degree of discretisation. To properly analyse the effect of discretisation error on numerical reflection from a PML interface, Chapter 3 derives a closed form expression for the numerical dispersion and numerical reflection as a function of frequency, edge length and material tensors. This derivation builds on an existing analysis of numerical dispersion in finite element meshes and extends it to anisotropic media and the analysis of numerical reflections. Closed form expressions for the numerical dispersion and numerical reflection predicted at an interface between two biaxial materials in the finite element method are derived. These expressions are then verified against practical FEM simulations with good agreement achieved.

Chapter 4 applies the closed form expressions developed in Chapter 3 to a PML interface resulting in a closed form expression for the numerical reflection from a PML inter-
face in the FEM. Examination of these reflection error relations reveals that the magnitude of reflection is largely governed by the edge length in the direction normal to the PML interface. Based on this observation a novel and highly efficient technique for improving the performance of the PML through a one dimensional mesh compression is developed. This technique is verified by numerical experiment and comparison to published work, with significant improvements in the efficiency of implementation achieved.

In Chapter 5 the compressed PML truncation derived in Chapter 4 is applied to three eigenvalue simulations. The devices simulated are a simple RF microstrip line, a coplanar waveguide electrode of a Mach-Zehnder optical intensity modulator on the anisotropic substrate LiNbO₃, and mode propagation and radiation in a radially bent integrated optic waveguide. The first two simulations demonstrate the use of the PML as a means of truncating the evanescent tails of the modes of lossless waveguides as well a means of absorbing radiation from leaky waveguides. A factor of three improvement in the required solution time is achieved. The final simulation demonstrates the ability of the PML to absorb radiation from a leaky waveguide and hence the range of application of the two dimensional waveguide model is extended to leaky waveguides. Comparison with published results is made with good agreement achieved.

The findings of the investigations conducted in this thesis are summarised in Chapter 6. Items requiring further investigation are identified and areas in which the results of this work could be applied are suggested for future work.

Appendix A provides derivations of the integral equations used in the implementation of the finite element simulator. Appendix B and Appendix C detail methods by which the numerical dispersion and numerical reflection respectively, can be obtained from practical finite element simulations. Appendix D re-derives the integral equations used in the implementation of the Eigenvalue FEM in cylindrical coordinates and comments on the use of conformal mapping to examine waveguide bends.
Chapter 2

Generalising the PML to Biaxial Materials

2.1 Introduction

A significant problem encountered in electromagnetic simulations is the implementation of a computational boundary. Usually, a perfect electric conductor (PEC) boundary, enforcing zero tangential field at the computational boundary to be zero, is sufficient. A particular problem arises, however, when attempting to model radiating structures. In these situations, electromagnetic power propagates away from the structure into free space and is thus lost. A PEC boundary reflects this power back into the structure, and hence provides a poor model of the physical situation.

It is evident that a boundary condition that absorbs radiated power is required. The reported alternatives basically fall into two categories, absorbing boundary conditions (ABCs) which are locally defined annihilation operators, and non-local boundary conditions that effectively match all the elements on the boundary of the internal problem to a set known forms in the exterior. A good summary can be found in Kuzuoglu [2]. The advantage of local ABCs is that they are easily implemented and maintain the local sparse nature of the matrix resulting from many finite methods. Their disadvantage is that they can often be ineffective and must be used inefficiently to perform well. The alternative non-local boundary conditions offer excellent performance at the expense of coupling all of the unknowns on the boundary and hence ruining the sparsity of the problem. Furthermore, for eigenvalue simulations, this coupling can be dependent on the eigenvalue itself, requiring the matrix to be refilled and solved iteratively reducing efficiency.

Recently a very promising boundary condition that is as efficient to implement as a local boundary condition, but can be as effective as a non-local boundary condition, has been suggested. This boundary is the perfectly matched layer (PML).
As stated in Chapter 1, a major goal of this thesis is to improve the efficiency of electromagnetic simulations involving the biaxial material LiNbO$_3$. As is shown in Chapter 5, the PML boundary can be used for this purpose. The current form of the PML in the literature is only suitable for use with isotropic materials, and thus it is necessary to generalise the PML for use with biaxial materials.

It is the goal of this chapter to develop such a PML. Firstly, in Section 2.1.1 the PML is introduced and a literature survey tracing the development of the PML from its proposal to the current state of the art is presented. Section 2.2 presents the derivation from first principles, of a new generalised PML suitable for application to biaxial materials that does not require the modification of Maxwell’s equations. The effectiveness of the biaxial PML in a practical finite element simulation is then demonstrated in Section 2.4 and a brief discussion of the implications of this generalised PML is presented in Section 2.5. Section 2.6 summarises the findings of this Chapter and briefly notes some of the shortcomings of the PML observed in Section 2.4, which form the basis of the investigations conducted in Chapters 3, 4 and 5.

2.1.1 Literature Survey

The perfectly matched layer (PML) was initially proposed by Bérenger in 1994 [1] as a method of bounding open region finite difference time domain (FD-TD) problems. This PML was developed by modifying the differential form of Maxwell’s equations in the time domain by splitting field components into subcomponents. A region of the solution governed by these equations could be coupled to a free space region governed by standard Maxwell’s equations without incurring a reflection at the interface, irrespective of incident angle or frequency. Owing to the split field modification, a conductivity can be introduced to the PML region without altering the reflectionless properties of the interface. Radiated fields from the interior thus pass into the PML without reflection from the PML but are then absorbed by the introduced conductivity, making it an almost ideal absorbing boundary condition (ABC).

Bérenger’s initial proposal was developed using a 2D FD-TD formulation. To reduce numerical reflections, he suggested the use of a quadratically tapered conductivity profile within the PML region, and provided a demonstration indicating orders of magnitude better performance than traditional ABCs. The proposal of the Bérenger PML was a landmark development and has had a major impact on the FD-TD modeling community.

The potential of the PML for use in FD-TD was realised immediately by the modeling community with the new PML being extended to 3D [4], demonstrated in curvilinear and

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1 A recent and independent paper by Teixeira et al. has extended this [3]
non-orthogonal coordinates [5] (later developed by [2, 6, 7, 8, 9]) and demonstrated as a means of truncating guided waves [10], including a demonstration of the termination of a dielectric waveguide indicating that the PML could be used for the truncation of dielectric regions as well as free space.

In the same year, an alternative approach to producing a perfectly matched medium for the truncation of open regions in FD-TD simulations was proposed by Chew and Weedon [11]. In their approach, Maxwell’s equations are modified by stretching the coordinates within the absorbing layer along each axis by complex factors, again resulting in a layer that is perfectly matched to a neighbouring region governed by standard Maxwell’s equations. The complex factors introduced allow for the introduction of material absorption in the modified region. The resulting form of the PML is similar to that proposed by Bérenger [1], however it can be implemented more efficiently in FD-TD simulations.

Shortly afterward, and apparently independently, Rappaport [12] proposed a PML formulation very similar to that of Chew and Weedon [11]. Rappaport’s formulation had the important difference that it was formulated in the frequency domain for use with finite difference frequency domain (FD-FD) simulations. Like Chew and Weedon [11], efficiency gains over Bérenger’s original PML [1] are claimed.

Following the stretched coordinate formulation, an important development was reported by Sacks et al. [13]. In their formulation of the PML, instead of scaling the coordinate axis within the modified layer, a diagonally anisotropic material tensor with variable components was introduced that could be set such that the material exhibited the PML properties previously reported. The importance of this development is that the governing equations within the PML are exact Maxwell’s equations, with modifications made only to the material tensor of the PML layer. The implication of this is that any finite method, and in particular the finite element method (FEM), that can model diagonally anisotropic materials can now use the PML without any modification of its functionality.

Recognising the work of Sacks et al. [13], but being concerned that the resulting PML may be invalid due to embedded sources, Mittra and Pekel [14] return to the split field formulation of Bérenger [1]. They cast the split field formulation in the frequency domain and made several illuminating observations. In particular, they note that in order to formulate a PML that satisfies Maxwell’s equations, non-physical materials must be used and similarly, if physical materials are to be used, Maxwell’s equations must be modified. Shortly afterward Pekel and Mittra demonstrated this frequency domain split field PML in a FEM simulation [15], and then in conjunction with a numerical ABC [16]. It was later shown that the PML described by Sacks et al. [13] is actually passive [17], [18].

1995 also saw researchers become more critical of the PML, with a comparative anal-
ysis by Andrew et al. [19] showing that traditional ABCs could perform as well as the PML boundary. Several researchers began investigating the shortcomings of the PML with respect to its ability to absorb evanescent and near cut-off waves [20],[21], and modifications to allow it to match lossy material [22] and to absorb evanescent waves [23] were proposed. The ability for the PML to absorb evanescent waves was developed further by Fang et al. [24] and Zhao and Cangellaris [25]. It was noted that an appropriate choice of PML parameter can be used to effectively absorb evanescent waves, however, Bérenger[26] has developed his original split field formulation to absorb evanescent waves by introducing a further splitting of the already split fields.

Discussions of optimisation and design methods for PML implementation continued into 1996 and 1997. A lengthy overview by Wittwer and Ziolkowski [27] discusses design considerations, while suggestions for optimum frequency profiles [28], taper profiles [29] were proposed. A link between discretisation levels in the PML layer and PML performance became evident with several studies attempting to analyse the relationship through numerical experiments [30, 31, 32, 33, 34]. Of particular note is the use of numerical reflection errors in the FD-TD by Fang and Wu [31] to produce a closed form expression for the reflection error from a PML interface in the FD-TD.

Also in 1996, reports of the PML's use in other finite methods were reported with Huang et. al. demonstrating the boundary condition both in a finite difference beam propagation method (FD-BPM) [35] and in a 1D FD eigenvalue solution for the radiating modes of a leaky waveguide [36]. Vassallo and Keur [37] present a development of use of PML in the FD-BPM, and Hyun et al. [38] present a further eigenvalue simulation demonstrating the PML as a means of truncating the exterior of a Fabry-Perot resonator in a 1D FEM simulation.

Of interest, Ziolkowski [17], discusses various attempts to realise physical media with characteristics approximating those of the PML using engineered artificial materials.

This brings the investigation of the PML almost to the present day. The final area of interest found in the literature is the extension of the PML to matching anisotropic media. Garcia et al. [39] present an attempt to extend the PML to match uniaxial media. Their work is based on Bérenger's split field formulation [1], and demonstrates that within this formalism only diagonally anisotropic media may be matched. Later this split field technique is further developed to perfectly match anisotropic media at any orientation [40], however as observed by Zhao et al. [41] this formulation is restricted to two dimensions and precludes the implementation of corner regions, even when the anisotropy is of the form of a diagonal tensor. Zhao et al. propose an alternative by reformulating the finite method to include the electric and magnetic displacement. Although this allows the definition of a more general PML that may be applied to corner regions, it requires the use of
special and more computationally expensive finite methods including electric and magnetic displacement vectors. A more general approach developed by Teixeira and Chew [42] develops the split field PML in a far more mathematically abstract fashion, demonstrating that in a general sense, anisotropic, dispersive and lossy media can be treated in exactly the same manner as Bérenger's original PML [1].

The above mentioned techniques are all non-Maxwellian in that they are derived from Bérenger’s split field formulation [1] and thus require the simulation algorithm to be modified in the PML region. As a final word on the extension of the PML to general linear materials, Teixeira and Chew [3] have developed an entirely general formulation of the PML using the metric invariance of Maxwell’s Equations. In this new approach too, the PML is applicable to lossy dispersive and indeed bianisotropic media. Furthermore this PML remains Maxwellian allowing it to be used in any finite method with the capability of modeling general tensors. The method is shown however to be inappropriate for application to non-linear problems. A non-linear version of the split field formulation has been recently published by Zhao [43] and no doubt an un-split variant will follow shortly.

The present work, comprising the remainder of this Chapter and published in [18] is a formulation of a Maxwellian PML for matching biaxial media. It is an extension of the Maxwellian approach to the PML derivation proposed by Sacks et. al [13] and thus differs from [39] [40] [41] and [42] all of which are based on the Bérenger split field formulation.

Unfortunately, the general formulation of [3] was not available until late 1998, as the approach is entirely applicable to the problems analysed in this thesis. Had it been available earlier, the derivation of [3] could have replaced the biaxial derivation of Section 2.2.

### 2.2 Derivation of a generalised PML

As mentioned in the previous section, the anisotropic PML as suggested by Sacks et al. [13] is applicable only to problems consisting of isotropic media. Since a major goal of this thesis is to improve the efficiency of eigenvalue simulations involving the uniaxial material LiNbO₃, and it has been proposed that the PML may be suitable for this purpose, the development of a generalised PML capable of truncating biaxial and uniaxial materials is necessary. It is thus the goal of this section to develop such a PML.

As mentioned previously, the anisotropic PML is simply a fictitious material that can be matched to a real material such that no reflection occurs at their interface irrespective of angle of incidence and frequency. The important property of the PML is that it is not

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2 recently remedied by Teixeira et. al [3]
CHAPTER 2.

Figure 2.1: A plane wave incident on the interface between two general biaxial media.

identical to the material to which it is matched, allowing for the introduction of loss for absorbing transmitted waves or other modifications.

Since in this Section a PML capable of matching a general biaxial material is sought, the derivation begins by defining two general biaxial materials, and then use Maxwell’s equations to apply boundary conditions at their interface that enforce zero reflection. The conditions that the PML material must satisfy to ensure zero reflection for all angles of incidence and frequencies is deduced.

The following derivation can be applied to plane waves traveling in an arbitrary direction in three dimensional space [18], however since the primary goal of this thesis is to examine the application of the PML to two dimensional cross-section eigenvalue problems, and for clarity, the following derivation considers only plane waves traveling in the x-y plane. The resulting form of the PML is identical using either approach.

2.2.1 Some preliminary definitions

Consider the situation depicted in Figure 2.1. Material 1 is the material to be matched and is a general biaxial material with permittivity and permeability given by tensors

$$
\begin{align*}
\varepsilon_1 &= \begin{bmatrix}
\varepsilon_{x1} & 0 & 0 \\
0 & \varepsilon_{y1} & 0 \\
0 & 0 & \varepsilon_{z1}
\end{bmatrix}, \\
\mu_1 &= \begin{bmatrix}
\mu_{x1} & 0 & 0 \\
0 & \mu_{y1} & 0 \\
0 & 0 & \mu_{z1}
\end{bmatrix}
\end{align*}
$$

(2.1)
Similarly the PML material, Material 2, has permittivity and permeability tensors

\[ \varepsilon_2 = \begin{bmatrix} \varepsilon_{x2} & 0 & 0 \\ 0 & \varepsilon_{y2} & 0 \\ 0 & 0 & \varepsilon_{z2} \end{bmatrix}, \quad \mu_2 = \begin{bmatrix} \mu_{x2} & 0 & 0 \\ 0 & \mu_{y2} & 0 \\ 0 & 0 & \mu_{z2} \end{bmatrix} \] (2.2)

Also depicted in Figure 2.1 are the incident and transmitted plane waves. If the TM to z polarisation is considered, with electric field directed only in the z-direction, it is possible to write the propagating plane wave in Material i, where i can be 1 or 2, as

\[ \vec{E}_i = A_i e^{-j k_{x_i} x} e^{-j k_{y_i} y} e^{-j k_{z_i} z} \] (2.3)

where

\[ k_{x_i} = k_0 \sqrt{\varepsilon_{x_i} \mu_{y_i}} \cos \theta_i \] (2.4)
\[ k_{y_i} = k_0 \sqrt{\varepsilon_{z_i} \mu_{z_i}} \sin \theta_i \] (2.5)

Using Maxwell’s equations it is possible to calculate the magnetic field as

\[ \vec{H}_i = -\frac{\vec{E}_i}{\omega \mu_0} \left[ -\frac{k_{y_i}}{\mu_{x}} \hat{x} + \frac{k_{z_i}}{\mu_{y}} \hat{y} \right] \] (2.6)

### 2.2.2 Matching the boundary conditions

The magnitude of the incident field in Material 1 may be arbitrarily set to 1 \( (A_1 = 1) \). Assuming that there is no reflection from the PML interface, this incident wave actually represents the total field in Material 1. The magnitude of the transmitted field in Material 2 is thus \( A_2 = T \), where T is the transmission coefficient. Equation (2.3) in Materials 1 and 2 thus completely describes the fields on either side of the interface. Using this information it is possible to enforce the boundary conditions

\[ \hat{n} \cdot \vec{D}_1 = \hat{n} \cdot \vec{D}_2 \] (2.7)
\[ \hat{n} \cdot \vec{B}_1 = \hat{n} \cdot \vec{B}_2 \] (2.8)
\[ \hat{n} \times \vec{E}_1 = \hat{n} \times \vec{E}_2 \] (2.9)
\[ \hat{n} \times \vec{H}_1 = \hat{n} \times \vec{H}_2 \] (2.10)

where \( \hat{n} \) is the direction normal to the interface, \( E \) and \( H \) represent the electric and magnetic fields respectively and \( B \) and \( D \) represent the magnetic and electric displacement. Assuming that the interface is axially aligned it is possible to choose \( \hat{n} = \hat{x} \) as depicted in Figure 2.1, with the interface located at \( x = 0 \). Since the incident field is polarised TM to z, the boundary conditions of Equations (2.7 - 2.10) may be simplified to
Substituting Equations (2.3) and (2.6) into Equations (2.11 - 2.13) yields

\[ V = f_{x1} \sin(\theta_1) \quad V = f_{x2} \sin(\theta_2) \]  
\[ V = f_{y1} \cos(\theta_1) \quad V = f_{y2} \cos(\theta_2) \]  
\[ e^{-j\kappa_{x1} y} = T e^{-j\kappa_{x2} y} \]  

Evidently there are three equations: (2.14), (2.15), and (2.16), but four unknowns: \( T, f_{x2}, f_{y2} \) and \( \varepsilon_{x2} \). It is thus possible to arbitrarily choose

\[ \varepsilon_{x2} = a_{pml}\varepsilon_{x1} \]  

Substituting this back into Equations (2.14) and (2.15), yields

\[ \sqrt{\varepsilon_{x1}\mu_{x1}} \sin(\theta_1) = \sqrt{\varepsilon_{x2}\mu_{x2}} \sin(\theta_2) \]  
\[ \sqrt{\frac{\varepsilon_{x1}}{\mu_{y1}}} \cos(\theta_1) = \sqrt{\frac{\varepsilon_{x2}}{\mu_{y2}}} \cos(\theta_2) \]  

Squaring both sides of each of the above and rearranging results in

\[ \frac{\mu_{x1}}{\mu_{x2}} \sin^2(\theta_1) = a_{pml} \sin^2(\theta_2) \]  
\[ \frac{\mu_{y2}}{\mu_{y1}} \cos^2(\theta_1) = a_{pml} \cos^2(\theta_2) \]  

The conditions under which both Equations (2.20) and (2.21) are satisfied for all \( \theta_1 \) are

\[ \frac{\mu_{x1}}{\mu_{x2}} = \frac{\mu_{y2}}{\mu_{y1}} = a_{pml} \]  

and hence \( \theta_2 = \theta_1 \).

Thus in summary, the PML tensor components derived are

\[ \mu_{x2} = \frac{\mu_{x1}}{a_{pml}} \]  
\[ \mu_{y2} = a_{pml}\mu_{y1} \]  
\[ \varepsilon_{x2} = a_{pml}\varepsilon_{x1} \]
By duality, it is possible to immediately state the equivalently solution for the TE polarisation by exchanging \( E \) and \( H \), and \( \mu \) and \( \varepsilon \). The result is

\[
\begin{align*}
\varepsilon_{x2} &= \frac{\varepsilon_{x1}}{b_{pml}} \\
\varepsilon_{y2} &= b_{pml}\varepsilon_{y1} \\
\mu_{x2} &= b_{pml}\mu_{x1}
\end{align*}
\]  

(2.26) \hspace{1cm} (2.27) \hspace{1cm} (2.28)

where \( b_{pml} \) is an independent and arbitrary parameter. Since in most cases it is desirable to treat both polarisations equivalently, it is possible to set \( b_{pml} = a_{pml} \) and thus,

\[
\begin{align*}
\varepsilon_{pml} &= \begin{bmatrix} 1/a_{pml} & 0 & 0 \\ 0 & a_{pml} & 0 \\ 0 & 0 & a_{pml} \end{bmatrix} \begin{bmatrix} \varepsilon_{x1} & 0 & 0 \\ 0 & \varepsilon_{y1} & 0 \\ 0 & 0 & \varepsilon_{x1} \end{bmatrix} \\
\mu_{pml} &= \begin{bmatrix} 1/a_{pml} & 0 & 0 \\ 0 & a_{pml} & 0 \\ 0 & 0 & a_{pml} \end{bmatrix} \begin{bmatrix} \mu_{x1} & 0 & 0 \\ 0 & \mu_{y1} & 0 \\ 0 & 0 & \mu_{x1} \end{bmatrix}
\end{align*}
\]  

(2.29) \hspace{1cm} (2.30)

2.3 The PML implementation

In Section 2.2, the PML was generalised such that it can be matched along an axial interface to general biaxial materials. In this section, the means by which this PML can be used as an effective truncation, including the mechanism by which incident waves are absorbed and range of validity, is discussed.

Consider the situation depicted in Figure 2.2. A plane wave is incident on a PML layer at an arbitrary angle \( \theta \). It is then transmitted without reflection through the interface into the PML material. Within the PML material, the propagation constant of the wave can be found from Equations (2.4), (2.5) and (2.29-2.30) to be

\[
\begin{align*}
k_{x2} &= a_{pml}k_{x1} \\
k_{y2} &= k_{y1}
\end{align*}
\]  

(2.31) \hspace{1cm} (2.32)

Thus the wave’s propagation constant within the PML material in the direction normal to the interface is scaled by \( a_{pml} \). If this variable parameter is chosen with an imaginary component, exponential decay in the direction normal to the interface can be achieved. This is typically how the PML is used to absorb propagating waves. The PML layer is however finite and must itself be truncated. Figure 2.2 indicates truncation by a perfect electric conductor (PEC) a distance \( x = d \) from the interface. The transmitted wave
Figure 2.2: The path of a plane wave incident on a layer of PML material truncated by a PEC boundary.

reflects from this truncation, as indicated, and returns back through the PML material to the interface where it is again perfectly transmitted. The ratio of the amplitude of the wave emerging from the conductor backed truncation to the incident wave is thus

\[ \Gamma = e^{-jk_x d \tan \theta_1} e^{-j\alpha_{pml} k_x d} \]  

(2.33)

It is thus evident that the absorption of the PML layer is proportional to \( k_x \). As \( k_x \) approaches zero the effect of the PML layer also approaches zero. Thus the PML cannot absorb waves at glancing incidence, or equivalently, modes propagating in the normal direction near cut-off.

### 2.4 Demonstration of the biaxial PML

Section 2.3 outlined how the generalised PML, derived in Section 2.2, could be used to absorb incident waves. It is the purpose of this section to demonstrate the effectiveness of such a PML truncation in a practical finite element simulation.

The geometry of the simulation investigated is depicted in Figure 2.3, with dimensions as indicated in the caption. The problem consists of a terminated parallel plate waveguide, filled with biaxial material of dielectric tensor
Figure 2.3: The geometry of the simulation used to demonstrate the effectiveness of the biaxial PML; \( d = 1\text{cm}, l = 0.2\text{cm}, h = 4\text{cm} \) with triangles of approximate area \( 10^{-5}\text{cm}^2 \) used throughout. The excitation port is Port 1.

\[
\varepsilon = \begin{bmatrix} 2.5 & 0 & 0 \\ 0 & 2.0 & 0 \\ 0 & 0 & 1.0 \end{bmatrix} \tag{2.34}
\]

and \( \mu = 1 \). The waveguide is truncated at one end with a conductor backed PML layer, with PML variable parameter

\[
a_{pml} = 2 - j \tag{2.35}
\]

resulting in the PML material tensors of

\[
\varepsilon_{pml} = \begin{bmatrix} 2.5/(2 - j) & 0 & 0 \\ 0 & 4 - 2j & 0 \\ 0 & 0 & 2 - j \end{bmatrix}, \quad \mu_{pml} = \begin{bmatrix} 1/(2 - j) & 0 & 0 \\ 0 & 2 - j & 0 \\ 0 & 0 & 2 - j \end{bmatrix} \tag{2.36}
\]

Modes launched at Port 1 proceed to the PML truncation, traverse the PML layer where they are attenuated, reflect from the PEC termination and re-emerge at Port 1. The ratio of the power in the wave emerging from Port 1 to that of the launched wave is calculated as a function of frequency. The finite element method used to perform this simulation is described in Appendix A. In this instance, edge basis functions are used.

The results of the simulation for the fundamental TEM mode is presented in Figure 2.4. The data points depict the reflected power resulting from the finite element simulation,
Figure 2.4: The results of the finite element simulation of the truncation of the TEM fundamental mode by a generalised biaxial PML.

Figure 2.5: The results of the finite element simulation of the truncation of the TM₁ first order mode by a generalised biaxial PML.
while the solid line indicates the magnitude expected from Equation (2.33), with

\[
k_x = \sqrt{k_0^2 \varepsilon_y - \frac{\varepsilon_y}{\varepsilon_x} \left( \frac{m \pi}{h} \right)^2}
\]  
(2.37)

for the TM\(_m\) mode. Although significant absorption across the range of frequencies examined is evident, significant deviation from the expected absorption is evident at higher frequencies.

The results of the simulation for the first order TM\(_1\) mode is presented in Figure 2.5, with the data points depicting the reflected power from the FEM simulation, while the solid line indicates the reflection expected from Equations (2.33) and (2.37). Here, absorption is observed both when the wave is propagating and when it is evanescent. This is due to the fact that the PML variable parameter was chosen with a real component as well as an imaginary component. This ability to absorb evanescent waves makes the PML boundary condition suitable for the truncation of eigenvalue simulations as is demonstrated in Section 5.

At cut-off the wave is not propagating in the x-direction and thus according to Equation (2.33), the observed zero absorption at this frequency is to be expected. Again, deviation from the predicted absorption is evident at higher frequencies.

In neither of the above investigations did the PML behave in exactly the manner predicted. It has been suggested [30] that these deviations are due to numerical reflection from the PML interface caused by approximations made in the finite element method itself. Since it is these numerical reflections that are the major limiting factor to the efficient implementation of the PML in the finite element method [44], a significant proportion of this thesis is dedicated to the understanding of these limitations. Chapter 3 investigates the nature of numerical reflection and dispersion in the finite element method, and Chapter 4 then examines the numerical reflection at a PML interface and develops a technique for efficiently reducing their effect.

The above discussion is not limited to the biaxial PML as derived in Section 2.2, but is applicable to PML’s of isotropic media as well. There are however a few points of interest that are specific to the biaxial PML. These are discussed briefly in the following section.

### 2.5 Implications of the biaxial PML

As mentioned previously, the observations made in Section 2.4 are not specific to the biaxial PML as derived in Section 2.2, being equally applicable to PMLs of isotropic media. There are however several implications of the biaxial PML in particular that are worth noting.
Although the biaxial PML as derived in Section 2.2 seems limited in application to the narrow range of problems involving biaxial materials, PMLs of this form, although they have not been identified as such, have already been demonstrated in several less specific applications. If it is noted that a PML layer of an isotropic material is itself uniaxial in form, then to place a second PML adjacent to the first in manner that does not produce reflections would require both PMLs to be matched to one and other. Two instances where such interfaces have been demonstrated are multi-layer graded PML’s and corner regions.

2.5.1 Multilayer Graded PML’s

As a means of minimising the numerical reflections from PML interfaces, the use of graded PML’s has been suggested, originally by Bérenger [1]. As a means of achieving this, Polycarpou et al. [30] suggest subdividing the PML region into a number of steps of constant PML variable parameter as depicted in Figure 2.6. The PML variable parameter is graded polynomially from unity to some large value such that the contrast between any two adjacent layers is minimal.

If the PML variable parameter for each layer is \( a_{pml}(x_j) \) then the tensors of layer \( j \) can be written

\[
\begin{align*}
\bar{\varepsilon}_{pml}(x_j) &= \begin{bmatrix} 1/a_{pml}(x_j) & 0 & 0 \\ 0 & a_{pml}(x_j) & 0 \\ 0 & 0 & a_{pml}(x_j) \end{bmatrix} \cdot \bar{\varepsilon}_r
\end{align*}
\] (2.38)

\[
\begin{align*}
\bar{\mu}_{pml}(x_j) &= \begin{bmatrix} 1/a_{pml}(x_j) & 0 & 0 \\ 0 & a_{pml}(x_j) & 0 \\ 0 & 0 & a_{pml}(x_j) \end{bmatrix} \cdot \bar{\mu}_r
\end{align*}
\] (2.39)

and the tensors for layer \( j+1 \)

\[
\begin{align*}
\bar{\varepsilon}_{pml}(x_{j+1}) &= \begin{bmatrix} 1/a_{pml}(x_{j+1}) & 0 & 0 \\ 0 & a_{pml}(x_{j+1}) & 0 \\ 0 & 0 & a_{pml}(x_{j+1}) \end{bmatrix} \cdot \bar{\varepsilon}_r
\end{align*}
\] (2.40)

\[
\begin{align*}
\bar{\mu}_{pml}(x_{j+1}) &= \begin{bmatrix} 1/a_{pml}(x_{j+1}) & 0 & 0 \\ 0 & a_{pml}(x_{j+1}) & 0 \\ 0 & 0 & a_{pml}(x_{j+1}) \end{bmatrix} \cdot \bar{\mu}_r
\end{align*}
\] (2.41)

which may be re-written

\[
\begin{align*}
\bar{\varepsilon}_{pml}(x_{j+1}) &= \begin{bmatrix} a_{pml}(x_j) & 0 & 0 \\ 0 & a_{pml}(x_{j+1}) & 0 \\ 0 & 0 & a_{pml}(x_{j+1}) \end{bmatrix} \cdot \bar{\varepsilon}_{pml}(x_j)
\end{align*}
\] (2.42)
Figure 2.6: A graded PML. The matched media has dielectric $\varepsilon_r$, the first layer of the PML has PML variable parameter $a$, while the second has PML variable parameter $b$. The PML permeabilities are not shown.

Thus the layer $j+1$ is a PML of the layer $j$ with a PML parameter $a_{pml}(x_{j+1})/a_{pml}(x_j)$. Hence, in the absence of numerical reflections, any grading profile should be possible with no reflection from any interface.

2.5.2 Corner regions

If a PML truncation is used in a two or three dimensional problem, there will be places where PML truncations with orthogonal normal directions meet. The suggested method for implementing such corner regions is in fact the use of a biaxial PML[45].

Consider the situation depicted in Figure 2.7. Again, treating the PML layers as biaxial media, the corner region must be able to match the PML with normal in the $x$ direction across an interface in the $y$-direction. Thus if the $x$-directed PML has the form

\[
\bar{\varepsilon}_{pmlx} = \begin{bmatrix}
1/a_{pmlx} & 0 & 0 \\
0 & a_{pml} & 0 \\
0 & 0 & a_{pmlx}
\end{bmatrix} \cdot \bar{\varepsilon}_r,
\bar{\mu}_{pmlx} = \begin{bmatrix}
1/a_{pmlx} & 0 & 0 \\
0 & a_{pmlx} & 0 \\
0 & 0 & a_{pmlx}
\end{bmatrix} \cdot \bar{\mu}_r
\] (2.44)

\[
\bar{\mu}_{pml} (x_{j+1}) = \begin{bmatrix}
\frac{a_{pml}(x_j)}{a_{pml}(x_{j+1})} & 0 & 0 \\
0 & \frac{a_{pml}(x_{j+1})}{a_{pml}(x_j)} & 0 \\
0 & 0 & \frac{a_{pml}(x_{j+1})}{a_{pml}(x_j)}
\end{bmatrix} \cdot \bar{\mu}_{pml} (x_j)
\] (2.43)
then the corner region must be of the form

\[
\begin{align*}
\varepsilon_{\text{pml}} &= \begin{bmatrix}
\alpha_{\text{pml}x}^{\text{car}} & 0 & 0 \\
0 & 1/\alpha_{\text{pml}y}^{\text{car}} & 0 \\
0 & 0 & \alpha_{\text{pml}y}^{\text{car}}
\end{bmatrix} 
\begin{bmatrix}
1/\alpha_{\text{pml}x} & 0 & 0 \\
0 & \alpha_{\text{pml}x} & 0 \\
0 & 0 & \alpha_{\text{pml}x}
\end{bmatrix} \cdot \begin{bmatrix}
\varepsilon_r \\
\mu_r
\end{bmatrix} 
\end{align*}
\]

Similarly matching the y directed PML to the corner results in

\[
\begin{align*}
\varepsilon_{\text{pml}} &= \begin{bmatrix}
1/\alpha_{\text{pml}x}^{\text{car}} & 0 & 0 \\
0 & \alpha_{\text{pml}y}^{\text{car}} & 0 \\
0 & 0 & \alpha_{\text{pml}y}^{\text{car}}
\end{bmatrix} 
\begin{bmatrix}
\alpha_{\text{pml}y} & 0 & 0 \\
0 & 1/\alpha_{\text{pml}y} & 0 \\
0 & 0 & \alpha_{\text{pml}y}
\end{bmatrix} \cdot \begin{bmatrix}
\varepsilon_r \\
\mu_r
\end{bmatrix} 
\end{align*}
\]

It is evident that making

\[
\alpha_{\text{pml}x}^{\text{car}} = \alpha_{\text{pml}x} 
\]
satisfies both conditions.

The resulting form for the corner region is thus

\[
\begin{align*}
\varepsilon_{\text{pm1}}^{\text{cnr}} &= \varepsilon_{\text{pm1}} \\
\mu_{\text{pm1z}}^{\text{cnr}} &= \mu_{\text{pm1}} \\
\end{align*}
\]

as reported in [45].

\section*{2.6 Conclusions}

In this chapter a generalised form of the PML suitable for application to biaxial materials is derived. The use of this material as a means of truncating finite element simulations involving biaxial materials is discussed and the performance of such a truncation in a practical finite element simulation is demonstrated. Several limitations of this PML truncation are identified. The newly derived biaxial PML is also presented as a means for explaining previously suggested methods of implementing PML corners and proves that in the absence of numerical errors, any PML may be arbitrarily graded in the normal direction without incurring any reflection.

During the practical demonstration of the PML in truncating the parallel plate waveguide in Section 2.4, it is evident that numerical reflections can limit the performance of the PML. As has been discussed in [44], this is one of the major limitations of the PML and it significantly reduces the efficiency of the PML in practice. It is thus the goal of the following chapters to investigate the nature of these reflections and present some techniques for their efficient minimisation.
Chapter 3

The Nature of Numerical Errors in the Finite Element Method

3.1 Introduction

The perfectly matched layer (PML) has been widely used as a means of truncating the solution region of numerical problems. In the main it has found use in finite difference time domain (FDTD) simulations [1], where it is an excellent solution to the problem of radiated energy returning into the solution region causing late time instabilities. More recently, it has found equivalent use [15][30] in the finite element method (FEM) where it can be used to model transitions into free space that would otherwise need to be treated with integral equation based radiation boundary conditions.

In Chapter 2 a generalisation of the PML suitable for the truncation of regions consisting of biaxial materials was developed. Further, it was proposed that this PML, or others for that matter, would be well suited to the truncation of frequency domain eigenvalue problems often encountered in waveguide models. The role of the PML in these instances is to reduce the number of unknowns that are required to model the infinite space surrounding a problem.

Many authors have investigated the performance and optimisation of the PML for truncating problems in finite difference methods[31]. A few, notably [30][44], have investigated the performance of the PML when used with a deterministic finite element method. Investigators of the FDTD method have developed implementations with PML layers that are only four elements deep[31]. The same is not true for the finite element method. The authors of [44] discovered vast quantities of unknowns are required for comparably effective PML boundaries.

If the PML is to be used as a means of reducing the number of unknowns required to accurately model waveguide problems, its implementation must be efficient. The number
of unknowns required to sufficiently implement the PML must be small enough so as not to outweigh the gains due solution space reduction. It is thus important to analyse the performance of the PML in detail to discover guidelines for its optimal design.

To this end, it is necessary to consider the mechanism by which the PML fails in practical situations. Chapter 2 has shown that the PML is entirely transmitting irrespective of frequency, angle of incidence and material properties. In practical numerical simulations, the levels of reflection from PML truncations are larger than would be expected from the ideal theory [30]. Ripples in the observed reflection response over frequency suggest reflections between discontinuities which in turn suggest that the solution region/PML interface is not reflectionless.

In this Chapter the important differences between the physical electromagnetics, as governed by Maxwell’s equations, and that modeled by the finite element method are examined. In particular numerical dispersion and numerical reflection errors, resulting from the finite element method, for interfaces between general biaxial materials, are investigated in detail. The dependencies of these numerical errors for the particular case of a PML interface are identified and hence methods for optimal reduction of undesirable reflections are developed. Finally, an improved PML scheme is proposed and verified against published schemes.

### 3.2 Numerical dispersion

In numerical methods, the solutions are never exact. In the limit of infinite unknowns, and hence infinite mesh density, the numerical solution should approach the exact solution, and for the finite element method this is shown to be the case shortly. A good characteristic parameter to evaluate the effect of finite element mesh discretisation on a solution is the dispersion that is modeled, incorporating both the phase velocity and the attenuation of a propagating wave. The dispersion modeled by a numerical method is often termed the numerical dispersion, and the difference between this and the exact dispersion is termed the numerical dispersion error.

For obvious reasons, it is not possible to solve a problem with infinite mesh density and often it is not practical to solve problems with even large mesh densities. In most cases it is desirable to solve a problem with the minimum required unknowns to achieve a nominal tolerable error. To do this efficiently, such that you can choose the correct mesh density for a given dispersion error before solving the problem, it is necessary to understand the relationship between numerical dispersion and discretisation.

Warren and Scott [46][47][48] have derived the numerical dispersion for a number of mesh types including triangular, rectangular and quadrilateral for both edge and node ba-
sis functions and for various interpolation orders. These have, however, been calculated assuming isotropic media. This thesis deals with anisotropic materials, in particular the PML. Hence, an investigation of the numerical dispersion resulting from discretisation of anisotropic materials must be conducted to discover more efficient means of implementing PML solution region truncation.

3.2.1 Derivation of the numerical dispersion relations

The formulation of the finite element method used in this study is detailed in Appendix A. The two dimensional coordinate system is depicted in Figure 3.1. Since the z-direction is infinite and unvarying, the plane wave solutions to Maxwell’s equations in this coordinate system can be divided into transverse electric (TE) solutions with electric field directed only in the z-direction, and magnetic field in the plane of the problem and transverse magnetic (TM) solutions with electric field directed in the plane of the problem and magnetic field in the z-direction only. Since any solution to Maxwell’s equations can be made up of a superposition of plane wave solutions, it suffices to consider only these solutions.

The field formulation of the FEM used in this investigation, can have two equivalent implementations, either solving for unknowns representing the electric field, from which the magnetic field can be calculated or conversely where the unknowns represent the magnetic field, from which the electric field may be calculated. These are called the E-field and H-field formulations respectively. Thus in the E-field formulation, a TE mode would be modeled using node basis functions and the TM using edges. Throughout this chapter only the TE polarisation will be considered. Thus to investigate the nodes, the E-field formulation will be used with the nodes representing the z-directed E-field component of the TE mode, and to investigate the edges, the H-field formulation will be used with the edges representing the H-field component of the TE mode in the x-y plane. To alternate between E-field and H-field formulations it is simply a matter of exchanging the material parameters \( \varepsilon \) and \( \mu \) and the PEC and PMC boundary conditions.

In this investigation elements of the form of equilateral triangles are assumed. This assumption was made since the mesh generator used in this study [49] aims to provide equilateral triangles. It will be shown later that this assumption approximates the actual situation of a random distribution of imperfect triangular elements.

**Derivation of the numerical dispersion relation for node basis functions**

Consider the portion of mesh depicted in Figure 3.2. Following the procedure in [47], a TE polarised plane wave propagating in the x-y plane is placed on this mesh. The field at any point can be related to that at any other point by a phase shift. In the particular case
Figure 3.1: Coordinate system and definition of TE and TM polarisation

of Figure 3.2, all nodes can be related to node $E_1$ by,

$$
E_2 = e^{-ja}e^{jb}E_1 \quad (3.1)
$$

$$
E_3 = e^{-ja}e^{-jb}E_1 \quad (3.2)
$$

$$
E_4 = e^{-2jb} \quad (3.3)
$$

$$
E_5 = e^{ja}e^{-jb}E_1 \quad (3.4)
$$

$$
E_6 = e^{ja}e^{jb}E_1 \quad (3.5)
$$

$$
E_7 = e^{2jb} \quad (3.6)
$$

where

$$
a = k_x \sqrt{3} L/2 \quad (3.7)
$$

$$
a = \sqrt{3}/2k_0\sqrt{\varepsilon_{zz}\mu_{yy}} L \beta \cos(\theta) = \sqrt{3}/2c_y \beta \cos(\theta) \quad (3.8)
$$

$$
b = k_y L/2 \quad (3.9)
$$

$$
b = 1/2k_0\sqrt{\varepsilon_{zz}\mu_{zz}} L \beta \sin(\theta) = 1/2c_x \beta \sin(\theta) \quad (3.10)
$$

in which

$$
c_x = k_0\sqrt{\varepsilon_{zz}\mu_{zz}} L \quad (3.11)
$$

$$
c_y = k_0\sqrt{\varepsilon_{zz}\mu_{yy}} L \quad (3.12)
$$

and $\beta$ is the normalised numerical dispersion, which should ideally be 1.

The general local matrix for a triangular finite element is given in 3.11. If the triangle is assumed to be an equilateral triangle as depicted in Figure 3.2, then the local matrices can be expressed as:

$$
-k_0^2 \varepsilon_{zz} L^2 \sqrt{3}/48 \begin{bmatrix}
2A & B & B \\
B & 2C & D \\
B & D & 2C
\end{bmatrix}
\begin{bmatrix}
E_1 \\
E_2 \\
E_3
\end{bmatrix}
$$

(3.11)

for both the upward and downward pointing triangle where
Figure 3.2: a) A portion of hexagonally symmetric finite element mesh with node basis functions labelled. b) A single element with dimensions shown.

For a single unknown, $E_1$ in Figure 3.2, is considered, the residual contributions from all of the surrounding nodes can be summed to give

$$(4A + 8C)E_1 + 2D(E_4 + E_7) + 2B(E_3 + E_6 + E_2 + E_5) = 0. \quad (3.16)$$

Substituting Equations (3.1-3.6), and eliminating $E_1$ results in

$$(A + 2C) + D(\cos(2\theta)) + 2B \cos(a) \cos(b) = 0. \quad (3.17)$$

For a given $c_x$, $c_y$ and $\theta$, this is a transcendental expression that may be solved numerically to yield the normalised numerical dispersion $\beta$. This solution can be found using the simplex method, or other basic complex root finding algorithm. This relationship suggests that the dispersion is affected equally by changes in material parameters $\mu$ and $\epsilon$, mesh dimensions $L$, frequency $k_0$. Taking the limit as $L$ approaches 0, yields the expression

$$\beta^2 + O(c_x^2, c_y^2) = 1 \quad (3.18)$$

where $O(c_x^2, c_y^2)$ represents terms in $c_x$ and $c_y$ of the second order and beyond. This suggests that the calculated solution should approach the exact solution ($\beta = 1$) quadratically with $c_x$ and $c_y$. 

\[ A = 1 - \frac{8}{c_y^2} \quad (3.12) \]
\[ B = 1 + \frac{8}{c_y^2} \quad (3.13) \]
\[ C = 1 - \frac{6}{c_x^2} - \frac{2}{c_y^2} \quad (3.14) \]
\[ D = 1 + \frac{12}{c_x^2} - \frac{4}{c_y^2}. \quad (3.15) \]
Figure 3.3: The anisotropy induced by a perfect hexagonally symmetric mesh on an otherwise isotropic problem for node basis functions. $c_x = 0.1$, (a) normalised dispersion error as a function of propagation angle to the x axis, (b) the same plot presented in polar form to highlight the low level of anisotropy.
It is interesting to note that in the case of an isotropic medium, when \( c_x = c_y \), there is still a dependence on \( \theta \), and hence anisotropy that is imposed by the mesh. Figure 3.3 shows the normalised numerical dispersion, defined

\[
\delta_\beta = \left| 1 - \beta_{\text{calc}} \right|
\]

as a function of propagation angle through the mesh depicted in Figure 3.2, with the material constants of air. It can be seen that this anisotropy is negligible. In a random mesh, as has been assumed here, this anisotropy is averaged due to the random orientation of the triangles within the mesh. In the special case of the PML, \( c_x \) and \( c_y \) will become related to a single variable. The significance of this in the design and optimisation of a PML is discussed in Chapter 4.

**Edge basis function numerical dispersion in a hexagonally symmetric triangular mesh**

![Diagram](image)

Figure 3.4: a) A portion of hexagonally symmetric finite element mesh with edge basis functions labelled. b) A single element with dimensions shown

Consider the portion of mesh depicted in Figure 3.4. A TE polarised plane wave, propagating in the x-y plane, is projected onto this mesh. The H field formulation is used to investigate the edges and thus edge unknowns correspond to the x-y directed H-field. The whole mesh can be spanned by three edge functions, \( \vec{H}_1, \vec{H}_2, \vec{H}_3 \) translated by appropriate phase shifts. In this particular case

\[
H_4 = e^{-ja}e^{jb}H_2
\]
\[
H_5 = e^{-ja}e^{-jb}H_3
\]
\[
H_6 = e^{-2jb}H_3
\]
\[
H_7 = e^{ja}e^{-jb}H_1
\]
where, \(a\) and \(b\) are defined in Equations (3.7) and (3.8) respectively. The closed form local matrix for the equilateral finite element, relating the edges, is

\[
\frac{\sqrt{3}}{72\epsilon_{zz}} \begin{bmatrix}
A & B & B \\
B & C & D \\
B & D & C \\
\end{bmatrix}
\]

(3.26)

for both the upward and downward pointing triangle where

\[
A = -c_x^2 - 9c_y^2 + 96
\]

(3.27)

\[
B = -c_x^2 + 3c_y^2 + 96
\]

(3.28)

\[
C = -7c_x^2 - 3c_y^2 + 96
\]

(3.29)

\[
D = 5c_x^2 - 3c_y^2 + 96.
\]

(3.30)

Summing the contributions from the four elements depicted in Figure 3.4 results in

\[
2AH_1 + B(H_2 + H_4 + H_3 + H_5) = 0
\]

(3.31)

\[
B(H_1 + H_7) + 2CH_2 + D(H_3 + H_6) = 0
\]

(3.32)

\[
B(H_1 + H_8) + D(H_2 + H_9) + 2CH_3 = 0.
\]

(3.33)

Substituting Equations (3.20) - (3.25) into Equations (3.31)-(3.33) yields a system of equations that may be rewritten in terms of a matrix as

\[
\begin{bmatrix}
2A & B(1 + e^{-ja}e^{jb}) & B(1 + e^{ja}e^{-jb}) \\
B(1 + e^{ja}e^{-jb}) & 2C & D(1 + e^{-2jb}) \\
B(1 + e^{ja}e^{jb}) & D(1 + e^{2jb}) & 2C \\
\end{bmatrix}
\begin{bmatrix}
H_1 \\
H_2 \\
H_3 \\
\end{bmatrix} = 0.
\]

(3.34)

Solving this system results in the relationship

\[
D(AD - B^2) \cos^2(b) + (C - D)B^2 \cos(a) \cos(b) - C(AC - B^2) = 0.
\]

(3.35)

Again, for given \(c_x\), \(c_y\), and \(\theta\), this transcendental equation may be solved to obtain the normalised numerical dispersion \(\beta\). It can again be seen that for a given direction of propagation the numerical dispersion is determined by the two parameters \(c_x\) and \(c_y\). In the limit as \(c_x\) and \(c_y\) approach zero, Equation (3.35) reduces to

\[
96c_y^2(\beta^2 - 1) + (6c_y^4\beta^2 - 2c_x^2c_y^2)(\beta^2 - 1) + c_y^2(c_y^2 - c_x^2\beta^2) + \\
(12c_x^2c_y^2 - 10c_y^4 - 2c_x^4)\beta^2 \cos^2 \theta + (4c_x^2c_y^2 - 6c_y^4 + 2c_x^4)\beta^4 \cos^4 \theta + \\
12c_x^2(c_y^2 - c_x^2)\beta^4 \cos^4 \theta + O(c_x^6, c_y^6) = 0
\]

(3.36)
If the material is isotropic, \( c_x = c_y = c \), this reduces to
\[
(96 + 6c^2\beta^2 - 2c^2)(\beta^2 - 1) + O(c_x^4, c_y^4) = 0
\]
(3.37)

Alternatively, if the material is anisotropic, then the expression reduces to
\[
(\beta^2 - 1) + O(c_x^2, c_y^2) = 0.
\]
(3.38)

Thus, in the anisotropic case, the error is quadratic with \( c_x \) and \( c_y \). This suggests that the errors in an isotropic mesh should approach the exact solution far more rapidly with reducing \( c_x \) and \( c_y \) than that of an anisotropic mesh for the edge elements. Since the node basis function dispersion error has been found to be quadratic also, it would be expected that the dispersion of both edges and nodes in an anisotropic media should vary with \( c_x \) and \( c_y \) in a similar fashion.

Equation (3.35) has a dependence on \( \theta \) and thus anisotropy due to the discretisation of the problem would again be expected. The dispersion error for a plane wave, propagating at an angle to a perfect hexagonal mesh through an isotropic material, as a function of propagation angle, is shown in Figure 3.5. It is evident that the anisotropy is very strong (approximately 1 : 2), and that the overall level of dispersion error is very much lower than that calculated for the nodes in Section 3.2.1.

To examine the effects of anisotropy on the predicted numerical dispersion, anisotropy of \( c_y = 1.1c_x \) was introduced. The dispersion error of a plane wave traveling through this mildly anisotropic material, as a function of propagation angle is depicted in Figure 3.6. Extreme anisotropy of orders of magnitude is evident, and a much larger maximum numerical dispersion is evident. This suggests that the numerical dispersion of edge basis functions is very sensitive to even small amounts of material anisotropy. Implications of this is discussed in Section 3.2.3.

### 3.2.2 Verification of the numerical dispersion calculation

The derivation in Section 3.2.1 was conducted assuming that the mesh in question was composed of identical equilateral triangles configured in a hexagonally symmetric pattern. In most practical problems this will not be the case. Most mesh generators will attempt to produce equilateral triangles of a given area, but are constrained to fit the geometry of the problem. It is the purpose of this section to demonstrate that the biaxial dispersion simulated for a practical finite element problem on a non-ideal mesh is approximated well by the ideal derivations of the previous sections.
Figure 3.5: The anisotropy induced by a perfect hexagonally symmetric mesh on an otherwise isotropic problem for edge basis functions. $c_x = 0.1$, (a) normalised dispersion error as a function of propagation angle to the x axis, (b) the same plot presented in polar form to highlight the high level of anisotropy.

Figure 3.6: The anisotropy induced by a perfect hexagonally symmetric mesh on a mildly anisotropic problem for edge basis functions. $c_x = 0.1$, (a) normalised dispersion error as a function of propagation angle to the x axis, (b) the same plot presented in polar form to highlight the high level of anisotropy.
CHAPTER 3.

The parallel plate waveguide as a test geometry

A parallel plate waveguide, as depicted in Figure 3.7, is used to characterise the dispersion properties of a practical finite element mesh. This is chosen for its simplicity, well confined geometry, and the existence of a closed form solution. The phase shift and attenuation experienced by a wave propagating through a length of this waveguide should reveal the dispersion properties as modeled by the finite element method.

The task becomes more complex, however, when the method by which a guided mode enters and exits the solution region is considered. An exact closed form solution is coupled between an input or output port and the solution region using the method described in Section A. Since the exterior mode is an exact solution of the parallel plate waveguide, it will have ideal dispersion. This is coupled to a finite element approximation to the waveguide with a slightly different numerical dispersion, and therefore some small reflection at the port interface would be expected.

Thus to accurately extract the numerical dispersion in this waveguide, the effects of these reflections need to be removed from the calculated reflection and transmission results. This process is called de-embedding. The procedure used for de-embedding in this particular case is detailed in Appendix B.

![Figure 3.7: Geometry of a parallel plate waveguide used in the investigation of numerical dispersion. Path of a guided mode incident at port one and subject to multiple reflections shown.](image-url)
3.2.3 Numerical experiments to verify the numerical dispersion relations

In Appendix E, a procedure by which the dispersion of waves propagating through a finite element mesh could be isolated from the reflections at the input and output ports is derived. Thus it is possible to extract the dispersion that is modeled by an imperfect finite element mesh under various conditions, and compare this with both the exact dispersion as predicted by Maxwell’s equations and the predicted dispersion error of Section 3.2.1.

Two test cases are considered. Firstly the simple case of propagation of the fundamental mode through a parallel plate waveguide loaded with isotropic dielectric are investigated. This case is used to determine the relevant parameters of the problem that affect the numerical dispersion and how well these match those indicated by the expressions derived in Section 3.2.1.

The parallel plate waveguide is also used to investigate propagation through a biaxial medium. For these investigations, however, the fundamental mode can not be used, since it travels along an axis of the material and hence interacts with only one of the tensor components of the biaxial material. It is thus necessary to examine the propagation of higher order modes of the parallel plate waveguide as these interact with more than one of the tensor components of the material. A higher order mode of a waveguide can be thought of as the superposition of two plane waves traveling at equal and opposite angles to the overall propagation axis. This angle is

\[
\sin(\theta) = \left( \frac{m \pi}{W} \right) \frac{1}{k_0 \sqrt{\varepsilon_{zz} \mu_{xx}}}.
\]

where \( m \) is the order of the mode and \( W \) is the width of the waveguide. Thus, by using this angle in Equations (3.17) and (3.35), it is possible to arrive at an approximate numerical dispersion for a higher order mode of a parallel plate waveguide filled with biaxial media.

In both the expression for the node basis dispersion, Equation (3.17), and the edge basis dispersion, Equation (3.35), the equations are characterised by the two variables \( c_x \) and \( c_y \). In the isotropic case these variables are identical and hence the dispersion depends on a single variable \( c \). In each of the following investigations dispersion error is measured as a function of these parameters.

Verification of the numerical dispersion of nodes

In this Section, the numerical dispersion that is observed in a practical mesh of nodal basis functions is investigated. The investigation is conducted firstly for an isotropic medium by examining the dispersion calculated for the fundamental mode of a parallel plate waveguide, and then for a biaxial material through examination of higher order modes of a
material filled parallel plate waveguide. The parallel plate waveguide geometry is depicted in Figure 3.7, with a width of 4 cm, and lengths of 0.2 cm and 0.25 cm used for de-embedding.

The isotropic numerical dispersion is investigated by simulating the propagation of the fundamental TE mode through the parallel plate waveguide, using the E-field formulation, and de-embedding the numerical dispersion as described in Section B. This numerical dispersion is plotted as a function of the parameter $c_x = c_y$ as defined in Equation (3.9). To verify that it is possible to consider the material constant, mesh edge length and frequency as aspects of a single variable parameter, the value of $c_x$ is varied by adjusting each of these parameters as detailed in Table 3.1. It is worth noting that the lengths of the waveguides used in the varying mesh density simulation were tripled to 0.6 cm and 0.75 cm to accommodate the larger triangle of the more coarse mesh densities used.

The results of this simulation are plotted in Figure 3.8. The normalised numerical dispersion errors resulting from varying material constant, mesh density and frequency are denoted by diamonds, crosses and squares respectively. A log-log scale is used for easy comparison of the polynomial order of dependence on $c_x$. It is evident that the influence of these parameters on the numerical dispersion error is equivalent. The theoretical numerical dispersion, resulting from the solution of Equation (3.17), is represented by a solid black line. A very good match to the finite element calculation is seen, in particular the quadratic dependence on $c_x$ predicted by Equation (3.18) is clear.

The biaxial numerical dispersion is investigated by simulating the propagation of the first order TE through the parallel plate waveguide. Again the calculated numerical dispersion error is plotted as a function of the parameter $c_x$. For this investigation only the mesh density is varied, as variations in frequency and material constant would alter the guiding properties of the mode. The range of values used in these simulations is given in Table 3.2.

The results of this investigation are plotted in Figure 3.9. The diamonds represent the normalised numerical dispersion error extracted from the finite element simulation, and the solid line represents the theoretical dispersion error resulting from the solution of Equation (3.17) with an angle given by Equation (3.39). Again, very good agreement is observed between the theory and the practical finite element calculation.

The dispersion appears quadratic, as noted by Warren and Scott [47], and it is evident that varying the three different variables of the problem have had very similar effects on the numerical dispersion observed. The solid line in this figure represents the magnitude of the theoretical numerical dispersion error as calculated by subtracting the solution of Equation (3.17) from the closed form waveguide solution. Excellent agreement is observed, despite the fact that the meshes used were not perfectly hexagonal arrangements.
Table 3.1: Variables used in the investigation of numerical dispersion of the fundamental TE mode of a parallel plate waveguide loaded with isotropic dielectric.

<table>
<thead>
<tr>
<th>Case</th>
<th>$k_0$ (cm)</th>
<th>$l$ (cm)</th>
<th>$\sqrt{\epsilon_\infty \mu_\infty}$</th>
<th>$c_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ranging frequency</td>
<td>1 - 3</td>
<td>0.045</td>
<td>1</td>
<td>0.045-0.135</td>
</tr>
<tr>
<td>Ranging edge-length</td>
<td>1</td>
<td>0.03-0.1</td>
<td>1</td>
<td>0.03-0.1</td>
</tr>
<tr>
<td>Ranging dielectric</td>
<td>1</td>
<td>0.045</td>
<td>1 - 4</td>
<td>0.045-0.18</td>
</tr>
</tbody>
</table>

Verification of the numerical dispersion of edges

The procedure used to verify the nodes in Section 3.2.3, is repeated for the edge basis functions. Firstly, the dispersion of the fundamental mode of a parallel plate waveguide propagating through an isotropic medium is considered. Since the fundamental mode of the parallel plate waveguide has its electric field directed in the y direction, the E-field formulation, as described in Section 3.2.1, was used for the following investigations. The parameters used in the simulation are again as given by Table 3.1 and dispersion error as a function of material constant, mesh density and frequency is examined.
Figure 3.9: Comparison of dispersion error observed and predicted for the anisotropic waveguide simulation as a function of \( e_x \) using nodes. The dispersion error resulting from varying the mesh edge length is denoted by diamonds while the dispersion error that would be expected for a perfect hexagonal mesh is denoted by a solid line.
Table 3.2: Variables used in the investigation of numerical dispersion of the first order TE mode of a parallel plate waveguide loaded with anisotropic dielectric.

<table>
<thead>
<tr>
<th>Case</th>
<th>$k_0$</th>
<th>$l$ (cm)</th>
<th>$\sqrt{\varepsilon_x \mu_z}$</th>
<th>$\sqrt{\varepsilon_y \mu_z}$</th>
<th>$c_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ranging frequency</td>
<td>1 - 3</td>
<td>0.045</td>
<td>1</td>
<td>2</td>
<td>0.045-0.135</td>
</tr>
<tr>
<td>Ranging edge-length</td>
<td>1</td>
<td>0.03 - 0.1</td>
<td>1</td>
<td>2</td>
<td>0.03-0.1</td>
</tr>
<tr>
<td>Ranging dielectric</td>
<td>1</td>
<td>0.045</td>
<td>1 - 4</td>
<td>2 - 8</td>
<td>0.045-0.18</td>
</tr>
</tbody>
</table>

Figure 3.10 shows the results of this investigation. The de-embedded dispersion error with varying material constant, mesh density and frequency is indicated by diamonds, crosses and squares respectively. The solid line corresponds to the numerical dispersion that results from the solution of Equation (3.35). Stark contrast is evident between the numerical dispersion error extracted from the finite element simulation and that predicted for a perfect hexagonal mesh. Not only is the theoretical dispersion error many orders of magnitude less than that observed, but the predicted dispersion errors dependence on $c_x$ and $c_y$ is of the fourth order, as predicted by Equation (3.37), while this dependence for the de-embedded dispersion error is clearly quadratic.

Recalling the discussion in Section 3.2.1 predicting large differences between the dispersion error for the edge basis functions in isotropic and even mildly anisotropic cases, a possible explanation is that practical meshes exhibit some sort of mild anisotropy. The theoretical dispersion error resulting from the solution of Equation (3.35) with an anisotropy of 1:1.1, averaged over all angles, appears in Figure 3.10 as a dashed line. This provides a much better match to the observed dispersion error, both in its overall level, and more particularly in its quadratic dependence on $c_x$ as predicted by Equation (3.38). It is shown later, in Section 4.5.1, that compressing or expanding an equilateral triangle has the same effect on dispersion error as the introduction of equivalent anisotropy. Further investigation of the deviations of the triangles from perfectly equilateral could yield an approximate overall mesh anisotropy that could provide an accurate model for the dispersion error of edges in an isotropic medium. This investigation is considered beyond the scope of this work.

Observation of the dispersion error for edge basis functions in a biaxial medium yields a very different result. The propagation through a biaxial medium is again studied by simulating the propagation of higher order modes through a parallel plate waveguide filled with biaxial material, as described in Section 3.2.3. The range of values used are detailed in Table 3.2. The de-embedded results are displayed in Figure 3.11, with the observed numerical dispersion exhibited by the finite element simulation depicted by diamonds, and the theoretical numerical dispersion resulting from the solution of Equation (3.35) as a solid line. Surprisingly, excellent agreement is evident. Since the material is al-
ready strongly anisotropic, 1:2, low levels of anisotropy introduced by mesh variations, as described above, would have minimal effect.

### 3.2.4 Summary of the findings for the investigation of dispersion error in the finite element method

In the preceding sections, the numerical dispersion that is expected for a perfect hexagonal mesh using both node and edge basis functions has been derived. A method of extracting the numerical dispersion from a practical finite element simulation has been developed and this has been used to examine the behavior of the numerical dispersion under various conditions. It has been discovered that the ideal hexagonal mesh may be used as a reasonable approximation to practical meshes for the node basis function.

The observed dispersion error for the edge basis functions for isotropic media is strikingly different to that predicted by Equation (3.35), and seems to behave as though it were mildly anisotropic. The numerical dispersion for the edge basis functions in an anisotropic media is, however, well matched by this theory, suggesting that perhaps mild anisotropy due to random mesh variations may need to be considered for an accurate model of the isotropic case. The equivalence of the dependence of numerical dispersion on material constant, mesh edge length and frequency has also been demonstrated, with all practical meshes exhibiting a quadratic dependence on $c_x$ as defined by Equation (3.9).

### 3.3 Numerical reflection

Recalling that the goal of this study is to analyse and optimise the performance of the PML absorber, and that this is limited by artificial numerical reflections, it is now necessary to consider what happens at an interface between two materials in the finite element method. As shown in Section 2, when modeled perfectly, the interface between the solution region and a PML absorber should produce no reflection whatsoever. From the findings in Section 3.2 it seems likely that errors in the numerical dispersion of the two layers may give rise to a small amount of reflection at such an interface. It is also possible that the numerical approximations made in the finite element method may somehow affect the mechanism by which the reflection itself is modeled.

Therefore in this Section, expressions are derived for the numerical reflection that is modeled by the finite element method for an interface between two materials. This derivation is done for general biaxial materials assuming a uniform hexagonal mesh across the boundary. These expressions are compared to the observed reflection error for both edge and node simulations in a number of test cases using imperfect meshes. Thus it is shown
Figure 3.10: Comparison of dispersion error observed and predicted for the isotropic waveguide simulation as a function of $c_x$ using edges. Diamonds, crosses and squares denote the dispersion error resulting from varying the material constant, mesh edge length, and frequency, respectively. The dispersion error that would be expected for a perfect hexagonal mesh is denoted by a solid line.

Figure 3.11: Comparison of dispersion error observed and predicted for the anisotropic waveguide simulation as a function of $c_x$ using edges. The dispersion error resulting from varying the mesh edge length is denoted by diamonds while the dispersion error that would be expected for a perfect hexagonal mesh is denoted by a solid line.
that the assumption of a perfect hexagonal mesh is an adequate model for the analysis and minimisation of numerical reflection errors in typical finite element simulations.

### 3.3.1 Derivation of the numerical reflection relations

In the following Sections the numerical reflection coefficient modeled by the finite element method for both node and edge basis functions is derived. This procedure parallels that used in Section 3.2.1 to obtain expressions for the numerical dispersion. A plane wave solution to Maxwell’s equations is projected onto a mesh constructed from ideal equilateral triangles that straddles the material boundary. To model reflection, the finite element local matrices are used to eliminate the unknown field amplitudes and isolate the reflection coefficient. Again, due to the infinite z-dimension, any propagating wave may be decomposed into TE and TM components and hence the node and edge basis functions may be considered separately.

**Derivation of the numerical reflection relation for node basis functions**

Consider the portion of mesh depicted in Figure 3.12. A TE polarised wave, propagating in the $x$-$y$ plane is projected onto the mesh with $x = 0$ occurring on the material boundary. Since it is the nodes that are of interest, the E-field formulation is used and hence the unknown field amplitudes correspond to the $z$-directed E-field.

If the reflection coefficient from the interface is labeled $r$, the unknown fields can be related by this coefficient and the appropriate phase shifts as

\[
\begin{align*}
E_1 &= (1 + r) \\
E_2 &= e^{-j a_1}e^{+jb_1} + re^{j a_1}e^{+jb_1} \\
E_3 &= e^{-j a_1}e^{-jb_1} + re^{j a_1}e^{-jb_1} \\
E_4 &= (1 + r)e^{-2jb_1} \\
E_5 &= (1 + r)e^{ja_2}e^{-jb_2} \\
E_6 &= (1 + r)e^{ja_2}e^{jb_2} \\
E_7 &= (1 + r)e^{2jb_2}
\end{align*}
\]

where $a_i$ and $b_i$ are as defined in Equation (3.7) and (3.8) for Material $i$. Note that the nodes along the boundary must be shared by incident, reflected and transmitted plane waves to assure continuity of the $z$-directed tangential field. Note also that translation of the nodes along the boundary must result only in a phase shift, and that phase shift must be common to the fields in both media, implying
Figure 3.12: A portion of the hexagonal mesh straddling an interface between Material 1 and Material 2 with nodes labeled. The plane wave angle of incidence and transmission, $\theta_i$ and $\theta_t$ respectively, are also indicated.

\[ b_1 = b_2 = b. \]  

This is actually a statement of Snell’s law of refraction. Using the local matrix of Equation (3.11) to relate the unknown fields and substituting (3.41 - 3.46) results in

\[
\begin{align*}
\epsilon_{z1} \left[ & (2A_1 + 4C_1)(1 + R) + 2D_1 \cos \theta b(1 + R) + 4B_1 \cos \theta \left( e^{-ia_1} + Re^{ja_1} \right) \right] + \\
\epsilon_{z2} \left[ & (2A_2 - 4C_2)(1 + R) + 2D_2 \cos \theta b(1 + R) + 4B_2 \cos \theta \left( e^{ja_2} + e^{-ja_2} \right) \right] = 0.
\end{align*}
\]

This can be rearranged

\[
\begin{align*}
-r \{ & \epsilon_{z1} \left[ (A_1 + 2C_1) + D_1 \cos \theta b \cos a_1 + 2B_1 \cos \theta \sin a_1 \right] + \\
& \epsilon_{z2} \left[ (A_2 + 2C_2) + D_2 \cos \theta b \cos a_2 + 2B_2 \cos \theta \sin a_2 \right] \} = \\
& \epsilon_{z1} \left[ (A_1 + 2C_1) + D_1 \cos \theta b \cos a_1 - 2B_1 \cos \theta \sin a_1 \right] + \\
& \epsilon_{z2} \left[ (A_2 + 2C_2) + D_2 \cos \theta b \cos a_2 + 2B_2 \cos \theta \sin a_2 \right].
\end{align*}
\]

Recalling the dispersion relation of Equation (3.17), this may be reduced to

\[
r = \frac{\epsilon_{z1}B_1 \sin a_1 - \epsilon_{z2}B_2 \sin a_2}{\epsilon_{z1}B_1 \sin a_1 + \epsilon_{z2}B_2 \sin a_2} \quad \text{(3.49)}
\]

For given $c_{x1}$, $c_{x2}$, $c_{y1}$, $c_{y2}$ and incident angle, the input numerical dispersion can be obtained from Equation (3.17) for Material 1, while the output numerical dispersion and
transmission angle can be found by solving Equation (3.17) for Material 2, and Equation (3.47) simultaneously. Again, the dependence on \( c_x \) and \( c_y \), as defined in Equations (3.9) and (3.10), suggests that the reflection error is affected equally by changes in material parameters \( \epsilon \) and \( \mu \), mesh dimensions \( L \), frequency \( k_0 \).

Taking the limit as \( c_{xi} \) and \( c_{yi} \) approach zero yields the expression,

\[
\tau_{num} = \tau_{ideal} - \left( \epsilon_{x1} \cos \theta_1/c_{y1} (8\delta_{y1} + c_{y1}^2 \sin^2 \theta_1) + \epsilon_{x2} \cos \theta_2/c_{y2} (8\delta_{y2} + c_{y2}^2 \sin^2 \theta_2) \right) \tau_{ideal} + \left( \epsilon_{x1} \cos \theta_1/c_{y1} (8\delta_{y1} + c_{y1}^2 \sin^2 \theta_1) - \epsilon_{x2} \cos \theta_2/c_{y2} (8\delta_{y2} + c_{y2}^2 \sin^2 \theta_2) \right) + O(c_{xi}^4, c_{yi}^4)
\]

where

\[
\tau_{ideal} = \frac{\epsilon_{x1} \cos \theta_1/c_{y1} - \epsilon_{x2} \cos \theta_2/c_{y2}}{\epsilon_{x1} \cos \theta_1/c_{y1} + \epsilon_{x2} \cos \theta_2/c_{y2}}.
\]

and \( \delta_{y1} \) and \( \delta_{y2} \) are the dispersion errors Material 1 and Material 2. In most cases Equation 3.50 can simply be expressed

\[
\tau_{num} = \tau_{ideal} + O(c_{xi}^2, c_{yi}^2),
\]

suggesting that the numerical reflection should approach the exact reflection quadratically with reducing \( c_x \) and \( c_y \). For a given frequency and material parameters, a small mesh dimension may be chosen to reduce reflection errors, and so increasing the mesh density, as was discussed in [30], is one option for reducing reflection error at the expense of increased unknowns. It is also worth noting that each of \( c_{xi} \) and \( c_{yi} \) should be of the same small size to effectively minimise reflection errors. Thus if the material parameters on one side of the interface are significantly larger than those on the other, then perhaps only the mesh dimension on that side need be reduced to compensate. These observations suggest a number of alternative options for efficient reduction of numerical reflections. More detailed investigation of these options in the context of reflections from a PML boundary can be found in Chapter 4.

Inspection of Equation (3.51) reveals the reflection error terms of order \( O(c_{xi}^2, c_{yi}^2) \) are dependent on incident angle. To investigate this relationship between incident angle and reflection error, Equation (3.50) is solved for an interface between two isotropic materials and for an interface between an isotropic material and an anisotropic material. The numerical reflection error is defined as

\[
\delta_r = \frac{|\tau_{num} - \tau_{ideal}|}{\tau_{ideal}}.
\]
Figure 3.13 shows the reflection error as a function of incident angle, for an interface between two isotropic materials \(c_2 = \sqrt{2}c_1\). The reflection error for \(c_{x1} = 0.001 \times 3^n\), \((n = 0, \ldots, 6)\) are shown. The reflection error is evidently fairly uniform with angle of incidence and scales quadratically with \(c_x\).

Closer examination of Equation (3.50) reveals that for a certain angle of incidence, satisfying
\[
8(\delta_{\beta1} - \delta_{\beta2}) = c_{y1}^2 \sin^2 \theta_1 - c_{y2}^2 \sin^2 \theta_2,
\]
Equation (3.50) reduces to
\[
r_{num} = r_{ideal} + O(c_{xi}^A, c_{yi}^A).
\]

Evidently, at this angle of incidence, the second order reflection error exactly cancels the second order dispersion error. It is thus possible, for some material combinations, that the reflection error as a function of incident angle will exhibit a resonance as the condition of Equation (3.54) is met.

Figure 3.14 shows the reflection error as a function of incident angle, for an interface between an isotropic material with dielectric constants \(\varepsilon_1 = 1\), and an anisotropic material with \(c_{x2} = c_1, c_{y2} = \sqrt{2}c_1\). Again the reflection errors for \(c_1 = 0.001 \times 3^n\), \((n = 0, \ldots, 6)\) are shown. The above mentioned resonances are evident at an angle of incidence of approximately 0.6 radians. Again the response scales quadratically with edge length as expected.

**Derivation of the numerical reflection relation for the edge basis functions**

Consider the portion of mesh depicted in Figure 3.15. As with the derivation of Section 3.3.1, a TE polarised plane wave, propagating in the x-y plane is projected onto this mesh with \(x = 0\) corresponding to the material boundary. Since in this instance it is the edge basis functions that are of interest, the H-field formulation, as described in Section 3.2.1, is chosen and thus the unknown fields will be the H-field components in the x-y plane. Labelling the reflection coefficient at the interface \(r\) and using this along with the appropriate phase shifts, it is possible to relate the unknown field amplitudes as follows

\[
\begin{align*}
H_1 &= (1 + r) \\
H_6 &= e^{-j\beta_1}(e^{-j\alpha_1} + re^{j\alpha_1}) \\
H_7 &= (1 + r)e^{j\alpha_2}e^{-j\beta_2} \\
H_8 &= (1 + r)e^{j\alpha_2}e^{j\beta_2} \\
H_9 &= e^{j\beta_1}(e^{-j\alpha_1} + re^{j\alpha_1}) \\
H_{10} &= H_5e^{-2j\beta_1}
\end{align*}
\]
Figure 3.13: The numerical reflection error as a function of angle of incidence for an interface between two isotropic materials with \( c_2 = \sqrt{2}c_1 \). \( c_1 = 0.001 \times 3^n \), \( n = 0, \ldots, 6 \) are shown.

Figure 3.14: The numerical reflection error as a function of angle of incidence for an interface between an isotropic material and a biaxial material with \( c_{x2} = c_1 \), and \( c_{y2} = \sqrt{2}c_1 \). Plots for \( c_1 = 0.001 \times 3^n \), \( n = 0, \ldots, 6 \) are shown.
CHAPTER 3.

\[ H_{11} = H_4 e^{-2jb_2} \]  \hspace{1cm} (3.62) \\
\[ H_{12} = H_3 e^{2jb_2} \]  \hspace{1cm} (3.63) \\
\[ H_{13} = H_2 e^{2jb_1}. \]  \hspace{1cm} (3.64)

Relating these fields using the finite element local matrix of Equation (3.26), substituting Equations (3.57 - 3.64), noting \( b_1 = b_2 \), and re-arranging in matrix form leads to

\[
\begin{bmatrix}
2C_1 e^{jb} & 0 & 0 & 2D_1 \cos(b) & B_1(e^{ja_1} + e^{jb})
\end{bmatrix}
\begin{bmatrix}
H_2 \\
H_3 \\
H_4 \\
H_5 \\
H_6
\end{bmatrix}
+ \begin{bmatrix}
2C_2 e^{jb} & 2D_2 \cos(b) & 0 & B_2(e^{ja_2} + e^{jb}) \\
0 & 2D_2 \cos(b) & 2C_2 e^{-jb} & 0 & B_2(e^{ja_2} + e^{-jb}) \\
0 & 2D_1 \cos(b) & 2C_1 e^{-jb} & B_1(e^{ja_1} + e^{-jb})
\end{bmatrix}
\begin{bmatrix}
H_7 \\
H_8 \\
H_9 \\
H_{10} \\
H_{11}
\end{bmatrix}
\begin{bmatrix}
B_1(e^{jb} + e^{-ja_1}) \\
B_2(e^{jb} + e^{ja_2}) \\
B_2(e^{-jb} + e^{ja_2}) \\
B_1(e^{-jb} + e^{-ja_1}) \\
(A_1 + A_2)
\end{bmatrix}
= 0.
\]

Figure 3.15: A portion of the hexagonal mesh straddling an interface between Material 1 and Material 2 with edges labeled. The plane wave angle of incidence and transmission, \( \theta_1 \) and \( \theta_2 \) respectively, are also indicated.

Using the MapleV5 software [50] the following solution is achieved

\[ r = \frac{Z_1 - Z_2}{Z_1 + Z_2} \]  \hspace{1cm} (3.66)
where

\[ Z_i = \frac{(D_i^2 \cos^2 b - 4C_i^2)}{\sin \alpha_i B_i^2 (D_i - 2C_i)} \]  

(3.67)

Thus again for a given \( c_{x1}, c_{x2}, c_{y1}, c_{y2} \) and incident angle, the input numerical dispersion can be found by solving Equation (3.35), and the transmitted numerical dispersion and transmission angle may be found by solving Equation (3.47) and Equation (3.35) simultaneously. The numerical reflection can then be found from Equation (3.66).

In the limit as \( c_{x1} \) and \( c_{y1} \) approach zero, it can be shown that

\[ r = \frac{\sqrt{\varepsilon_{x1} \mu_{x2} \cos \theta_i} - \sqrt{\varepsilon_{y2} \mu_{y1} \cos \theta_i}}{\sqrt{\varepsilon_{x1} \mu_{x2} \cos \theta_i} + \sqrt{\varepsilon_{y2} \mu_{y1} \cos \theta_i}} + O(c_{x1}^2, c_{x2}^2, c_{y1}, c_{y2}), \]  

(3.68)

suggesting that the reflection error scales quadratically with the square root of material constant, edge length and frequency. Unlike the node basis functions, the reflection error of the edges does not have a simple dependence on angle of incidence and it seems unlikely that there exists a real angle that will cause this numerical expression to become exact. Further investigation of the occurrence of these resonances, in the context of reflection from a PML interface is conducted in Section 4.2.

The dependence of the reflection error on incident angle was investigated by solving Equation (3.66) for an interface between two isotropic materials with \( c_2 = \sqrt{2} c_1 \). Figure 3.16 shows the reflection error as a function of angle for \( c_1 = 0.001 \times 3^n, \ (n = 0, \ldots, 6) \). A quadratic dependence on edge length is evident. Figure 3.17 depicts the reflection error as a function of incident angle for an interface between an isotropic material and a biaxial material with \( c_{x2} = c_1 \) and \( c_{y2} = \sqrt{2} c_1 \), for \( c_1 = 0.001 \times 3^n, \ (n = 0, \ldots, 6) \). Again quadratic scaling with \( c_x, c_y \) is evident. With the exception of the extreme case of \( c_1 = 0.001 \), only shallow resonances appear in the response suggesting nearby angles in the complex plane where the numerical reflection becomes exact.

### 3.3.2 Verification of the theoretical reflection error

To use the theoretical reflection error derived in the previous section as a tool for analysing and minimising the reflection errors introduced by the finite element method, it is necessary to verify that these expressions are good models for the behavior of typical finite element meshes. This verification is treated in a similar fashion to the verification of the numerical dispersion in Section 3.2.2.

Again the parallel plate waveguide test case is used; however, in this instance, the waveguide is loaded with two different materials as depicted in Figure 3.18. The observed reflection from the interface as shown, is compared to that predicted by Equation (3.49) and Equation (3.66) for nodes and edges respectively. As before, the input and output
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Figure 3.16: The numerical reflection error as a function of angle of incidence for an interface between two isotropic materials with \( c_2 = \sqrt{2}c_1 \). Plots for \( c_1 = 0.001 \times 3^n \), \((n = 0, \ldots, 6)\) are shown.

Figure 3.17: The numerical reflection error as a function of angle of incidence for an interface between an isotropic material and a biaxial material with \( c_{x2} = c_1 \), and \( c_{y2} = \sqrt{2}c_1 \). Plots for \( c_1 = 0.001 \times 3^n \), \((n = 0, \ldots, 6)\) are shown.
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ports of the problem are expected to cause reflections as a transition is made from an ideal closed form solution to the imperfect solution modeled by the finite element method. Thus to accurately gauge the numerical reflection from an interface, it will be necessary to derive a de-embedding procedure for these reflection test cases. A detailed description of the de-embedding process used for the investigation of numerical reflection errors can be found in Appendix C.

![Geometry of a parallel plate waveguide](image)

Figure 3.18: Geometry of a parallel plate waveguide, used in the investigation of numerical reflection with reflection coefficients for the various interfaces labeled

### 3.3.3 Numerical experiments to verify the numerical reflection relation

Having derived a de-embedding procedure in Appendix C, it is now possible to extract the numerical reflection error resulting from an interface in the finite element method from a parallel plate waveguide simulation. Using a similar approach to that used to verify the numerical dispersion relations in Section 3.2.3, the expressions arrived at for the numerical reflection will be compared to the actual reflections observed in practical finite element meshes.

In each case the reflections for a dielectric interface within the parallel plate waveguide is investigated. Again the edge and node basis functions are examined separately and for each of these, two cases have been conducted. These are the interface between an isotropic material and a second isotropic material of twice the material constant, and the case of the interface between an isotropic material and an anisotropic material.

The isotropic/isotropic interface is investigated by modeling the propagation of the fundamental TE mode of the waveguide and varying the three parameters, edge length,
material constant and frequency and comparing the de-embedded reflection to that predicted for a normal incident plane wave by Equation (3.50) for node basis functions and Equation (3.66) for edge basis functions.

The isotropic/anisotropic interface is examined by simulating the reflection of the first order TE mode of the waveguide, since the fundamental TE mode will only interact with a single element of the material tensor. Only mesh edge length is varied in this instance, as frequency and material constant will affect the guiding properties of the higher order mode. The results of the simulation are compared with the solution of Equation (3.50) for node basis functions and Equation (3.66) for edge basis functions for a plane wave traveling at an angle given by Equation (3.39).

**Verification of the numerical reflection error of nodes**

The numerical reflection error are examined for two cases in the parallel plate waveguide as described previously in Section 3.3.3. Table 3.3 presents the details of each case, specifying the parameters indicated in Figure 3.18, which are varied to produce the range of \( c_x \) values. The reflection from the interface was de-embedded using the procedure outlined in Appendix C for each of these cases and the result was compared with that predicted by Equation (3.49).

The normalised reflection error, as defined by Equation (3.53), is depicted in Figure 3.19. A very good match between the de-embedded simulation and the solution of Equation (3.50) is evident. Also, the effects of varying each of mesh density, dielectric constant and frequency are seen to be equivalent. Notice the resonance that appears in the case of varying dielectric as the problem becomes electrically large. Uncertainties in the de-embedding procedure become more significant at this resonance producing abrupt behavior.

To demonstrate the validity of Equation (3.50) in a more general case involving bi-axial material, the numerical reflection of the first order TE mode of the waveguide from an interface between an isotropic material and a biaxial material was simulated. Only the mesh density was varied since frequency and material parameters affect the guiding properties, and hence effective incident angle of higher order modes. Table 3.4 summarises the variables of the two materials that are used in this investigation.

Figure 3.20 shows the de-embedded reflection error as a function of mesh edge length. The solid line depicts the solution to Equation (3.50) at an angle given by Equation (3.39). The de-embedded reflection error is evidently more erratic for the higher order mode than for the fundamental. It is suspected that the reflection error is more sensitive to the random variations in the individual triangles of the mesh. Further investigation may be required to identify the actual source of these fluctuations.
Figure 3.19: Comparison of reflection error observed and predicted for the isotropic/isotropic waveguide interface simulation as a function of $c_x$ using nodes. The reflection error resulting from varying the material constant, mesh edge length, and frequency, are denoted by diamonds, crosses and squares respectively. A solid line denotes the reflection error that would be expected for a hexagonal mesh.

Figure 3.20: Comparison of reflection error observed and predicted for the isotropic/anisotropic waveguide interface simulation as a function of $c_x$ using nodes. The reflection error resulting from varying the mesh edge length is denoted by diamonds while the dispersion error that would be expected for a hexagonal mesh is denoted by a solid line.
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<table>
<thead>
<tr>
<th>Variable</th>
<th>( l_1 ) (cm)</th>
<th>( l_2 ) (cm)</th>
<th>( k_0 )</th>
<th>( L_{\text{edge}} ) (cm)</th>
<th>( \sqrt{\varepsilon_{x1}\mu_{z1}} )</th>
<th>( \sqrt{\varepsilon_{x2}\mu_{z2}} )</th>
<th>( c_x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>frequency</td>
<td>0.25</td>
<td>0.25</td>
<td>1 - 3</td>
<td>0.045</td>
<td>1</td>
<td>2</td>
<td>0.045-0.135</td>
</tr>
<tr>
<td>edge-length</td>
<td>0.75</td>
<td>0.75</td>
<td>1</td>
<td>0.03 - 0.1</td>
<td>1</td>
<td>2</td>
<td>0.03-0.1</td>
</tr>
<tr>
<td>dielectric</td>
<td>0.25</td>
<td>0.25</td>
<td>1</td>
<td>0.045</td>
<td>1 - 4</td>
<td>2-8</td>
<td>0.045-0.18</td>
</tr>
</tbody>
</table>

Table 3.3: Variables used in the investigation of numerical reflection of the fundamental TE mode from an interface between two isotropic dielectric materials within a parallel plate waveguide.

Table 3.4: Variables used in the investigation of numerical reflection of the first order TE mode from an interface between an isotropic and an anisotropic dielectric material within a parallel plate waveguide.

Verification of the numerical reflection of edges

The numerical reflection error resulting from finite element simulation using edge basis functions is investigated similarly to that of the node basis function in Section 3.3.3. Again two cases are examined, reflection from an interface between two isotropic materials and then, more generally reflection from an interface between an isotropic material and an anisotropic material. The parallel plate waveguide and de-embedding procedure described in Appendix C is used in each investigation.

To investigate the reflection error at an isotropic/isotropic interface, the zeroth order TE mode was used in an H-field formulation finite element simulation. The simulation studied is again that of Figure 3.18, with parameters given by Table 3.3. The results of the finite element simulation are processed using the de-embedding procedure described in Appendix C and the results are presented in Figure 3.21. As before, the three variables, material parameter, mesh edge length and frequency were varied, and the results of each investigation are represented by diamonds, crosses and squares respectively. The solid line shows the solution of Equation (3.66). Good agreement between this predicted reflection error and that obtained from the simulation is evident. This is surprising since it is evident from the findings of Section 3.2.3 that the numerical dispersion predicted for the edges in isotropic media differs greatly from that observed in the practical simulation. This suggests that the errors in the reflection are dominated by errors in the reflection simulation itself, rather than indirect errors in the numerical dispersion on either side of the discontinuity.

The reflection error from the interface between an isotropic material and a biaxial
material produced by the edge basis functions, was also investigated as in Section 3.3.3. The first order TE mode, using the H field formulation was used to ensure that both material tensor elements in the x-y plane would interact with the wave. The simulation geometry is as presented in Figure 3.18 with parameters as given in Table 3.4. Only the mesh was varied to avoid altering the guiding properties of the mode.

The results of this investigation, after de-embedding are presented in Figure 3.22. The observed reflection error, obtained from the finite element simulation is represented by diamonds, while the predicted reflection error, obtained through the solution of Equation (3.66) is shown by a solid line. Good agreement is evident.

3.3.4 Summary of the findings for the investigation of the numerical reflection

In the preceding sections, the numerical reflection that is expected from an interface between two general biaxial materials at an arbitrary angle of incidence, has been derived. This derivation has been conducted for both edges and nodes assuming a uniform hexagonal mesh across the interface. A method for isolating the numerical reflection and transmission of the interface from the overall results of a finite element simulation has been developed and this has been used to compare the derived numerical reflection expressions to practical examples. It is evident that the expressions are an adequate model for the practical simulations examined.

In some material configurations, the numerical reflection for the node basis functions as predicted by Equation (3.49) exhibits a resonance where the error goes to zero at a particular angle. Observed fluctuations and low error levels in the simulated reflection response of the interface between an isotropic material and a biaxial material suggest a nearby resonance, and hence support this prediction. As with the findings for the numerical dispersion, in Section 3.2, the effect of variations in material parameters, mesh dimension and frequency are found to be equivalent, producing a quadratic change in the reflection error.

3.4 Conclusion

At the beginning of this chapter the numerical errors in the finite element method were identified as a possible cause for the failure of the PML boundary condition in practical finite method simulations. It was proposed that in order to understand and remedy the shortcomings of the PML in practical situations, it would first be necessary to understand the numerical errors intrinsic to the finite element method itself. Thus it was the aim of
Figure 3.21: Measured reflection error from an interface between two dielectric materials within a parallel plate waveguide and the reflection error that would be expected from an ideal mesh.

Figure 3.22: Measured reflection error from an interface between two dielectric materials within a parallel plate waveguide and the reflection error that would be expected from an ideal mesh.
this chapter to investigate the numerical dispersion and reflection errors produced by the first order edge and node basis functions in the finite element method were used to model interfaces between general biaxial materials.

To this end, models for the numerical dispersion and reflection errors for the edge and node basis functions have been developed assuming a perfect hexagonal mesh. The applicability of these models to practical simulations has been investigated, summaries of which may be found in Section 3.2.4 and Section 3.3.4. From these investigations it is evident that the relations for numerical dispersion Equations (3.17) and (3.35), and numerical reflection Equations (3.49) and (3.66) for node and edge basis functions respectively, provide good models for the imperfect meshes of practical simulations.

With these expressions derived and verified, it is now possible to use them as tools to design solutions to the problem of numerical reflections from an interface between the solution region and a PML boundary. The following chapter will explore possibilities for efficient reduction of numerical reflection leading, ultimately to the development of a highly efficient scheme for the implementation of the PML in a practical mesh.
Chapter 4

Highly Efficient PML Implementation using a Compressed Mesh

4.1 Introduction

Chapter 3.4, investigates the mechanism by which the finite element method models transmission and reflection within anisotropic media. In particular, the numerical dispersion and numerical reflection for the case of a regular, perfect hexagonal mesh has been derived and compared to the dispersion and reflection resulting from a practical finite element simulation. It is shown that the assumption of such a perfect mesh is adequate to model the behavior of numerical dispersion and reflection in the less structured meshes that can be expected from typical mesh generators.

Now that these models have been derived and verified, it is possible to analyse them in more detail to discover the parameters that control numerical reflection from a PML interface. By identifying these important parameters it should be possible to suggest methods to tailor interfaces to minimise numerical reflection. Since the PML, when applied to a practical finite element problem, is limited by numerical reflections, reducing the amount of numerical reflection error that occurs at an interface, in a manner that incurs minimal increase in unknowns, leads to a more efficient and effective PML.

The performance of a PML truncation scheme can be quantified using several parameters. Two inter-related parameters are the numerical reflection that occurs at the PML interface and the number of unknowns required to implement such a PML truncation. To be both effective and efficient, a compromise where both of these parameters are minimal needs to be devised. There is a third parameter that affects the solution of a finite element problem, namely the matrix condition number. It will be shown shortly that the introduction of a PML boundary can have a significant impact on the finite element matrix conditioning and thus must be considered when designing a PML boundary.
The following two sections will investigate the performance of a PML layer in terms of these three quantities. Firstly, Section 4.2 will examine the numerical reflection equations derived in Section 3.3 in the context of the boundary between a solution region and a PML boundary. In this section the relationship between the numerical reflection from a PML boundary, the mesh density and the PML variable parameter is identified. Section 4.3 then discusses the importance of the matrix condition number and describes a brief empirical analysis of the impact of the PML properties on this quantity.

With these measures of performance for the PML identified, Section 4.4 describes a basic PML implementation consisting of a solution region truncated by a single layer of PML backed by a perfect electric conductor. Here the work of Polycarpou et al. [44] investigating such PML layers in the finite element method is introduced. Analysis of their findings in terms of the theory and observations of Sections 4.2 and 4.3 is presented.

The numerical reflection from a PML interface is then re-examined theoretically in Section 4.5. A method by which mesh distortion can be used to improve the performance of the PML is proposed and theory to describe numerical dispersion and reflection from such a distorted mesh is derived. Solving these closed form relationships numerically, an optimum distortion for minimum numerical reflection from a PML interface is found. This theory is then verified by finite element simulation. Using the investigation of [44] and Section 4.4 as a benchmark, this scheme is shown to be a vast improvement over currently used PML implementations.

A brief discussion of limitations of this approach and possible approaches for its extension are discussed in Section 4.6, then finally Section 4.7 summarises the findings of this chapter and outlines the method for the application of this new technique to practical finite element problems.

4.2 The numerical dispersion and reflection in the context of a PML boundary

Having determined the numerical dispersion and reflection in Sections 3.2 and 3.3, it is now possible to examine the nature of these discretisation errors in the context of a PML boundary. Recall from Chapter 2 that, for an interface with normal in the x direction, the material tensors of a PML boundary can be expressed as

\[
\begin{bmatrix}
\epsilon_{1x}/a_{pml} & 0 & 0 \\
0 & \epsilon_{1y}/a_{pml} & 0 \\
0 & 0 & \epsilon_{1z}/a_{pml}
\end{bmatrix},
\begin{bmatrix}
\mu_{1x}/a_{pml} & 0 & 0 \\
0 & \mu_{1y}/a_{pml} & 0 \\
0 & 0 & \mu_{1z}/a_{pml}
\end{bmatrix}
\] (4.1)
where

\[
\begin{bmatrix}
\varepsilon_{1x} & 0 & 0 \\
0 & \varepsilon_{1y} & 0 \\
0 & 0 & \varepsilon_{1z}
\end{bmatrix}, \quad
\begin{bmatrix}
\mu_{1x} & 0 & 0 \\
0 & \mu_{1y} & 0 \\
0 & 0 & \mu_{1z}
\end{bmatrix}
\]

(4.2)

are the material parameters of the solution region bounding the PML and \(a_{pml}\) is the PML variable parameter which, to absorb fields within it, is often set to be a complex number with large imaginary component.

Recall from Section 3.2 and 3.3, that the amount of dispersion and reflection error was related to the general parameters \(c_x\) and \(c_y\) defined in Equations (3.9) and (3.10). Referring to Equation (4.1), \(c_x\) and \(c_y\) in a PML material may be rewritten

\[
c_{x2} = k_0\sqrt{\varepsilon_{1x}\mu_{1x}}L, \quad \text{\text{(4.3)}}
\]

\[
= c_{x1} \quad \text{\text{(4.4)}}
\]

\[
c_{y2} = k_0\sqrt{a_{pml}^{2}\varepsilon_{1y}\mu_{1y}}L. \quad \text{\text{(4.5)}}
\]

\[
= a_{pml}c_{y1}. \quad \text{\text{(4.6)}}
\]

Some interesting deductions may be drawn from this. Firstly, it is surprising that \(c_{x2}\) is independent of the PML parameter, and is always equal to \(c_{x1}\). Secondly, since \(c_{y2}\) scales linearly with \(a_{pml}\), it is evident that the reflection error from a PML interface scales quadratically with increasing \(a_{pml}\).

Since it is only \(c_{y2}\) that is affected by \(a_{pml}\), some dependence of reflection error on incident angle could be expected. To investigate this, the material tensors of Equations (4.1) and (4.2) were substituted into the reflection Equations (3.49) and (3.66), for node and edge basis functions respectively, and the reflection error was plotted as a function of \(a_{pml}\) and incident angle \(\theta_1\).

Figure 4.1 shows the reflection error for the node basis functions as a function of incident angle, \(\theta_1\) and PML variable parameter \(a_{pml}\) resulting from the solution of the numerical reflection relationship for the node basis functions: Equation (3.49), with \(c_{x1} = c_{y1} = 0.001\). The solid lines show the reflection error as a function of angle for values of \(a_{pml} = 3^n\) \((n = 1, \ldots, 7)\). Since the PML will ultimately be a lossy material, this calculation was repeated with the loss tangent of \(a_{pml}\) set to 1 giving \(a_{pml} = 3^n e^{-j\pi/4}\) \((n = 1, \ldots, 7)\). The reflection error for this complex \(a_{pml}\) is shown by dashed lines. It is evident that aside from the extremes of very large and near unity \(a_{pml}\), the reflection error of the two cases are almost indistinguishable. Note also that the reflection error scales as \(|a_{pml}|^2\). This is true almost independent of angle suggesting that \(c_y\), which is proportional to \(a_{pml}\), dominates \(c_x\). A resonance appears at \(\theta_1 = 0.6\) radians, where, as described in
Section 3.3.1, it is proposed that the numerical dispersion error exactly compensates the numerical reflection.

The above procedure was repeated for the edge basis functions with the results presented in Figure 4.2. Again, the solid and dashed lines depict the reflection error as a function of angle resulting from the solution of Equation (3.66) for PML interfaces with loss tangents of 0 and 1 respectively for the above values of $|a_{pm1}|$. As with the node basis functions, the effect of loss tangent on reflection error is negligible. The reflection error again scales as $|a_{pm1}|^2$, but unlike the node basis functions, the edge basis reflection error exhibits a resonant angle only in the most extreme case. Note the discontinuities in the most extreme cases. At these points the gradient root finding technique becomes unstable, hence it is not clear whether the behaviour in the extreme case of $a_{pm1} = 3$ is a numerical artifact. This occurs at such a small value of reflection error as to be insignificant for the case of this study.

From the two investigations above, it is evident that for both edges and nodes the reflection error scales as $|a_{pm1}|^2$ and that this is independent of angle. It is also evident that the reflection error depends only on the magnitude of $a_{pm1}$ independent of loss tangent.

These observations can now be used in the analysis of current PML schemes and the development of more efficient PML implementations. This is done shortly in Sections 4.4 and 4.5. Before this can be done, it will be necessary to define the performance of the PML more precisely. Previously the performance of the PML has been characterised only in terms of the reflection error and the number of unknowns required for its implementation. There is another important parameter that the introduction of a PML boundary affects that this study has as yet neglected, and that is the matrix condition number.

### 4.3 The matrix condition number

It is the objective of the deterministic finite element method to express the electromagnetic problem to be solved as a single large sparse matrix equation. To then discover the electromagnetic field distribution that satisfies Maxwell’s equations, it is simply a matter of solving this matrix equation. An eigenvalue finite element method expresses the problem as a pair of large sparse matrices for which a general eigensolution is sought. For the remainder of this discussion the deterministic finite element solution will be assumed; however the findings will apply equally to both implementations. The case with which a solution to a matrix equation can be found can be quantified by the matrix condition number.

The condition number can be defined as the ratio of the largest to smallest eigenvalues of a matrix and can be calculated as a by-product of an LU factorisation as is done by the
Figure 4.1: The predicted numerical reflection from a PML interface for various values of PML parameter $a$ using the node basis function. Solid lines show the reflection from a lossless PML, dashed lines show reflection from a PML with a loss tangent of 1.

Figure 4.2: The predicted numerical reflection from a PML interface for various values of PML parameter $a$ using the edge basis function. Solid lines show the reflection from a lossless PML, dashed lines show reflection from a PML with a loss tangent of 1.
matrix solution routine Sparse1.3 [51] for each solution. In practical terms, the condition number is related to the number of iterations that an iterative matrix solver will require to converge [52, page 85]; the larger the condition number, the more iterations required. For some matrix solvers a large condition number precludes iterative solution altogether. For direct solution, as is the case for this study, the condition number affects the amount of roundoff error that is introduced and hence indicates the level of accuracy that the solution will exhibit. In any event, a large condition number is undesirable.

Many factors can influence the matrix condition number. Most significant of these is the matrix order. Often the condition number will scale with the matrix order, growing with increasing problem size. Noting that the matrix order is equal to the number of unknowns which in turn scales as the square or cube of the problem domain dimension, for 2D and 3D problems respectively, it can be seen that the condition number can become impractically large for even moderately sized problems. So effectively reducing the solution region dimension not only makes the solution more rapid, but should also make it more accurate due to improved matrix conditioning. These are the primary functions of the PML boundary.

Unfortunately, there are other factors that affect the matrix condition number. These include widely varying material parameters and mesh densities, and strong anisotropy in both material parameter and mesh dimension. The PML boundary, as discussed in Chapter 2 is likely to have strong anisotropy, and radically different material parameters to the neighboring solution region. This, coupled with the very fine mesh densities needed for an effective PML [30], can lead to large condition numbers and hence inaccurate and inefficient solution. For these reasons, the PML in its current implementation does not seem an attractive candidate for improving the efficiency of finite element simulations.

To demonstrate the effects of these parameters on the condition number of the finite element matrix, three cases have been constructed for each of the node and edge basis functions. The basic geometry consists of a parallel plate waveguide, filled half with air, half with PML as is used in the investigation of numerical reflection in Section 3.3, and depicted in Figure 3.18. This geometry was chosen to be consistent with the investigations of Chapter 3.4.

In the first case, the PML parameter was set to 10, the frequency was set to 5 GHz and the condition number ( \( L_\infty \) [51]) of the finite element matrix was calculated for various mesh densities. Since the matrices for all of the considered simulations are symmetric, \( L_\infty \equiv L_1 \). Figure 4.3 shows the dependence of the condition number on the number of unknowns as solid and dashed lines for the node and edge basis functions respectively. A log scale has been used for clarity, but it is evident that the condition number scales linearly with the number of unknowns in both cases. It is interesting to note that the con-
Figure 4.3: The dependence of the $L_\infty$ condition number\cite{51} on the number of unknowns for node and edge basis functions represented by solid and dashed lines respectively.

Condition number for the edge basis functions is more than an order of magnitude larger than the condition number for the node basis functions at the same number of unknowns.

To investigate the contrast between the condition numbers of the node and edge basis functions, this case was simulated with an average finite element edge length of 0.1 mm and frequency varied between 10 MHz and 100 GHz. Figure 4.4 presents the dependence of the condition number on the solution frequency, with solid and dashed lines representing node and edge basis functions respectively. The condition number of the finite element matrix based on nodes decreases linearly with frequency while the matrix formed by the edge basis functions exhibits a condition number that decreases quadratically with frequency. This indicates that the edges become more rapidly ill conditioned at low frequencies when compared to the nodes.

Examination of the local matrices of Equations (3.11) and (3.26), in Chapter 3.4, show that the effect of varying edge length, and frequency should be equivalent. This would suggest that for a given frequency using a very fine mesh will produce a poorly conditioned matrix, particularly for the edge basis functions. A possible explanation can be arrived at by noting that the edge basis functions intrinsically describe curl\cite{53, pages232-244}. At low frequencies or on a very small scale, the problem approaches static conditions, and thus edges are a poor choice of basis function. Node basis functions are possibly better suited to these situations. From this finding it is evident that care must be taken in refining the mesh when using edge basis functions. Further investigation...
of this is required to attain a better understanding of the optimum number of unknowns required for minimal reflection and dispersion errors while maintaining practical matrix conditioning. It is possible that the introduction of higher order elements may improve this situation.

Finally, to examine the effect of a PML boundary on the condition number the previous cases were examined with an edge length of 0.02 mm and a frequency of 500 MHz. Figure 4.5 depicts the effect of the PML parameter on condition number with solid lines and dashed lines representing node and edge basis functions respectively. It is evident that for small PML parameters, the condition number hits the threshold set by the basic problem in the absence of the PML. As the PML parameter increases, the condition number rises almost proportionally. At an extreme value of $|\alpha_{pml}| \approx 300$, the condition number of the edge basis function matrix exhibits a strong resonance. It is hypothesised that this turning point in the condition number is due to the large dielectric magnitude of the PML increasing the dielectric size of the edge basis function, and hence improving the condition number as observed above. Further investigation is needed to understand this behavior; however, this is considered beyond the scope of this work.

Thus it can be concluded that the condition number is proportional to the number of unknowns for both edges and nodes. It is evident that the dependence of matrix conditioning on solution frequency is linear for nodes and quadratic for edges, suggesting that edge basis functions may be a poor choice for certain problems. Finally, the dependence of the condition number on the PML variable parameter is found to be complex but significantly detrimental for realistic values.

It is thus expected that these effects could compound in a PML implementation significantly increasing the effort required to obtain a finite element matrix solution. In the following sections it is therefore important to closely monitor the matrix condition number to ensure that a technique to improve the reflection error or PML attenuation does not have an adverse effect.

### 4.4 A single layer, conductor backed, PML boundary

In Section 4.2, the performance of the PML is investigated in terms of the numerical reflection that would be expected from the interface between it and the enclosed problem. Although numerical reflection limits the amount of field that is transmitted across the PML boundary, the overall effectiveness of the PML is determined by the amount of this field that the PML can absorb. In practical implementations the PML must be of finite thickness and is usually truncated by a perfect electric conductor. Thus fields that enter the PML region, traverse its thickness, reflect from the PEC boundary, pass once more
CHAPTER 4.

Figure 4.4: The dependence of the condition number on the solution frequency for node and edge basis functions represented by solid and dashed lines respectively.

Figure 4.5: The dependence of the condition number on the magnitude of the PML variable parameter $|\alpha_{pml}|$ for node and edge basis functions represented by solid and dashed lines respectively.
through PML layer and then re-enter the solution region. It is thus important the the PML variable parameter is large enough so that it sufficiently absorbs the fields that enter it.

This situation evidently requires a compromise. Increasing the thickness of the PML to increase the overall boundary absorption increases the problem domain and hence increases the number of unknowns. Increasing the loss of the PML increases the amount of numerical reflection at the surface, requiring a denser mesh to compensate, similarly increasing the number of unknowns. Investigations of these trade offs can be found in [30] [44] and [31] among others.

In this section, the investigation of [44] is analysed in more detail. The authors of [44] investigate two forms of PML boundary and then use the second in a full vector three dimensional finite element simulation. The first boundary examined, which is also the focus of [30], consists of an inhomogeneous PML layer where the PML variable parameter is tapered with depth. A discussion of tapered PML boundaries is postponed until Section 4.6. The second boundary investigated is that of a homogeneous PML layer of set thickness. The investigation examines the total reflection from this boundary for a range of mesh densities and PML conductivities. This investigation is repeated here to obtain additional information regarding the number of unknowns and the matrix condition number. Further, this investigation is used as a benchmark for assessing the performance of the improved PML scheme to be introduced in Section 4.5.

For clarity the details of the investigation are briefly outlined here. The test case
consists of a parallel plate waveguide, terminated by a PEC short circuit lined with a layer of PML as depicted in Figure 4.6. The loss in the PML is expressed as a conductivity so that for a constant PML thickness all frequencies should be attenuated equivalently. The interior of the waveguide is filled with air and thus the material tensors of the PML material are given

$$\begin{pmatrix}
\frac{1}{\kappa} & 0 & 0 \\
0 & \kappa & 0 \\
0 & 0 & \kappa
\end{pmatrix}$$

(4.7)

where

$$\kappa = 1 - j \frac{\delta}{k_x d},$$

(4.8)

and

$$\delta = \ln \left( \frac{1}{R} \right)$$

(4.9)

in which, R is the desired reflection coefficient, d is the PML layer thickness and $k_x$ is the x directed wavenumber of the incident wave.

In the investigation of [44], the PML thickness d is set to 2 cm, the waveguide width is 4 cm, the frequency is 100 MHz and the resulting reflection coefficient modeled by the finite element method for the TEM mode is recorded as a function of desired reflection R for finite element edge lengths of 2.0 mm, 1.0 mm and 0.5 mm. Although the authors of [30] use only edge basis functions in their investigation, both nodes and edges are investigated here. These investigations are detailed in the following sections.

### 4.4.1 Node basis functions

The case depicted in Figure 4.6, is simulated using the fundamental TEM mode at the port. To model the problem using node basis functions, the E field formulation of the finite element method is used. The results of this simulation are depicted in Figure 4.7 for node basis functions. The reflection resulting from the PML layer with finite element edge lengths of 2.0 mm, 1.0 mm, and 0.5 mm are depicted. The ideal reflection, expected in the absence of discretisation error is also shown as a solid line. Each of the curves follows the ideal line to a point at which the reflection error at the PML interface dominates. The level of PML absorption that can be used without the onset of significant reflection errors increases with increasing mesh density. Strong resonances appear in the reflection coefficient response for large $\delta$. Surprisingly, two of these resonances exceed a reflection coefficient of 1. This is clearly not physical; however, it can be shown that if $c_x$ or $c_y$ in Equation (3.49) can no longer be considered small, dispersion errors that may introduce gain can be realised. Thus the use of such large PML losses with the node basis functions is clearly outside the range of validity for the finite element method.
CHAPTER 4.

The behavior of the finite element condition number, as obtained from SparseI.3 [51], for each of 2.0 mm, 1.0 mm and 0.5 mm edge length cases above is depicted in Figure 4.8, with the ideal reflectance depicted by a solid line. It is evident that in each case the condition number becomes worse with increasing δ. The condition number increases also as the mesh is refined, possibly reflecting the increase in the number of unknowns. The resonances in the condition number responses can be identified with a corresponding resonance in the reflection coefficient response of Figure 4.7.

It seems evident that at this low frequency (100 MHz) and resulting high PML absorption coefficient that an unrealistic number of unknowns must be used to effectively implement the PML boundary. It is also evident that aside from having to manipulate larger vectors and matrices, the condition number of these matrices worsens, compounding the effort required for solution. Further, implementation of this form of PML boundary in a 3D method would incur still more unknowns since the matrix order increases with the inverse cube of edge length. Ultimately it would seem that the implementation of the PML in this manner for nodal unknowns is not attractive.

4.4.2 Edge basis functions

The investigation of Section 4.4.1 is repeated for the edge basis functions by using the H field formulation of the finite element method. This case was presented in [44] and will be referred to for comparison. The geometry as described in Section 4.4 was again used, with the simulated reflection coefficient for edge lengths within the PML of 2.0 mm, 1.0 mm and 0.5 mm shown in Figure 4.9. The ideal reflection response, in the absence of numerical reflection is shown as a solid line. Again, the reflection coefficient for each mesh follows the ideal case with increasing PML loss up to the point at which the numerical reflection from the PML surface dominates. At this point the total reflection coefficient turns and gradually increases as more of the field is numerically reflected from the abrupt interface at the PML surface. As with the nodes, it is evident that the level of PML absorption that can be used before the onset of numerical reflection increases as the mesh is refined.

The response of the coarsest mesh for the edge basis functions is more effective than even the finest mesh used with the node basis functions. The absence of resonances in the response suggests that the reflection error for the edges does not introduce gain as it does for the nodes. Taking the limit of the numerical reflection relation Equation (3.66) for large $c_x$ and $c_y$ verifies this. Thus for very large values of $\alpha_{pml}$ it would seem that the edge basis functions are far more suitable.

The behavior of the condition number for the edge basis functions is shown in Figure 4.10 for edge lengths of 2.0 mm, 1.0 mm and 0.5 mm. The condition number for each
Figure 4.7: The reflection modeled by the finite element method using node basis functions for various values of PML loss parameter, \( \delta = \ln(1/R) \) where \( R \) is the ideal overall reflection coefficient. \( L \) refers to the finite element edge length and \( N \), to the number of unknown nodes in the mesh.

Figure 4.8: The condition number of the finite element matrix using the node basis functions for various values of PML loss parameter, \( \delta = \ln(1/R) \) where \( R \) is the ideal overall reflection coefficient. \( L \) refers to the finite element edge length and \( N \), to the number of unknown nodes in the mesh.
Figure 4.9: The reflection modeled by the finite element method using edge basis functions for various values of PML loss parameter, \( \delta = \ln(1/R) \) where \( R \) is the ideal overall reflection coefficient. \( L \) refers to the finite element edge length and \( N \), to the number of unknown edges in the mesh.

Figure 4.10: The condition number of the finite element matrix using the edge basis functions for various values of PML loss parameter, \( \delta = \ln(1/R) \) where \( R \) is the ideal overall reflection coefficient.
case starts at a fairly high level, then rapidly becomes larger with a small increase in the PML parameter. Remarkably, increasing the PML parameter further results in a rapid decrease in the condition number until a threshold is reached. Interestingly, this threshold condition number is lower for the two cases of edge length 1.0mm and 0.5mm than that when the PML parameter is zero, suggesting that the introduction of PML material to the problem actually improves the matrix conditioning. Further investigation is needed to determine the nature of the matrix conditioning and its relationship to the PML variable parameter.

It is evident that the performance of a single layer PML implementation using edge basis functions is more effective than that using node basis functions. This advantage, however, is at the cost of increased condition number and hence reduced computational efficiency.

4.5 Improving the PML

In Section 4.4 a traditional single layer implementation of the PML boundary, as investigated by [44], is examined. It is concluded that in this form, the PML is not an attractive option for the truncation of solution regions in the finite element method. The authors of [44] reach the same conclusion:

\textit{At present, the use of an ABC in FEM is computationally more efficient than PML, but not necessarily more accurate. Future developments on the subject suggest that the PML will most likely be the preferred approach to truncating the finite element domain.}

Clearly a more efficient implementation is essential for the PML to be considered a viable alternative to existing absorbing boundary conditions (ABCs) in finite element analysis. Tapering the PML, as is discussed briefly in Section 4.6, certainly improves the performance of the PML boundary, as shown in [30]; however, this comes at the cost of additional geometric complexity and is only an incremental improvement. Polycarpou et al. also suggest that mesh refinement only be applied to the PML region. This is a valid approach as was mentioned in Section 3.3, and will reduce the number of unknowns required throughout the volume of the finite element problem. Even so, for a 3D finite element simulation, the number of unknowns required for the PML implementation rises as the cube of PML layer thickness and mesh density requiring an impractical number of unknowns to implement effectively. For the PML to be a better alternative than traditional ABCs its computational efficiency must be improved by orders of magnitude without compromising its effectiveness. It is the purpose of this section to show how the nature of
the numerical reflection relations derived in Section 3.3 and then analysed in Section 4.2 may be exploited to produce such a PML implementation.

4.5.1 Numerical dispersion and reflection in a compressed mesh

Recall from Section 4.2, the observation that \( c_y \) depends on the PML variable parameter, \( |a_{pml}| \), while \( c_x \) remains independent. Thus, the numerical reflection for large values of \( a_{pml} \) are attributable to a large value of \( c_y \) only. Since \( c_y \) is the product of \( k_0, a_{pml}\sqrt{\varepsilon_\mu} \) and \( L \), compensation for a large \( a_{pml} \) can be made by reducing one of \( k_0, \sqrt{\varepsilon_\mu} \) or \( L \). Since the frequency and material constants are set by our problem, only the edge length \( L \) may be used to compensate. With edge lengths in the \( x \) and \( y \) directions equal, a reduction in \( L \) will reduce both \( c_x \) and \( c_y \) by equal amounts, with any reduction in \( c_x \) wasted. The task is thus to find a method of reducing \( L \) that only affects \( c_y \). This suggests anisotropic compression of the mesh.

To discover whether it is possible to reduce the edge length that appears in \( c_y \) at a boundary without affecting \( c_x \) by compressing the mesh anisotropically, it is necessary to re-derive the numerical dispersion and reflection for both edges and nodes in such a mesh. This section derives the numerical dispersion and reflection for both edge and node basis functions for a compressed mesh. The resulting relations are then examined, in the context of the PML to identify the relevant parameters required to optimally compensate for the magnitude of the PML parameter and hence reduce reflection errors. A simulation of the effect of these parameters as a function of angle, similar to the investigation of Section 4.2, is conducted to estimate the ideal performance of this new implementation. Finally, a single layer implementation of this compressed PML is analysed using the finite element method, similar to the analysis of Section 4.4. The performance of this new implementation of the PML is compared to the results of Section 4.4 in terms of effective absorption, unknowns required and matrix conditioning. Finally, some conclusions are drawn regarding the applicability of this new implementation of the PML to various finite element problems.

Numerical dispersion and reflection modeled by node basis functions in an anisotropically compressed finite element mesh

Consider the portion of mesh depicted in Figure 4.11 a). Following directly the procedure detailed in Section 3.2.1, the fields can be related by

\[
E_2 = e^{-j\alpha'} e^{j\beta'} E_1 \quad (4.10)
\]
\[
E_3 = e^{-j\alpha'} e^{-j\beta'} E_1 \quad (4.11)
\]
\[ E_4 = e^{-2jy'} \]  
\[ E_5 = e^{ja} e^{-jy'} E_1 \]  
\[ E_6 = e^{ja} e^{jy'} E_1 \]  
\[ E_7 = e^{2jy'} \]  

where

\[ \alpha' = k_x \sqrt{3} L_x / 2 \]  
\[ = \sqrt{3} / 2 k_y \sqrt{\varepsilon_{xx} \mu_{yy}} L_x \beta \cos(\theta) \]  
\[ = \sqrt{3} / 2 c'_{xy} \beta \cos(\theta), \]  
\[ y' = k_y L_y / 2 \]  
\[ = 1/2 k_0 \sqrt{\varepsilon_{xx} \mu_{yy}} L_y \beta \sin(\theta) \]  
\[ = 1/2 c'_{yy} \beta \sin(\theta) \]

in which

\[ c'_{xx} = k_0 \sqrt{\varepsilon_{xx} \mu_{xx}} L_y, \]  
\[ c'_{yy} = k_0 \sqrt{\varepsilon_{xx} \mu_{yy}} L_x. \]  

and \( \beta \) is the normalised numerical dispersion.

The general local matrix for a triangular finite element is given in 3.11. If the triangle is assumed to be a compressed equilateral triangle as depicted in Figure 4.11 b), then the local matrices can be expressed as:

\[ -k_0^2 \varepsilon_{xx} L_x L_y \frac{\sqrt{3}}{48} \begin{bmatrix} 2A' & B' & B' \\ B' & 2C' & D' \\ B' & D' & 2C' \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \]  

for both the upward and downward pointing triangle where

\[ A' = 1 - \frac{8}{c'_{yy}^2} \]  
\[ B' = 1 + \frac{8}{c'_{yy}^2} \]  
\[ C' = 1 - \frac{6}{c'_{xx}^2} - \frac{2}{c'_{yy}^2} \]  
\[ D' = 1 + \frac{12}{c'_{xx}^2} - \frac{4}{c'_{yy}^2}. \]
It is evident that these expressions are identical to those of Section 3.2.1, with the exception that $c_x$ uses $L_y$ and $c_y$ uses $L_x$ where previously they both used the value $L$. Having established this, it is evident that the numerical dispersion will again be the solution to

\[ (A' + 2C') + D'(\cos(2b)) + 2B' \cos(a) \cos(b) = 0 \] (4.25)

Having identified that the mesh compression can be modeled using the simple modification to $c_x$ and $c_y$ presented in Equations (4.18) and (4.19) it is trivial to derive the expression for the numerical reflection at an anisotropically compressed interface.

Consider the interface between material 1 and material 2 as shown in Figure 4.12. Material 1 is meshed in a uniform fashion with edge length $L_1$. Material 2 is discretised with an anisotropically compressed mesh such that the triangles are as depicted in Figure 4.11 b), with edge lengths $L_x2$ and $L_y2$. Note that since the two meshes must share edges at their interface, $L_y2 = L_1$. The numerical reflection can be easily shown to be

\[
r = -\frac{L_{x1}L_{y1}\epsilon_{x1}B_1 \sin \alpha_1 - L_{x2}L_{y2}\epsilon_{x2}B_2 \sin \alpha_2}{L_{x1}L_{y1}\epsilon_{x1}B_1 \sin \alpha_1 + L_{x2}L_{y2}\epsilon_{x2}B_2 \sin \alpha_2}.
\] (4.26)

where $L_{x1} = L_{y1} = L_{y2} = L_1$ and $L_{x2}$ is the edge length in the compressed dimension.

The previous derivation has made available an extra variable $L_{x2}$ that does not affect the finite element problem outside the PML. This variable affects only the value of $c_y$ leaving $c_x$ unchanged. From the investigation in Section 4.2 it was found that the PML variable parameter, for matching across a plane with normal in the x direction, only affected the variable $c_y$. Thus it seems that the suggested mesh compression may indeed allow for the efficient compensation for large PML, only in the dimensions where it is required. Verification of this prediction is presented in Section 4.5.3. Before this can be done, it will be necessary to repeat the above derivation for the edge basis functions to ensure that a similar benefit is possible.

**Numerical dispersion and reflection using anisotropically compressed edge basis functions**

The procedure of Section 4.5.1 is repeated for edge basis functions. Consider the portion of mesh depicted in Figure 4.13. Following directly the procedure detailed in Section 3.2.1, the fields can be related by

\[
H_4 = e^{-ja}e^{jb}H_2
\] (4.27)

\[
H_5 = e^{-ja}e^{-jb}H_3
\] (4.28)

\[
H_6 = e^{-2jb}H_3
\] (4.29)
Figure 4.11: a) A portion of an anisotropically compressed hexagonal finite element mesh with node basis functions labelled. b) A single element with dimensions shown.

Figure 4.12: A boundary between an uncompressed and compressed mesh with node basis functions labelled. The direction of propagation of Incident, reflected and transmitted is also shown.
where, $a'$ and $b'$ are defined in Equations (4.16) and (4.17) respectively. The closed form local matrix for the equilateral finite element, relating the edges, is

\[
\begin{bmatrix}
\sqrt{3} \\
72\varepsilon_{zz} \\
A' & B' & B' \\
B' & C' & D' \\
B' & D' & C'
\end{bmatrix}
\]

for both the upward and downward pointing triangle where

\[
A' = \frac{L_y}{L_x} \left( -c_x'^2 - 9c_y'^2 + 96 \right) 
\]

\[
B' = \sqrt{\left( \frac{L_y^2}{4L_x^2} + \frac{3}{4} \right) \left( -c_x'^2 + 3c_y'^2 + 96 \right)} 
\]

\[
C' = \frac{L_y}{L_x} \left( \frac{L_y^2}{4L_x^2} + \frac{3}{4} \right) L_x \left( -7c_x'^2 - 3c_y'^2 + 96 \right) 
\]

\[
D' = \frac{L_y}{L_x} \left( \frac{L_y^2}{4L_x^2} + \frac{3}{4} \right) \left( 5c_x'^2 - 3c_y'^2 + 96 \right) .
\]

Again, only simple substitution of these modified local matrix elements is required to determine the numerical dispersion and reflection in this compressed mesh. The dispersion may immediately be written

\[
D' \left( A'D' - B'^2 \right) \cos^2(b') + \left( C' - D' \right) B'^2 \cos(a') \cos(b') - C' \left( A'C' - B'^2 \right) = 0. 
\]

Similarly, the numerical reflection from an interface between two compressed meshes, as depicted in Figure 4.14, will be

\[
r = -\frac{Z_1 - Z_2}{Z_1 + Z_2} 
\]

where

\[
Z_i = \frac{(D_i^2 \cos^2 b - 4C_i^2)}{\sin a_i B_i^2 (D_i^2 - 2C_i^2)}
\]

In the context of the PML boundary, medium 1 would be the problem to be matched, and thus $L_{x1} = L_{y1}$ to avoid non-physical anisotropy. Since the meshes on either side of the boundary must share the edges on the boundary, $L_{y2} = L_{y1}$. The value of $L_{x2}$ may, however be freely chosen and thus, as with the node basis functions, an extra free variable has been introduced.
Figure 4.13: a) A portion of an anisotropically compressed hexagonal finite element mesh with edge basis functions labelled. b) A single element with dimensions shown.

Figure 4.14: A boundary between an uncompressed and compressed mesh with edge basis functions labelled. The direction of propagation of Incident, reflected and transmitted is also shown.
CHAPTER 4.

4.5.2 Using mesh compression to improve the PML

Having introduced the edge length in the x direction as a free variable of the PML boundary, it is now possible to investigate how it may be used to improve the efficiency of a PML boundary. To do this, an approach similar to that used in Section 4.2 is taken. The material tensors of Equations (4.1) and (4.2) were substituted into the reflection Equations (4.26) and (4.39), for node and edge basis functions respectively. The frequency was set to 5 GHz, the base edge length to 0.001 cm and the reflection error was plotted as a function of \( \alpha_{\text{pml}} \) and the ratio \( L_{2x}/L_{2y} \).

Figure 4.15 shows the family of curves resulting from the solution of Equation (4.26) to obtain the numerical reflection from the PML interface as modeled by node basis functions. The numerical reflection for \( \alpha_{\text{pml}} = 3^n \) for loss tangents of 0 and 1 are depicted by solid and dashed lines respectively. It is evident that compressing the mesh, should indeed improve the numerical reflection from a PML interface. For the case of the lossless PML (loss tangent of 0) the reflection error should actually null when \( L_{2y}/L_{2x} = \alpha_{\text{pml}} \). If mesh compression is continued beyond this optimal point, the reflection error increases asymptotically approaching a threshold that is independent of \( \alpha_{\text{pml}} \). For the case of PML with loss (loss tangent of 1), the reflection error does not exhibit a null at \( L_{2y}/L_{2x} = \alpha_{\text{pml}} \), but instead asymptotically approaches the same threshold level of the lossless case directly. It is shown in Section 4.6 that this threshold level is related to the frequency of the problem and the uncompressed edge length.

The same procedure was applied to the edge basis functions in an identical fashion with the results presented in Figure 4.16. The relationships can be seen to be almost identical. Note the noise in reflection of the highest PML value for low mesh compression. The very large PML value at this point makes the gradient based algorithm unstable in this region.

These observations suggest a number of possible methods of improving the PML. Firstly, interesting though it is, the removal of numerical reflection entirely from a PML interface by mesh compression cannot be applied to a practical PML boundary condition since the PML material needs to have a loss tangent of 0, rendering it non-absorbing to propagating waves. On the other hand, mesh compression of a PML with a nonzero loss tangent can significantly reduce numerical reflections from its surface while maintaining its absorption. Further the numerical reflection from PML material of any value of \( \alpha_{\text{pml}} \) can be reduced to the same low level given sufficient mesh compression. Finally, since the reflection error approaches a threshold with continued compression, over-compression will not have a detrimental effect on the numerical reflection. Thus for boundaries at which there is a range of edge lengths, as would be likely for all but perfect meshes, compression sufficient for the longest edge would suffice to provide the same reflection.
Figure 4.15: The predicted numerical reflection from a PML interface as a function of mesh compression in the normal direction, for various values of PML parameter $a$ using the node basis function. Solid lines show the reflection from a lossless PML, dashed lines show reflection from a PML with a loss tangent of 1.

Figure 4.16: The predicted numerical reflection from a PML interface as a function of mesh compression in the normal direction, for various values of PML parameter $a$ using the edge basis function. Solid lines show the reflection from a lossless PML, dashed lines show reflection from a PML with a loss tangent of 1.
level for all edges.

This approach to improving the reflection error occurring at a PML interface will be of great significance to improving its efficiency. The technique requires only a one dimensional compression of the mesh in the direction normal to the interface. When compressing a PML layer, the layer thickness should be maintained constant, to ensure the overall absorption of the layer remains constant and thus only the triangles within the layer should be compressed. This implies the addition of unknowns since the same space needs to be filled with thinner triangles, however the increase in unknowns is one dimensional, irrespective of the dimensionality of the problem. Thus even for a 3D problem, only a 1D mesh compression is required. An exception will occur at the corners where the PML boundaries meet. Here a 3D mesh compression is required, however the volume of these corners is expected to be small relative to the remaining PML region. In comparison to the alternative of increasing the mesh density throughout the PML region, as suggested by Polycarpou et al. [30], this technique should improve the computational efficiency of the PML by orders of magnitude, without compromising its effectiveness.

Though this technique seem a very promising proposal, this theory has been based on the assumption of a perfect hexagonal mesh. It is thus necessary to demonstrate that this technique can be applied to a PML interface within a random distribution of triangles as would occur in a practical finite element problem. This is the goal of the following section.

### 4.5.3 Verification

Section 4.5.2 presented a method by which the numerical reflection from a PML interface could be minimised through a one dimensional mesh compression. Numerical predictions for a perfect hexagonal mesh demonstrate that the technique is capable of reducing the reflection error by many orders of magnitude, while only incurring a minimal increase in the number of unknowns. It must be shown that this technique is applicable to the case of a practical finite element problem with imperfect triangular mesh as would result from a typical mesh generator. It is therefore the aim of this section to demonstrate the application of this technique to a practical finite element problem for both the node and edge basis functions.

The problem chosen is that presented by Polycarpou et al. in [44], and analysed further in Section 4.4. For this investigation, a finite element edge length of 2.0 mm, and frequency to 100MHz was chosen. As with the investigation of Section 4.4, the total reflection from the conductor backed PML layer, as modeled by the finite element method, is recorded as a function of the loss introduced to the PML. This is repeated for several
different mesh compressions.

If the PML thickness is $d$, a mesh compression in the PML of a factor of $C$ is achieved by beginning with a PML layer of thickness $Cd$. A finite element mesh is constructed in the usual fashion. A simple preprocessing program is used to scale all of the coordinates within the PML layer along the compression direction by $1/C$. The resulting PML layer will be of thickness $d$, but will be composed of triangles where $L_y/L_x = C$.

This procedure is applied to the PEC backed, PML truncated parallel plate waveguide problem of Section 4.4 for mesh compressions of $L_y/L_x = 2^n, (n = 0..8)$. Figure 4.17 shows the reflection coefficient resulting from the finite element simulation using node basis functions. The ideal reflection is depicted by a solid line while the simulated reflection for the various mesh compressions are depicted by dashed and dotted lines as described in the legend. It is evident that mesh compression does indeed improve the reflection error from the PML interface. Comparison with the increased mesh density approach of Section 4.4, shows that halving the edge length in the normal direction has an equivalent effect to halving the edge lengths in all directions, but produces only a linear increase in the number of unknowns. As mentioned previously, uniform mesh refinement in a 2D or 3D finite element simulation produces a quadratic or cubic increase in the number of unknowns.

Figure 4.18 shows the dependence of the finite element matrix condition number as a function of PML loss and mesh compression. It is evident that the mesh compression actually improves the condition number. This suggests that the mesh compression is not only countering the effects of the PML variable parameter, but is also countering the increase in condition number associated with an increase in the number of unknowns. Referring to Figure 4.8, depicting the dependence of condition number on PML variable parameter and mesh density for an uncompressed PML boundary, it can be seen that the condition number rises with a uniform decrease of edge length.

A one dimensional mesh compression thus offers a two fold improvement over the increased mesh density approach. Firstly it requires far less unknowns to produce an equally effective PML boundary, and thus less computational effort is required to solve the problem. This is already evident for even a two dimensional problem and will be an order of magnitude more significant for the truncation of a three dimensional problem. Secondly the mesh compression actually improves the condition number of the finite element matrix for the node basis functions, despite the increase in unknowns. Thus even less computational effort is required to attain a more accurate solution to the finite element method.

The above procedure was repeated for edges with the reflection coefficient as a function of PML loss and mesh compression presented in Figure 4.19. Again it is evident...
Figure 4.17: The reflection modeled by the finite element method using node basis functions for various values of mesh compression and PML loss parameter, $\delta = \ln(1/R)$ where $R$ is the ideal overall reflection coefficient. $L$ refers to the finite element edge length and $N$, to the number of unknown nodes in the mesh.

Figure 4.18: The condition number of the finite element matrix using the node basis functions for various values of mesh compression and PML loss parameter, $\delta = \ln(1/R)$ where $R$ is the ideal overall reflection coefficient. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
that mesh compression has a significant impact on the reflection error at a PML interface, with a one dimensional compression of the mesh providing equivalent improvement to the two dimensional compression shown in Figure 4.9 of Section 4.4. The mesh compression technique requires significantly less unknowns than mesh density technique. Figure 4.20 shows the condition number of the finite element matrix for this case. The effect of the mesh compression on condition number is evidently not as spectacular as for the nodes; however, the condition number of the matrix required to produce a specific reflection error is less than that required by the mesh density technique.

A new technique for implementing the PML in the finite element method has been derived and demonstrated in a practical problem. It is as effective for edges as it is for nodes and is evidently vastly more efficient than more traditional techniques, especially for 3D finite element simulation. Although this technique appears very promising, it is not quite the panacea that it appears. The next section explores some of its limitations and briefly discusses some possible approaches to address these problems.

4.6 Notes on frequency response and PML tapering

In the previous section, a technique for improving the effectiveness of a PML layer with minimal increase of unknowns is described and demonstrated for a practical finite element problem. An improvement in reflection coefficient from a PML interface of several orders of magnitude is achieved, while incurring only a linear increase in the number of unknowns. This technique is also shown in certain circumstances to improve the matrix condition number, hence further reducing the computational effort required to attain a solution.

Although this seems a very promising technique answering almost every point raised by Polycarpou et al. [44], there is a significant limitation that has been overlooked, namely the frequency response. In the previous investigations, the frequency was set to 100 MHz, and the average edge length 2.0 mm, \( L = \lambda /1500 \). This is a very fine mesh for this frequency, and thus it is not surprising that very low reflection errors can be attained. It is more typical to construct a mesh from edges where \( L \approx \lambda /10 \). This is the situation for the previous case at a frequency of 15 GHz. It is thus of interest to investigate the behaviour of these PML boundaries at higher frequencies.

To examine and compare the effects of mesh compression and mesh refinement over a range of frequencies, the simulations of Section 4.4 and Section 4.5.3 were repeated with \( \delta = 9 \) and frequency ranging from 100 MHz to 30 GHz.

Figure 4.21 presents the reflection coefficient of the simulation using node basis functions for uniformly meshed edge lengths of 2.0 mm, 1.0 mm and 0.5 mm. It is evident
Figure 4.19: The reflection modeled by the finite element method using node basis functions for various values of mesh compression and PML loss parameter, $\delta = \ln(1/R)$ where $R$ is the ideal overall reflection coefficient. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.

Figure 4.20: The condition number of the finite element matrix using the node basis functions for various values of mesh compression and PML loss parameter, $\delta = \ln(1/R)$ where $R$ is the ideal overall reflection coefficient. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
that although the reflection coefficient of the nodes is poor at low frequencies, it rapidly reaches an acceptable level as frequency increases, before gradually rising as frequency is increased further. It is proposed that the poor performance of the nodes at low frequency, as shown in Figure 4.7, is due to a breakdown in the finite element numerical dispersion due to the very large PML variable parameter. Interestingly, at higher frequencies, the distinction between the performance of the three meshes is not clear, with each of the meshes providing unsatisfactory reflection of around \(-30dB\).

The dependence of the condition number on frequency is depicted in Figure 4.22. It is evident that this parameter rises sharply with reduced frequency, due both to the large PML parameter and to the low frequency when compared to the edge length. Using the condition number as a guide, an iterative solution could take hundreds of times longer to solve at the lower frequency that it would at the higher frequencies.

Figure 4.23 presents the reflection coefficient for finite element simulations using the node basis function and an anisotropically compressed mesh with \(L_y/L_x = 1, 2, 4,\) and \(8\). The mesh compression clearly has a significant impact on the reflection coefficient at low frequencies, with the compression \(L_y/L_x = 2\) providing better performance than even the most dense uniform mesh of Figure 4.21. Interestingly, above about 5GHz, the mesh compression has negligible effect, providing a reflection coefficient of approximately the same value as the uniformly meshed cases.

Figure 4.24 presents the frequency dependence of the condition number of the compressed mesh. The condition number at lower frequencies is the same or better than the uncompressed mesh, but at higher frequencies, mesh compression worsens the condition number.

These observations can be easily understood by considering the fact that the PML variable parameter, being set as a conductivity defined in Equation (4.8), is a frequency dependent loss. At around 5GHz, for \(\delta = 9\), \(|a_{pml}| \approx 2\). Above this frequency \(|a_{pml}|\) approaches 1, thus it is evident, referring to Figure 4.15 that compressing the mesh beyond a factor of 2 will have little effect. This suggests that the numerical reflection is no longer due to the large value of \(|a_{pml}|\), but is instead limited by the edge length. Indeed at 15GHz, the edge length is \(\lambda/10\), the rule of thumb limit for finite element. It would thus seem that the technique of mesh compression is best suited to frequencies where the edge length is small, and \(|a_{pml}|\) is large, suggesting that the thickness of the PML layer should be small also. Further, it would appear that neither technique offers good performance over a broad range of frequencies, indicating that perhaps an assembly of different PML layers, or a taper of material parameter, similar to that demonstrated by Polycarpou [30], may need to be devised for wide band applications. It is worth noting that for similar reasons, the point at which the frequency response of the compressed mesh crosses that of the uncompressed
mesh, is approximately the frequency at which $|\alpha_{pm}| = \frac{L_y}{L_z}$.

The edge basis functions were examined in a similar manner with the frequency response of the reflection coefficient of the uniformly refined cases depicted in Figure 4.25. Unlike the node basis functions, the reflection coefficient using edge basis functions does not degrade at lower frequencies. As frequency is increased, the reflection coefficient, gradually increases in the same fashion as observed with the node basis functions, becoming unacceptable towards 30GHz.

The frequency response of the condition number for the uniformly refined cases is depicted in Figure 4.26. The matrix conditioning, degrades less sharply than for the node basis functions, but is significantly higher in general. This can be explained since, as shown in Figure 4.4, the edge based simulations produce a condition number that rises quadratically with reduced frequency, whereas the node basis function produce a linear relationship. Thus the rise in condition number of Figure 4.10 is due in part to the increased PML parameter and part to the reduced frequency.

The reflection coefficient for the compressed mesh implementation using edge basis functions is depicted in Figure 4.27. As with the node basis functions, at low frequencies, the mesh compression technique produces a more effective truncation than uniform refinement, while incurring less unknowns. At higher frequencies, the improvement is negligible.

The condition number as a function of frequency for the compressed cases is shown in Figure 4.28. An improvement over the uniformly refined case is observed, although less the the improvement observed for node basis functions. This is as expected, since the mesh compression only compensates for the PML parameter, and not the inherent increase with reduced frequency.

### 4.7 Conclusions

In summary, the relationships derived in Chapter 3 have proved to be powerful tools for the analysis, design and understanding of effective and efficient PML boundary conditions. Using these expressions a significantly improved PML implementation technique, using a one dimensional mesh compression, has been developed and verified, comparing favorably with the work of Polycarpou et al. [44]. The technique described can be used to reduce each of the reflection error, the required unknowns and the matrix condition number of a problem when compared to more traditional technique of uniform mesh refinement. Relying only a 1D mesh refinement, this technique will be of particular use in the efficient truncation of 3D finite element meshes.

Investigation of the performance of this technique over a range of frequencies indicate
Figure 4.21: The reflection modeled by the finite element method using node basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.

Figure 4.22: The condition number modeled by the finite element method using node basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
Figure 4.23: The reflection modeled by the finite element method using node basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.

Figure 4.24: The condition number modeled by the finite element method using node basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
Figure 4.25: The reflection modeled by the finite element method using edge basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.

Figure 4.26: The condition number modeled by the finite element method using edge basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
Figure 4.27: The reflection modeled by the finite element method using edge basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.

Figure 4.28: The condition number modeled by the finite element method using edge basis functions for various values of mesh compression and frequency, $\delta = 9$ in all cases. $L$ refers to the finite element edge length and $N$, to the number of unknown edges in the mesh.
that although the mesh compression technique performs well at lower frequencies where \( |a_{pml}| \) is large, it becomes ineffective at higher frequencies. This suggests that in its current state mesh compression is most applicable to thin, high \( |a_{pml}| \) layers at frequencies where the edge length is small. It is worth noting that the uniform mesh refinement approach offers no better performance at these higher frequencies and thus both techniques are unacceptable for use over these broad frequency ranges.

Some possible approaches for improving the efficiency of the PML over a range of frequencies can be suggested. Since the PML is limited primarily by the initial reflection from the PML interface, and consequently, the mesh density refined to reduce this initial reflection, sustaining this mesh refinement throughout the whole PML layer is unnecessary. Considering the amount of loss present in the PML, small reflections throughout the PML layer may be tolerated and thus a tapered implementation where the mesh becomes more coarse, or \( |a_{pml}| \) increases with depth can be devised to optimally reduce the number of unknowns required for a given reflection error. Further, a PML with zero loss tangent can be compressed in such a way as to cancel all numerical reflection and thus it is conceivable that a graded loss tangent could be used. Finally, since it has been demonstrated that mesh compression produces optimum results for \( L_y / L_x = a_{pml} \), and \( a_{pml} \) varies as a function of frequency, a range of mesh compressions an PML parameters could be used to provide broader bandwidth.

Thus there are now four variables that may be used in a graded PML, \( a_{pml} \), \( L_x \), \( L_y \) and the loss tangent. It is proposed that the relationships derived for the numerical reflection and dispersion may provide an excellent tool in the investigation of optimum combinations of these parameters. Such an investigation could attempt to identify optimum closed form solutions for a general class of taper, or, since it is possible to rapidly solve the relations numerically, more specific numerical optimisation routine could be used to locate specific combinations for a desired set of properties. In fact it can be imagined that a numerical optimisation routine, using these relations could be built into the preprocessor of a finite element package, producing an optimum PML to the users specifications.

It would also be worth applying the procedure of this Chapter, and of Chapter 3, to both edge and node higher order elements [54], [53, pages 123–135] as has been done for nodes in the isotropic case by [48]. It is almost certain that such basis functions will exhibit differing reflection error, and condition number responses, and consequently would suggest further investigation would be required for the optimum implementation of a PML boundary with these basis functions.

Although there is evidently a great deal of work that can be done in extending the frequency range of the PML, and developing these techniques for higher order elements, this is not necessary for the cases of interest to this study. In the following chapter, Chapter
5, a number of examples using the PML techniques developed here will be presented to demonstrate their effectiveness in practical situations. These will include the cases of the Mach-Zehnder co-planer waveguide electrodes on biaxial $LiNbO_3$, and the attenuation of a radially bent waveguide as described in Section 5. The RF electrode problem is of the order of $\mu m$'s, and the frequency range is between 1 and 100 GHz.
Chapter 5

Examples of the PML in Eigenvalue Simulations

5.1 Introduction

In Chapter 1, two specific devices were identified as targets for finite element eigenvalue simulation. These were the co-planar waveguide (CPW) electrodes of a Mach-Zehnder optical intensity modulator (MZM), and the radiating optical waveguides that result from bending channel waveguides. In each case, the imposition of truncating boundaries is problematic. These issues are briefly reiterated.

The accurate simulation of the traveling wave CPW electrodes of the MZM over a range of frequencies is critical to the effective design of broadband MZM devices. It has been shown [55], using finite difference and standard PEC boundaries, that an extremely large bounding region is required before the effect of truncations on the solution is negligible. This is an inefficient use of unknowns and leads to prolonged solution times and excessive computational requirements. The PML seems an obvious alternative to the standard PEC boundary condition, however since the substrate is LiNbO₃, a strongly uniaxial material, the generalised PML derived in Chapter 2 is required.

Many integrated optic device configuration require long thin sections of optical waveguide. For reasons of practicality and efficiency, it is desirable to reduce their length by folding the waveguide sections. Devices that make use of optical feedback [56], also require waveguide bends and often have small arc length as a criterion. This bending of an optical waveguide produces radiation losses, with tighter bends causing greater loss. In order to design tightly bent waveguides that exhibit minimal loss, a model capable of accurately modeling propagation in a bent waveguide, and the associated losses is essential.

A conformal mapping can be employed to allow a standard mode solver to model bent waveguides, however, this does not assist in modeling the radiation. Again the PML
seems an obvious choice to truncate the problem and absorb the radiated waves.

Surprisingly there seems a shortage of published works utilising the PML in eigen-value problems. In fact only two articles [36], and [38] have been found suggesting the concept. The authors of [36] apply a tapered conductivity profile PML to a one dimensional leaky optical slab waveguide. They have used a scalar finite element method which they have modified within the PML region to account for the vector nature of the PML. The authors of [38] have used a full wave finite element solution, again in one dimension, to calculate the resonances of a one dimensional Fabry-Perot cavity. In both studies the PML parameter is chosen in such a way as to only absorb the radiating waves, leaving the evanescent tails to be truncated in the usual fashion. As is observed in [36], this limits the size of the computational window. It is worth noting that radiation from a one dimensional problem can be easily modeled by assuming a complex exponential form outside the solution region [53, page 52]. Application of such a boundary condition to a two dimensional problem is possible, but leads to a situation where the matrix elements of the eigensolution themselves depend on the eigensolution, requiring iterative and highly computationally expensive matrix solution.

As was discussed in Chapter 2, and contrary to popular belief, the PML parameter can be chosen such that it will absorb propagating waves, evanescent waves or both simultaneously. This suggests that the PML boundary condition can be used to truncate the solution region for non-leaky modes. It is thus the aim of this Chapter to investigate and demonstrate the PML as a means of truncating 2D eigenvalue simulations using the finite element method. It is shown that the PML can be used equally well for truncating transversely propagating tails of radiating modes, or the transversely evanescent tails of guided modes. To ensure that the PML is implemented efficiently, without significantly compromising accuracy, the analysis and improved implementation schemes developed in Chapter 3 and Chapter 4 are employed to provide both effective and efficient PML truncations for each case investigated.

This Chapter examines three cases. Firstly, a simple microstrip line as analysed in [57] is simulated and the application of the PML for improved efficiency is analysed. This is a macroscopic problem with features of size in the order of a tenth of a wavelength. The next problem analysed is the CPW electrodes of an MZM. Although similar to the microstrip line problem, the modal solution to this problem is less tightly confined, is of a much smaller scale and is on an anisotropic substrate, hence requiring the use of the biaxial PML derived in Chapter 2. The final simulation is a brief investigation of the radiating modes of a bent integrated optic channel waveguide. This is a leaky structure and thus the ability of the PML to absorb radiated energy is demonstrated.

A summary of the findings for the application of the PML to 2D eigenvalues is then
presented along with guidelines for its application to eigenvalue problems in general.

5.2 Simple microstrip line

The first example is a simple microstrip line. A detailed examination of this geometry with the finite element method can be found in Slade [57]. For convenience, the geometry of this strip line is reproduced in Figure 5.1 with dimensions as stated. This example has been chosen since it is a simple macroscopic problem, with features of the order of a tenth of a wavelength. The investigation of [57] examines the frequency dependence of the propagation constant and characteristic impedance of higher order modes of this waveguide. Since the propagation constant and characteristic impedance are related to the eigenvalue and eigenvector respectively, they should be good indicators of the effect of the introduction of a PML boundary on the overall eigensolution.

The example presented in [57] is also a good candidate for PML truncation since the majority of unknowns are actually used to model the bounding space around microstrip to simulate an open region of space. The authors of [57] have used a bounding box of \( b = 10 \text{mm} \), or a third of a free space wavelength at 10 GHz. To determine how this dimension is chosen it is necessary to investigate the dependence of the solution on this boundary dimension. This investigation also serves as a benchmark by which to measure the performance of the PML boundary as an alternative truncation.

Figure 5.1: Geometry of microstrip example; substrate dielectric \( \varepsilon_r = 10 \), stripline width \( w = 1.0 \text{mm} \), dielectric thickness \( h = 1.0 \text{mm} \) and bounding box dimension \( b \) is varying.
5.2.1 Convergence analysis

A certain amount of empty space is required around the stripline in order for the problem to be considered open. To determine the amount of empty space required, a sequence of simulations with increasing boundary dimension $b$ was performed using the mixed edge-node eigenvalue formulation as described in Appendix A. The dependence of the eigenvalue on the parameter $b$ is presented in Figure 5.2. Also presented in Figure 5.2 is the characteristic impedance as a function of $b$, calculated as described in [57].

To assess the convergence of these simulations, the rate of change of each of these parameters with $b$ is also calculated and when this has reduced sufficiently, the solution is considered converged. Figure 5.3 presents the rate of change of the effective index and characteristic impedance as a function of $b$, normalised to the smallest boundary dimension. When this rate of change has reduced by two orders of magnitude, the solution is considered converged.

Examination of Figure 5.3 indicates convergence occurs at approximately $b = 14\text{mm}$, close to the choice of 10mm in [57]. It is worth noting that of the $14\text{mm} \times 14\text{mm}$ solution area only $1\text{mm} \times 0.5\text{mm}$ actually contains the features of the geometry. It is thus evident that if a PML boundary can be devised to reduce the amount of space required around the features of the geometry, then a significant improvement in the efficiency of the solution should be attained.

5.2.2 Application of PML boundary condition

In the previous section the large truncation boundary required for the accurate solution of the microstrip problem is found to be inefficient. In this section a PML boundary is developed that requires only a fraction of the computational resources of the PEC truncation, when applied to the microstrip problem, while maintaining the same level of accuracy in the solution. Following are a few observations that may help this development.

Firstly, since the structure does not radiate, no PML absorption of propagating waves is required, and hence the loss tangent of the PML may be set to zero. Referring to Section 4.5.2 it can be seen that a PML with zero loss tangent can be compressed such that no numerical reflection occurs at the surface. Since the wavenumber of plane waves within a PML layer in the normal direction, is $a_{\text{pml}}k_n$, were $n$ is denoted the direction normal to the interface, a perfectly compressed lossless PML layer, would be electrically thicker by a factor of $a_{\text{pml}}$. Thus using a large PML parameter should cause the eigenvalue solution to converge for a smaller boundary dimension.

Although this seems promising, recall that the optimum compression requires a factor of $a_{\text{pml}}$ more unknowns than an uncompressed layer, exactly the number of unknowns
Figure 5.2: The effective index and characteristic impedance of the microstrip line first order mode as a function of bounding box dimension $b$.

Figure 5.3: The rate of change of the effective index and characteristic impedance with boundary dimension.
that would be required to simply make the boundary $a_{pml}$ times larger. Thus to actually improve the efficiency, it will be necessary to devise a PML truncation, with variable parameter exceeding that which would produce zero reflection. Hence the numerical reflection at the surface is finite, but just below the level of significance for the problem.

It is thus the goal of this section to investigate the effect of a PML truncation on the microstrip eigenvalue problem and to identify an implementation that provides as accurately converged answer as can be achieved in the absence of PML while requiring a minimum number of unknowns.

Figure 5.4 presents the geometry of the microstrip line enclosed by a PML boundary. A PML layer thickness of 1mm was chosen, and a minimal boundary dimension of $b = 2.25$ was chosen so that only 0.25mm separates the features of the problem and the PML. To investigate the effect of the PML variable parameter on the simulation, a similar approach to that used in Section 4.5.3 is taken. Figures 5.5 and 5.6 show the effective index and characteristic impedance, resulting from the solution of the geometry depicted in Figure 5.4, as a function of $a_{pml}$ for a number of one dimensional mesh compressions as described in Section 4.5.1. The value shown is the difference between the simulated solution and a supposed exact solution, taken as the asymptote of Figure 5.2. For ease of comparison, this error is expressed in dB ($10\log n_{eff}$).

A striking resemblance to Figures 4.19 is evident and a parallel interpretation is possible. As the magnitude of $a_{pml}$ increases, the PML layer seems electrically thicker and thus the solution approaches the free space solution. As the magnitude of $a_{pml}$ is increased further, numerical reflections begin to occur at the PML interface. As these reflections be-
Figure 5.5: The normalised error in effective index of the microstrip line first order mode as a function of PML variable parameter $|\alpha_{pml}|$ for mesh compressions of $L_x/L_y = 1, 2, 4$ and 8. Comparison is made to an assumed ideal effective index value of $n = 2.698$.

Figure 5.6: The normalised error in characteristic impedance of the microstrip line first order mode as a function of PML variable parameter $|\alpha_{pml}|$ for mesh compressions of $L_x/L_y = 1, 2, 4$ and 8. Comparison is made to an assumed ideal characteristic impedance value of $Z = 50.92$. 
come more significant, the solution begins to diverge as the transversely evanescent tails of the mode are reflected back from the PML interface into the waveguide structure. Compression of the mesh compensates for the large value of $a_{pml}$ and thus large PML values may be used before the onset of numerical reflections. It is interesting to note that with no mesh compression, a PML variable parameter of $a_{pml} = 3$ provides an optimum solution.

To verify that the simulations with optimal $a_{pml}$ for each mesh compression are indeed converging correctly, the convergence analysis of Section 5.2 was repeated for these cases. The effective indices of the simulations with $L_n/L_t = 1, 2$ and 4 and optimum PML parameters, chosen from Figure 5.5, of $a_{pml} = 3, 4$ and 5.5, respectively as a function of boundary dimension are presented in Figure 5.7. The uncompressed case with unity PML is also shown. It is evident that the simulation converges more rapidly when enclosed by a PML layer. Note the fluctuations in the eigenvalue for these cases. It is proposed that these are caused by subtle changes to the structure of the mesh with increasing boundary size.

It would seem evident from Figures 5.7 and 5.8 that most rapid convergence is achieved by the most highly compressed case. Recall, however, that the mesh compression requires the addition of unknowns, and thus comparison on the basis of boundary dimension is misleading. Figures 5.9 and 5.10 present the same effective index and characteristic impedance of the above simulations as a function of the solution time on a k6-200 PC with 128MB RAM. Of note is the fact that all of the PML cases have merged, indicating that no one approach to the application of the PML boundary is more efficient, in terms of computation time, than the other. Figures 5.9 and 5.10 also demonstrates the improvement in efficiency achieved by the application of a PML boundary. The PML truncations take approximately one third of the time to achieve the same level of accuracy.

The eigenvalue solution method, described in Bathe [58], can require the iterative solution of a matrix. It is thus important to note the affect of the PML on the condition number of this matrix to ensure the accuracy and efficiency of this solution. Figure 5.11 presents the condition number as a function of boundary dimension for each of the cases. It is evident that the condition number is effectively constant for all cases.

5.2.3 Summary

The PML has been applied to the microstrip problem investigated in [57] and demonstrates the ability to provide an accurate termination with 3 times more efficient solution, with respect to the time required. Similar improvement to memory requirements are observed. Equivalence between low compression, low PML parameter layers and high compression, high PML parameter layers has been discovered in terms of the number of
Figure 5.7: The effective index of the microstrip line first order mode as a function of boundary dimension for the optimum combinations of PML parameter and mesh compression as indicated.

Figure 5.8: The characteristic impedance of the microstrip line first order mode as a function of boundary dimension for the optimum combinations of PML parameter and mesh compression as indicated.
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Figure 5.9: The effective index of the microstrip line first order mode as a function of solution time on a k6-200 CPU PC, for the optimum combinations of PML parameter and mesh compression as indicated.

Figure 5.10: The characteristic impedance of the microstrip line first order mode as a function of solution time on a k6-200 CPU PC, for the optimum combinations of PML parameter and mesh compression as indicated.
unknowns required to obtain a specified level of accuracy. This leaves the choice of PML parameter as a true free variable, provided the appropriate mesh compression is applied to compensate. It is expected that a tapered PML layer would provide further improvement to efficiency of the homogeneous PML layers presented here.

5.3 Co-planar waveguide Mach-Zehnder modulator electrode structure

The second example is a coplanar waveguide (CPW) traveling-wave electrode structure component of a broad-band, Mach-Zehnder optical intensity modulator (MZM). As mentioned earlier, the careful design of this electrode structure is critical to attaining the broadest possible bandwidth in a Mach-Zehnder device. A thorough analysis of this device and the associated electrode design, can be found in [55]. The general geometry is depicted in Figure 5.12. Since there are many significant variables associated with the electrode structure, the capability to efficiently and accurately simulate such a structure is essential.

The improvement of the efficiency of solution of this electrode structure is one of the major goals of this work. This section demonstrates that the use of the PML boundary condition can greatly improve the efficiency of this simulation, and is thus a significant
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Figure 5.12: Geometry of the CPW electrode structure for the MZ optical intensity modulator. hot electrode width $w = 10.0\mu m$, electrode gap $g = 20\mu m$, electrode thickness $t = 10\mu m$, SiO$_2$ thickness $d = 1\mu m$.

step towards this goal.

As described in [55], a great deal of empty space is required around the features of the structure to ensure convergence. A boundary $b$ of $150\mu m$ is suggested, which is only a minute fraction of a wavelength at $10GHz$. Although the density of the mesh can be graded to improve the efficiency, this gradation must be gradual and thus a significant number of unknowns are required. Further the existence of the thin ($< 1\mu m$), but very significant SiO$_2$ buffer layer requires a fine mesh to be continued all the way to the boundary. It is thus evident that a truncation of the solution region should offer a significant reduction in the computational requirements for solution. As demonstrated in Section 5.2, the PML can be used effectively in this manner.

There are, however, some important differences between the simulation described in this section and that described in Section 5.2. Firstly, the substrate is LiNbO$_3$ a strongly anisotropic material. Thus in order to use the PML to truncate the boundaries adjoining the LiNbO$_3$, it must be based on the generalised PML developed in Chapter 2. Another, more subtle, difference is the scale of the problem when compared to a wavelength. Since the edge lengths are only a minute fraction of an edge length, it is expected that numerical reflections will be smaller than in the previous case and that the threshold level identified in Section 4.5.1 will be lower allowing more efficiency to be achieved through the technique of mesh compression.
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Using a similar procedure to that of Section 5.2, a convergence analysis of the problem in the absence of a PML boundary is first performed.

5.3.1 Convergence analysis

As discussed in Section 5.3, a large amount of empty space is required around the CPW features such that the effects of the PEC truncation on the guided mode may be considered negligible. To determine the actual dimensions required, a sequence of eigenvalue simulations, as described in Appendix A, and subsequent characteristic impedance calculation, as described in [57], are performed with increasing boundary dimension $b$. The effective index and impedance resulting from these simulations at a frequency of 10 GHz are presented as a function of boundary dimension in Figure 5.13. Again to assess the convergence, the derivatives of these parameters with respect to $b$, are calculated and normalised to the results for minimal possible $b$. Figure 5.14 presents the normalised derivatives of these parameters as a function of $b$. The simulation is deemed converged once this derivative has reduced by two orders of magnitude.

It is evident from Figure 5.14 that convergence occurs at around $b = 150 \mu m$. Thus the total computational area is approximately $300 \mu m \times 150 \mu m$ compared to the region enclosing the features of $10 \mu m \times 40 \mu m$. Application of a PML truncating boundary to this problem, as described in Section 5.2.1, should reduce this area and hence improve the efficiency of solution.

5.3.2 Application of PML boundary condition

In Section 5.3.1, it is found that a large computational domain is required for the eigenvalue solution to be considered converged. In this section, a similar approach to that used in Section 5.2.2, is applied to the CPW example. The modified CPW problem geometry is depicted in Figure 5.15. A minimal solution region of $b = 40 \mu m$ was chosen to allow an equivalent amount of the ground electrode to be exposed from the PML layer as the hot electrode. As in Section 5.2.2, Figure 5.16 and Figure 5.17 show the effective index and characteristic impedance of the eigensolution as a function of PML variable parameter. Again comparison is made to the asymptote of Figure 5.3.1.

Comparing Figure 5.16 to 5.5, it is evident that there are some differences. In the previous example, the eigensolution approaches the ideal solution with increasing PML variable parameter, until the magnitude of the PML parameter becomes large enough to incur significant numerical reflections, at which point the solution diverges. Increasing the mesh compression reduces the amount of PML reflection and hence larger values of PML parameter can be used.
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Figure 5.13: The effective index and characteristic impedance of the CPW fundamental mode at 10GHz, as a function of bounding box dimension \( b \).

Figure 5.14: The rate of change of the effective index and characteristic impedance of the CPW fundamental mode at 10GHz with boundary dimension.
Figure 5.15: Geometry of the CPW electrode structure for the MZ optical intensity modulator. Hot electrode width $w = 10.0 \mu m$, electrode gap $g = 20 \mu m$, electrode thickness $t = 10 \mu m$, SiO$_2$ thickness $d = 1 \mu m$. PML layer thickness $p = 10 \mu m$ and bounding box dimension $b$ is varying.

In this instance, the effective index approaches the ideal solution with increasing PML variable parameter, but then exceeds it. This behavior is thought to be due to a resonance within the PML layer. As the PML variable parameter is increased, the reflection at the PML interface increases further, causing the propagation constant to diverge as before. The optimum PML parameter is not clear from Figure 5.16.

Fortunately, Figure 5.16 exhibits very similar form to Figure 5.6, and thus an optimum PML parameter can be deduced from this figure. Following the approach of Section 5.2.2, to verify the convergence of the PML truncated simulations, a convergence analysis of each of the optimal cases is performed.

As in Section 5.2.2, the convergence of the simulations with PML truncations are examined as a function of boundary dimension, with the results displayed in Figures 5.18 and 5.19. Again it is seen that the simulations with most mesh compression and hence larger optimum PML value converge most quickly. As noted earlier, this is deceptive as the more highly compressed cases require the application of further unknowns, thus Figures 5.20 and 5.21 present the same results as a function of the time for solution.

Again it can be seen that the simulations with the PML truncation are all approximately 3 times more efficient in terms of the time required for solution and again each of the PML truncations is effectively equivalent.
Figure 5.16: The normalised error in effective index of the coplanar waveguide fundamental mode as a function of PML variable parameter $|a_{pml}|$ for mesh compressions of $L_x/L_y = 1, 2, 4$ and 8. Comparison is made to an assumed ideal value of $n = 2.582$.

Figure 5.17: The normalised error in characteristic impedance of the coplanar waveguide fundamental mode as a function of PML variable parameter $|a_{pml}|$ for mesh compressions of $L_x/L_y = 1, 2, 4$ and 8. Comparison is made to an assumed ideal value of $Z = 45.3$. 
Figure 5.18: The effective index of the CPW fundamental mode as a function of boundary dimension for the optimum combinations of PML parameter and mesh compression as indicated.

Figure 5.19: The characteristic impedance of the CPW fundamental mode as a function of boundary dimension for the optimum combinations of PML parameter and mesh compression as indicated.
Figure 5.20: The effective index of the CPW fundamental mode as a function of solution time on a k6-200 CPU PC, for the optimum combinations of PML parameter and mesh compression as indicated.

Figure 5.21: The characteristic impedance of the CPW fundamental mode as a function of solution time on a k6-200 CPU PC, for the optimum combinations of PML parameter and mesh compression as indicated.
5.3.3 Summary

Application of the PML truncation to the CPW electrodes of a MZ optical intensity modulator has been demonstrated, and similar to the findings of Section 5.2, an improvement of around a factor of 3 in the solution time has been achieved. Similar gains in terms of memory requirements were also achieved. This simulation has utilised the biaxial PML developed in Chapter 2 to match the strongly uniaxial LiNbO₃ substrate. Again a variety of PML truncations are shown to be equivalent in terms of the improvement in accuracy that can be achieved for a given solution time. A tapered PML should improve the gains in efficiency further and the application of such a tapered PML will be the topic of future work.

5.4 Bending loss in an integrated optic rib waveguide

The final example is a brief examination of a bent integrated optic rib waveguide. As mentioned in the introduction, Section 5.1, waveguide bends can be used to effectively reduce device length by folding long waveguide sections. They can also be used in transitions such as the optical waveguide y-junctions of Mach-Zehnder optical modulators to provide rapid separation of split waveguides without incurring significant transition losses [55]. Further, for devices that rely on optical feedback for example, [56] [59], waveguide bends offer a low loss means of routing the optical signal back to an earlier stage.

For all of the above applications, bends that are as tight as possible are desirable. Unfortunately, as the radius of a waveguide bend is reduced, the propagation losses introduced rise dramatically. Thus the design of tight waveguide bends that do not introduce significant losses has become the topic of much interest. The capability to efficiently and effectively model mode propagation bent waveguides of arbitrary index profile would be of great use in the investigation of novel low loss waveguide bends.

The FEM waveguide mode solver used for the simulations of Section 5.2 and 5.3 can be used to model modal propagation in a bent waveguides by applying a conformal mapping to convert from Cartesian to polar coordinates as described in Appendix D. For isotropic optical problems, this mapping results in the refractive index at any point being scaled by its radial distance from the cylindrical axis.

The geometry presented in Figure 5.22 is analysed both theoretically and experimentally in [60] with significant bending loss evident at a radius of 2 mm or less. The aim of this section is to simulate the bending loss of the structure in Figure 5.22 at a radius of 2 mm, using the conformally mapped FEM using a PML absorbing boundary condition. The effectiveness of the PML truncation is verified by comparison to Vijaya et al. [60].
5.4.1 Bending loss convergence analysis

The fact that this simulation involves propagation loss renders a convergence analysis difficult. No simple PEC bounding box will be large enough to model the propagation loss since all radiated power eventually reflects from the PEC boundary and is returned to the problem. There is thus no advantage in performing a convergence analysis with the PML truncation absent.

To perform a convergence analysis, an absorbing layer must be used in the first instance. In this investigation, a likely PML is chosen using the guidelines set out in Chapter 2, with sufficient absorption to significantly damp any radiation. At the same time, a mesh density that minimises reflection errors at the PML interface is chosen according to the observations of Chapter 4. As noted by Bérenger [29], choosing an absorbing boundary condition with high numerical reflection results in a truncation that must be placed further from the details of the problem to achieve an accurate result.

The PML layer was chosen to produce less than -20dB of reflection at normal incidence. According to Equation (2.33), a PML layer as depicted in Figure 5.22, with \( \ell = 1\mu m \) and \( a_{pml} = 0.5 \) and \( k_x = 1.5 k_0 \) at a wavelength of 830 nm, should produce more than the required absorption. It is worth noting, however, that the since the wave is predominantly propagating in the \( \phi \) direction, the angle of incidence that the radiated waves will make with the PML interface will be great. This large angle of incidence is expected to reduce the effects of the absorption of the PML layer.

The discretisation of the problem was performed uniformly with an average edge length of approximately 100nm. Since all optical propagating modes can be considered
TEM with respect to the propagation direction $\phi$, the leaky mode will be modeled by edge basis functions. Thus, using Equation (3.66), and setting the average edge length within the PML region to 50 nm, produces the predicted reflection error depicted in Figure 5.23. A reflection error of less than -20 dB is evident at normal incidence.

![Figure 5.23: The predicted reflection error from the PML interface with edge length $\approx$ 50 nm.](image)

Having chosen the PML parameters for the absorbing layer, the convergence analysis follows that of Section 5.2 and 5.3. The eigenvalue simulation is performed on the geometry depicted in Figure 5.22 with the boundary dimension $b$ ranging from 2 $\mu$m, to 9.6 $\mu$m. Examination of the results reveals that the real component of the effective index remains constant at 1.4989 to five significant figures over this entire range. The propagation loss, represented by the imaginary component of the effective index, has a strong dependence on the box dimension. Figure 5.24 presents the cumulative attenuation that a mode propagating through a half-circle of this waveguide at a radius of 2 mm would exhibit, as a function of boundary dimension $b$. The normalised rate of change of this propagation loss with boundary dimension $b$ is presented in Figure 5.25.

It is clear, both from Figure 5.24 and Figure 5.25, that the simulation has converged by $b = 9.6$. The value of attenuation at this point is a little more than 5 dB, a figure that is in good agreement with the theoretical and experimental results reported by [60]. There is, however, a curious peak in Figure 5.24. This anomaly can be explained by considering the nature of radiation from cylindrically symmetric waveguides. The following section describes the origins of this peak and its implications for the use of the PML in improving the efficiency of solution in bent waveguide problems.
Figure 5.24: The bending loss for propagation around a semi-circle of radius 2mm.

Figure 5.25: The rate of change of the imaginary component of the effective index with boundary dimension.
5.4.2 Interpretation of the bending loss simulation results

To simplify the explanation of the peak observed in Figure 5.24, consider the one dimensional effective index approximation to the waveguide geometry presented in Figure 5.26. The effective index values used are those used by Vijaya et al. [60] in their theoretical analysis. If the conformal mapping described in [61], is approximated to the first order for waveguide features much smaller than the radius of curvature, it can be interpreted as a scaling of the refractive index by the radial position. The mapped profile for a bending radius of 2mm could then be represented as shown in Figure 5.27. The effective index of the guided mode of the unbent waveguide is also displayed in each Figure.

Notice that in Figure 5.27, the index profile crosses the effective index of the guided wave at a radial distance of around 7 μm from the center of the waveguide. Unguided light propagating at this radial distance travels with the same propagation constant as the guided mode and hence the two can couple. Since the index profile continues to increase with increased radial distance, the optical power coupled to this crossover point is unbounded on one side and hence radiates. This is the mechanism for radiation in bent waveguides.

To return to the explanation of the peak in Figure 5.24, it is worth noting that this peak begins as the boundary approaches a radial distance of around 7 μm. A possible interpretation is that before the boundary reaches this point, light does not couple from the waveguide, with the evanescent tail decaying in the radial direction until it is terminated by the PML boundary. As the boundary expands past the coupling point, light begins to couple into the PML region. However, with the boundary still close to this region, the light is contained by the PEC wall which effectively guides the light within the PML layer. Thus the optical mode is coupled from the bent waveguide to a second waveguide that is loaded with PML. The result is a drastic increase in the propagation loss as evidenced by the peak in Figure 5.24.

As the boundary expands further, the situation gradually approaches that of free space with power coupling out of the waveguide and into the cladding where it radiates into the PML absorber. Considering this, the minimal problem from which convergence should be assessed, is where the boundary is at the coupling point. Thus the problem should be deemed converged once the rate of change of propagation loss with respect to b has dropped 2 orders of magnitude from the peak in Figure 5.24, indicating that convergence is achieved at around b = 9 μm.

Directions in which to proceed

The simulations of the convergence analysis of Section 5.4.1 incur a great deal of unknowns. It would thus be advantageous to use the PML as it has been used in Sections
Figure 5.26: The 1D effective index profile as specified by [60]. The effective index of the guided mode is shown (dashed line).

Figure 5.27: The 1D effective index profile as specified by [60], mapped to cylindrical coordinates with a radius of 2mm. The approximate effective index of the guided mode is shown (dashed line).
5.2 and 5.3 to minimise the empty space surrounding the details of the problem. It has become apparent, however, that the exterior of the problem when mapped to cylindrical coordinates begins at around $b = 6 \mu m$, with the point at which the mapped index profile crosses the guided mode effective index being considered a significant detail of the index profile. Thus there is only the region between $b = 6 \mu m$ and $b = 9 \mu m$ to optimise using a PML truncation. Since this region represents only a minority of the unknowns of the simulation, reduction of its extent would not significantly improve overall computational efficiency.

To proceed with improving the efficiency of the simulation, it would be necessary to reduce the amount of space required between the waveguide features and the point at which it begins coupling into the continuum. It has yet to be seen whether a PML layer can be used for that task, however several reports of PML truncations derived in curvilinear coordinates have been published [2] [5] [6], [7], [8], and [9], and these may offer some advice on how to proceed. The task of improving the efficiency of this simulation will be the topic of future investigation. Since the point at which the optical mode begins coupling into the cladding is determined by the bending radius, it is expected that a smaller radius of curvature could result in a more compact simulation. Thus it is possible that this technique could be well suited to very tight bends in integrated optic waveguides such as those examined in [59].

5.4.3 Summary

The PML has been applied to a bending loss simulation, implemented by conformally mapping a two dimensional waveguide geometry from Cartesian to polar coordinates. The resulting bending loss compares well with the theoretical and experimental findings of Vijaya et al. [60].

Unfortunately, the simulation is found to be computationally expensive requiring a great deal of apparently featureless space around the device features for accurate simulation. It is proposed that this space could be reduced through the use of an evanescent PML as applied in Sections 5.2 and 5.3, adapted for use in cylindrical coordinates. Application of this technique to waveguides with low radius bends is also predicted to be more computationally efficient.

5.5 Conclusions

This Chapter has demonstrated the application of the PML absorbing boundary condition to the solution of both lossless and leaky waveguide simulations using a 2D finite element
eigenvalue model.

Section 5.2 demonstrated the simulation of the first order modes of a microstrip line with features of the order of a tenth of a wavelength. A PML boundary with real variable parameter was used to absorb the evanescent tails of the guided modes and hence truncate the computational domain in order to improve efficiency. Solution times reduced by a factor of three were realised without reduction in the accuracy of either the eigenvalue as represented by the effective index, or the eigenvector as represented by the characteristic impedance.

In Section 5.3 the same approach was applied to a coplanar waveguide structure on a biaxial substrate with features size of only a minute fraction of a wavelength. Again a PML with real variable parameter was used to reduce the computational domain size. To truncate the region filled with biaxial material, the generalised PML developed in Chapter 2 was used. Improvement in solution time of around a factor of three was again observed.

In each of the investigations of Section 5.2 and 5.3, the technique of compressing the PML in one dimension was employed to reduce reflection errors and hence allow the choice of a larger PML parameter. Although the performance of the PML improved with mesh compression as expected, the associated increase in number of unknowns rendered the boundary equivalent, in terms of efficiency, to the uncompressed boundary. Investigation of optimal methods using mesh compression will be the topic of future work.

The simulation of a leaky integrated optic waveguide was demonstrated in Section 5.4. A conformal mapping was used to convert the FEM mode solver from the Cartesian coordinate system to a cylindrical coordinate system to allow the simulation of mode propagation in radially bent waveguides. A PML truncation with complex variable parameter was used on the radial boundary to absorb radiation caused by the bend. Comparison was made to the approximate theoretical and experimental results of Vijaya et al. [60], with good agreement evident.

The choice of PML parameter and associated mesh density used in Section 5.4 were based on the reflection error relationships for biaxial materials derived in Chapter 3. The bending loss simulation, though achieving an accurate result, has proved to be computationally expensive, since the domain must extend past the radius at which the effective index profile exceeds the effective index of the guided wave. It is expected that a PML layer could be used to reduce the computational domain of this simulation also, however the derivation of such a PML is beyond the scope of this work.

In each of the above simulations, a PML truncation was used to simulate an open region of space. For simplicity, these PML truncations consisted of a single layer of uniform variable parameter and mesh discretisation. As suggested by Bérenger [1] a tapered variable parameter profile can be used, and it is expected that using such a tapered PML
would improve the efficiency and effectiveness of the PML truncations examined in this Chapter. As mentioned in Chapter 4, the numerical reflection relations for a PML boundary could be used to investigate the properties of tapered PML layers. Thus optimisation of PML tapers using these expressions and the application of the resulting PML boundaries to waveguide simulations such as those examined in this Chapter hold great potential for further investigation.

Finally, it is expected that the use of the closed form relations derived in Chapter 3 and Chapter 4, could be developed into a more formal scheme for choosing PML variable parameters and mesh discretisation levels in finite element simulation. Although some guidelines have been identified, further investigation is required to develop them into a rigorous methodology that can be applied to the implementation of the PML boundary condition in FEM simulations.
Chapter 6

Conclusions

The aim of this thesis was to improve the efficiency and functionality of electromagnetic mode solvers through the application of the PML boundary condition. Particular emphasis was placed on simulations of integrated optic devices based on the uniaxial material LiNbO$_3$. The key areas of investigation were extension of the PML boundary for application to anisotropic materials, analysis of factors contributing to the efficiency and effectiveness of the PML boundary, development of a more efficient implementation, and demonstration of the boundary as a means of improving the efficiency and accuracy of simulations of both lossless and radiating waveguide structures. Each of these goals has been realised with a summary of the major achievements of this work following.

6.1 Outcomes of this work

A primary outcome of this work was the development of a generalised PML, suitable for use with biaxial anisotropic material. The derivation of this boundary was detailed in Chapter 2. This development facilitates the application of the PML boundary to problems involving biaxial materials such as LiNbO$_3$. Observations about the role of this material in corner regions and PML gradations have been made and the new formulation were used to prove that PML/PML interfaces, present in graded PML implementations, should produce no reflection. This PML was demonstrated as an effective means of truncating a region of biaxial dielectric, however discrepancies from the predicted results were observed at higher frequencies. Literature on the subject attributed these discrepancies to numerical reflections in the finite element method itself and demonstrated a relationship between the discretisation density and the level of reflection from a PML interface. It was clear that to efficiently and effectively implement the PML boundary, the nature of the link between discretisation level and numerical errors would need to be identified.

The relationship between element edge length and numerical dispersion and numer-
ical reflection in the finite element method was investigated in Chapter 3. This investigation builds on an existing analysis of numerical dispersion in finite element meshes and extends it to anisotropic media and the analysis of numerical reflections. Closed form expressions for the numerical dispersion and numerical reflection predicted at an interface between two biaxial materials in the finite element method were derived. A hexagonally symmetric finite element mesh was assumed and both node and edge basis functions were considered. These expressions were verified by comparison to numerical errors observed in practical finite element simulations with good agreement. This demonstrates the applicability of these closed form expressions to imperfect hexagonal meshes as are encountered in practical simulations. An interesting result of this comparison was that the low error levels reported for edge elements using a hexagonally symmetric mesh are only realisable for a perfect mesh.

Chapter 4 uses the general expressions derived in Chapter 3 to examine the special case of numerical reflection from such a PML interface. A major result of this investigation was the discovery that the reflection error from a PML interface was largely dependent on the triangle edge length in the normal direction, and less affected by edge lengths in the other dimensions. This suggests that an equivalent effect on the PML performance should be achieved by a one dimensional mesh compression as was previously attained by a general increase in the mesh density. Simulations of reflection errors from PML layers with compressed meshes were demonstrated with performance exceeding that of uniformly meshed layers at a fraction of the expense. Hence the PML has been made significantly more efficient to implement in the FEM. A similar result is predicted for finite difference models.

In Chapter 5, the PML technique developed in Chapter 4 was demonstrated in three eigenvalue simulations. The simulations include a simple microstrip line, a coplanar waveguide electrode of an integrated Mach-Zehnder optical intensity modulator, and the radiating mode of a bent integrated optic rib waveguide. Important results include verification of the ability of the PML to absorb evanescent waves and the demonstration of this evanescent PML in truncating the area of the computational domain of lossless waveguide simulations. Improvements in the solution time for simulation by a factor of three were achieved, and hence the PML was demonstrated as a powerful technique for the reduction of unknowns in eigenvalue simulations. Further, the well known ability of the PML to absorb radiating waves was demonstrated in a two dimensional eigenvalue simulation where it used to absorb the radiated power from a bent integrated optical waveguide. Good agreement with published results were achieved.
6.2 Suggestions for future work

The primary goal of enhancing the eigenvalue solution of integrated optical waveguides has been met. Further, the investigations leading to this result have produced many useful discoveries and interesting observations. Further examination of these areas was recommended and thus below was a summary of areas that hold potential for future work.

Recent work [3] has developed a PML similar to that arrived at in Chapter 2, but was far more general being suitable for full tensor bianisotropic media. It was thus evident that further extension of the PML to more general media was unnecessary. However, following the interpretation of the biaxial PML in terms of corner regions this more general PML could allow for corners at any angle. The implementation of such corner regions should allow the external boundary of the problem to better fit the contours of the geometry under examination and hence provide more efficient use of unknowns.

The numerical dispersion and reflection error relations, derived in Chapter 3 for interfaces in biaxial materials, were performed for finite element edge and node basis functions of the first order only. The application of this analysis to higher order basis functions should lend insight to their efficient and effective use in the finite element method.

The examination of the numerical reflection performed in Chapter 4 indicated that the reflection from the PML was largely due to the reflection from the surface. A graded PML implementation was thus suggested. It should be possible to use the closed form expressions developed in Chapter 3 for a single interface, to produce a closed form expression for the numerical reflection from a graded PML as a function of frequency, PML grading profile and mesh compression/density profile. It was expected that such an investigation should be able to determine the combination of profiles for a given frequency range to optimally balance the required number of unknowns with the PML performance. Extension of this analysis to higher order elements is also suggested, since it was possible that the reduction in numerical errors and improvement of matrix conditioning achieved by an increase in order should offset the number of extra unknowns incurred.

The investigation of the application of the PML to eigenvalue problems presented in Chapter 5 was incomplete. Full use was not made of the analytic information derived in Chapters 3 and 4 in these simulations and it was expected that more highly optimised PML truncations could be devised. Further, if non-rectangular PML boundaries and graded PML profiles were applied to these simulations, further gains in terms of efficiency should be attainable. The brief bending loss simulation proved to be computationally expensive due to the necessity to extend the boundary to a point where the guided mode and conformally mapped cladding layer exhibit the same effective index. It was proposed that a PML layer could be devised to simulate this effect without the need to extend the boundary to
this extent. Improvement of the efficiency of the bending loss simulation was essential for it to be considered a practical alternative to current beam propagation methods.

In conclusion, the PML has been successfully applied to finite element eigenvalue simulations incorporating biaxial media. The PML boundary itself has been extended for application to biaxial materials, and its effectiveness demonstrated in a practical finite element simulation. The cause of the failure of the PML in certain circumstances has been identified as being caused by numerical errors in the finite method. The numerical errors in the finite element method have been analysed in detail and closed form expressions for numerical dispersion and reflections for cases involving biaxial media have been developed. These expressions have been used to quantify the causes of numerical error displayed by the PML boundary and a new technique for efficiently minimising these errors has been presented. Demonstration of application of this PML boundary condition to eigenvalue simulations has been presented. Improvement in efficiency by a factor of three with respect to solution time have been observed and accurate solution of a radiating waveguide problem using the absorbing properties of the PML has been achieved with good agreement to published experimental and theoretical results.
Appendix A

The Finite Element Method Implementation

This Appendix outlines the formulation of both forced and eigenvalue forms of the finite element method used in this thesis. A more detailed description of the finite element implementation can be found in Jin. [53]. The derivation presented here is extended to include anisotropic magnetic materials.

A.1 The basic integral expressions

The vector wave equation can be written

\[
\nabla \times \frac{\text{\mu}}{\text{\mu}^{-1}} \nabla \times \vec{E} - k_0^2 \epsilon \cdot \vec{E} = 0
\]

(A.1)

Invoking the Galerkin method, field solutions must satisfy

\[
\int_{\Omega} \vec{E}^+ \cdot \left( \nabla \times \frac{\text{\mu}}{\text{\mu}^{-1}} \nabla \times \vec{\bar{E}} \right) d\Omega - k_0^2 \int_{\Omega} \vec{E}^+ \cdot \bar{\epsilon} \cdot \vec{E} d\Omega = 0
\]

(A.2)

Where \( \Omega \) is the computational domain, and \( \vec{E}^+ \) denotes the \( \vec{E} \) field mirrored in the \( z \) plane. After manipulation using differential vector identities, Equation (A.2) can be written

\[
\int_{\Omega} \left( \nabla \times \vec{E}^+ \right) \cdot \frac{\text{\mu}}{\text{\mu}^{-1}} \left( \nabla \times \vec{\bar{E}} \right) - k_0^2 \vec{E}^+ \cdot \bar{\epsilon} \cdot \vec{E} d\Omega

= \int_{\Omega} \nabla \cdot \left[ \vec{E}^+ \times \left( \frac{\text{\mu}}{\text{\mu}^{-1}} \nabla \times \vec{\bar{E}} \right) \right] d\Omega
\]

(A.3)

The first two terms of Equation (A.3) describe the behavior of the field in the interior of the computational domain and will become the finite element matrix. The third term in
Equation (A.3) describes sources in the problem that appear at the computational boundary. If this source term is non-zero then the problem is forced and becomes a 'forced' problem. If this source term is zero, then the problem becomes an 'eigenvalue' problem. In the following a two dimensional formulation is assumed, with $z$ direction infinite. Also material tensors are assumed to be of the form

$$
\varepsilon = \begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & 0 \\
\varepsilon_{yx} & \varepsilon_{yy} & 0 \\
0 & 0 & \varepsilon_{zz}
\end{bmatrix},
\mu = \begin{bmatrix}
\mu_{xx} & \mu_{xy} & 0 \\
\mu_{yx} & \mu_{yy} & 0 \\
0 & 0 & \mu_{zz}
\end{bmatrix}
$$

(A.4)

**A.2 The forced problem formulation**

The formulation of the forced formulation of the FEM can be separated into formulation of the interior finite element matrix and formulation of the source boundary conditions.

**A.2.1 Interior coupling**

Having assumed an infinite an unvarying $z$ dimension, it is convenient to decompose the field into tangential and normal components

$$
\vec{E} = (\vec{E}_t + z\vec{E}_z), \quad \vec{E}^+ = (\vec{E}_t - z\vec{E}_z)
$$

(A.5)

Making this substitution it is possible to write

$$
\nabla \times \vec{E} = \frac{\partial E^+_x}{\partial y} \hat{x} - \frac{\partial E^+_y}{\partial x} \hat{y} + \left[ \frac{\partial E^+_y}{\partial x} - \frac{\partial E^+_x}{\partial y} \right] z
$$

(A.6)

$$
= -\hat{z} \times \nabla E_z + \nabla_t \times \vec{E}_t
$$

(A.7)

and similarly

$$
\nabla \times \vec{E}^+ = \hat{z} \times \nabla E_z + \nabla_t \times \vec{E}_t
$$

(A.8)

where

$$
\nabla_t = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, 0 \right]
$$

(A.9)

thus

$$
\left( \nabla \times \vec{E}^+ \right) \cdot \vec{\mu}^{-1} \left( \nabla \times \vec{E} \right)
= \left( \hat{z} \times \nabla E_z + \nabla_t \times \vec{E}_t \right) \cdot \vec{\mu}^{-1} \left( -\hat{z} \times \nabla E_z + \nabla_t \times \vec{E}_t \right)
= \left( \nabla_t \times \vec{E}_t \right) \frac{1}{\mu_{zz}} \left( \nabla_t \times \vec{E}_t \right) - \left( \hat{z} \times \nabla E_z \right) \cdot \vec{\mu}^{-1} \cdot \left( \hat{z} \times \nabla E_z \right)
$$

(A.10)
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where

$$\bar{\mu}_{tt} = \begin{bmatrix} \mu_{xx} & \mu_{xy} \\ \mu_{yx} & \mu_{yy} \end{bmatrix}$$  \hspace{1cm} (A.11)

Noting that

$$\bar{E}^+ \cdot \bar{e} = \bar{E}_t \cdot \bar{e}_{tt} \cdot \bar{E}_t - E_z \varepsilon_{zz} E_z$$  \hspace{1cm} (A.12)

Equation (A.3) can be written

$$\int_{\Omega} \left( \nabla \times \bar{E}_t \right) \frac{1}{\mu_{zz}} \left( \nabla \times \bar{E}_t \right) - k_0^2 \bar{E}_t \cdot \bar{e}_{tt} \cdot \bar{E}_t \, d\Omega$$

$$- \int_{\Omega} \left( \bar{z} \times \nabla E_z \right) \cdot \bar{e}_{tt}^{-1} \left( \bar{z} \times \nabla E_z \right) - k_0^2 E_z \varepsilon_{zz} E_z \, d\Omega$$

$$= \int_{\Omega} \nabla \cdot \left[ \bar{E}^+ \times \left( \bar{e}_{tt}^{-1} \nabla \times \bar{E} \right) \right] \, d\Omega$$  \hspace{1cm} (A.13)

If scalar node basis functions are used to represent $E_z$ and vector edge basis functions are used to represent $E_t$ then this provides the local matrix for each element Since basis functions span at least two element, a sparse matrix coupling neighboring elements results. For more details see Jin. [53, pages 158].

A.2.2 Exterior sources

In this case the source is assumed to be a port to a one dimensional waveguide. Any of the modes of the waveguide can be excited and hence coupled into or out of the problem. Recall the source term in Equation (A.3)

$$\int_{\Omega} \nabla \cdot \left( \bar{E}^+ \times \left( \bar{e}_{tt}^{-1} \nabla \times \bar{E} \right) \right) \, d\Omega$$  \hspace{1cm} (A.14)

Formulating $\bar{E}$ in terms of the closed form eigenfunction expansion of the power launched through the port and power returning from the waveguide through the basis functions $\bar{E}^+$, it is possible to couple the basis functions to the modes propagating in the port waveguide. The derivation follows that given in Jin. [53, pages 353–357], and will not be repeated here.

A.3 The eigenvalue formulation

The derivation of the eigenvalue formulation is very similar to the derivation of the forced formulation with two important differences. Firstly the source term in Equation (A.3) must be zero, and secondly, a propagating solution is assumed in the $z$ direction. Thus
Thus
\[ \nabla \times \vec{E} = -\vec{z} \times \left( j \gamma \vec{E}_t + \nabla_t E_z \right) + \left( \nabla_t \times \vec{E}_t \right) \]
and similarly
\[ \nabla \times \vec{E}^+ = \vec{z} \times \left( j \gamma \vec{E}_t + \nabla_t E_z \right) + \left( \nabla_t \times \vec{E}_t \right) \]
Again noting that
\[ \vec{E}^+ \cdot \vec{E} = \vec{E}_t \cdot \vec{E}_t - E_z \epsilon_{zz} E_z \]
and setting the source term to zero, Equation (A.3) can be rewritten as
\[ \int_{\Omega} \left( \nabla_t \times \vec{E}_t \right) \frac{1}{\mu_{zz}} \left( \nabla_t \times \vec{E}_t \right) d\Omega - k_0^2 \int_{\Omega} \vec{E}_t \cdot \vec{E}_t d\Omega \]
\[ = \int_{\Omega} \left[ \vec{z} \times \left( j \gamma \vec{E}_t + \nabla_t E_z \right) \right] \cdot \vec{E}_t^{-1} \cdot \left[ \vec{z} \times \left( j \gamma \vec{E}_t + \nabla_t E_z \right) \right] d\Omega \]
\[ - k_0^2 \int_{\Omega} E_z \epsilon_{zz} E_z d\Omega \] (A.19)
If the edge basis functions are used to represent \( E_t \), but the node basis functions are related to the \( z \) polarised fields by \( E_z = j \gamma e_z \) where \( e_z \) represents the node basis functions, then it is possible to rewrite Equation (A.19) as
\[ \int_{\Omega} \left( \nabla_t \times \vec{E}_t \right) \frac{1}{\mu_{zz}} \left( \nabla_t \times \vec{E}_t \right) d\Omega - k_0^2 \int_{\Omega} \vec{E}_t \cdot \vec{E}_t d\Omega \]
\[ = -\gamma_2 \int_{\Omega} \left( \vec{z} \times \vec{E}_t \right) \cdot \vec{E}_t^{-1} \cdot \left( \vec{z} \times \vec{E}_t \right) d\Omega \]
\[ -\gamma_2 \int_{\Omega} \left( \vec{z} \times \vec{E}_t \right) \cdot \vec{E}_t^{-1} \cdot (\vec{z} \times \nabla_t e_z) d\Omega \]
\[ -\gamma_2 \int_{\Omega} (\vec{z} \times \nabla_t e_z) \cdot \vec{E}_t^{-1} \cdot (\vec{z} \times \vec{E}_t) d\Omega \]
\[ -\gamma_2 \left[ \int_{\Omega} (\vec{z} \times \nabla_t e_z) \cdot \vec{E}_t^{-1} \cdot (\vec{z} \times \nabla_t e_z) d\Omega - k_0^2 \int_{\Omega} e_z \epsilon_{zz} e_z d\Omega \right] \] (A.20)
This specifies the local matrix to be used in the eigenvalue simulation. Since each triangular element has three edges and three nodes, and each of these edges and nodes is shared by at least one other element, performing the above integral for each edge and node of each element results in an eigenvalue problem composed of large sparse matrices of the form
\[ \begin{bmatrix} A_{tt} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} e_{tt} \\ e_{\phi\phi} \end{bmatrix} = \gamma_2 \begin{bmatrix} B_{tt} & B_{tz} \\ B_{zt} & B_{zz} \end{bmatrix} \begin{bmatrix} e_t \\ e_z \end{bmatrix} \] (A.21)
Further details can be found in Jin. [53, pages 244–247].
Appendix B

De-embedding waveguide propagation characteristics

The transmission and reflection from a parallel plate waveguide, as depicted in Figure B.1, depends on six unknowns. These are the reflection from the exterior of Port 1 ($s_{11}$), the reflection from the interior of Port 1 ($s_{22}$), the product of the transmission coefficients of Port 1 ($s_{21}s_{12}$), the dispersion ($k_x$), and the internal reflection and transmission of Port 2, ($r_2$) and ($t_{p2}$) respectively. Thus, if $r_{p2}$ and $t_{p2}$ in Figure B.1 are known, four separate measurements are needed to isolate each of the remaining unknowns.

Figure B.1: Geometry of a parallel plate waveguide used in the investigation of numerical dispersion. Path of a guided mode incident at port one and subject to multiple reflections shown.
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In general the reflection at Port 1 can be summed as an infinite series to yield

\[ r_{\text{general}} = s_{11} + r_{p2} s_{21} s_{12} e^{-2j k a l} + r_{p2}^2 s_{21} s_{12} s_{22} e^{-4j k a l} + \ldots \]  

(B.1)

or more simply as,

\[ r_{\text{general}} = s_{11} + \frac{r_{p2} s_{21} s_{12} e^{-2j k a l}}{1 - r_{p2} s_{22} e^{-2j k a l}} \]  

(B.2)

and the transmission

\[ t_{\text{general}} = t_{p2} s_{21} e^{-j k a l} + r_{p2} t_{p2} s_{21} s_{22} e^{-3j k a l} + \ldots \]  

(B.3)

or

\[ t_{\text{general}} = \frac{t_{p2} s_{21} e^{-j k a l}}{1 - r_{p2} s_{22} e^{-2j k a l}} \]  

(B.4)

The specific test geometries are now described in more detail.

1. The shorted parallel plate waveguide

To model a shorted parallel plate waveguide, a perfect electric conductor (PEC) boundary condition is used at port 2. Thus the electric field at Port 2 is forced to be 0. It can be shown that this leads to a reflection coefficient \( r_{p2} \) of exactly \(-1\), irrespective of material parameters, mesh density and frequency. The transmission \( t_{p2} \) is of course 0. Substituting \( r_{p2} = -1 \) and \( t_{p2} = 0 \) into Equation (B.2) gives

\[ r_{\text{PEC}} = s_{11} + \frac{s_{21} s_{12} e^{-2j k a l}}{1 + s_{22} e^{-2j k a l}} \]  

(B.5)

2. The open circuit parallel plate waveguide

To model the open circuit parallel plate waveguide, a perfect magnetic conductor (PMC) boundary condition is used at Port 2. Thus the electric field at Port 2 is unrestrained, which can be shown to ensure a reflection coefficient \( r_{p2} \) of exactly \(1\), irrespective of material parameters, mesh density and frequency. Again, the transmission \( t_{p2} \) is 0. Substituting \( r_{p2} = -1 \) and \( t_{p2} = 0 \) into Equation (B.2) yields

\[ r_{\text{PMC}} = s_{11} + \frac{s_{21} s_{12} e^{-2j k a l}}{1 - s_{22} e^{-2j k a l}} \]  

(B.6)

3. The matched parallel plate waveguide

If the parallel plate waveguide is matched identically at both ends, the same transmission and reflection can be assumed for both Port 1 and Port 2. Substituting \( r_{p2} = s_{22} \), and \( t_{p2} = s_{12} \), into Equation (B.2) and Equation (B.4) yields

\[ r_{\text{port}} = s_{11} + \frac{s_{21} s_{12} s_{22} e^{-2j k a l}}{1 - s_{22}^2 e^{-2j k a l}} \]  

(B.7)
and the transmission

\[ t_{\text{port}} = \frac{s_{21}s_{12}e^{-jk_xl}}{1 - s_{22}^2e^{-2jk_xl}}. \]  

(B.8)

4. A second matched section of parallel plate waveguide

A second waveguide case as above with a different length is needed to isolate the dispersion from the various reflections.

To perform the de-embedding it is desirable to obtain expression for each of the port characteristics in terms of the calculated reflection and transmission data. Some manipulation of Equations (B.5) - (B.7) results in the following expressions

\[ s_{22}^2 = \frac{2t_{\text{port}}e^{-jk_xl} - (r_{PMC} - r_{PEC})}{2t_{\text{port}}e^{-2jk_xl} - (r_{PMC} - r_{PEC})e^{-jk_xl}} \]  

(B.9)

\[ s_{21}s_{12} = t_{\text{port}}(1 - s_{22}^2e^{-2jk_xl})e^{-jk_xl} \]  

(B.10)

\[ s_{11} = r_{PMC} - \frac{t_{\text{port}}(1 - s_{22}^2e^{-2jk_xl})e^{-jk_xl}}{1 - s_{22}e^{-2jk_xl}}. \]  

(B.11)

Notice that the only unknown in the expression for \( s_{22} \) is the value \( k_x \). With these expressions it is now possible to ‘measure’ the numerical dispersion in the waveguide. To do this, note from Equation (B.7) and Equation (B.8) that

\[ r_{\text{port}} = s_{11} + s_{22}e^{-jk_xl}t_{\text{port}}. \]  

(B.12)

Thus the reflection from two, different lengths of waveguide are required to isolate \( s_{11} \) and \( s_{22} \). Subtracting the reflection from waveguide segments of lengths \( l_1 \) and \( l_2 \) yields

\[ r_{\text{port}1} - r_{\text{port}2} = s_{22}(e^{-jk_xl_1}t_{\text{port}1} - e^{-jk_xl_2}t_{\text{port}2}). \]  

(B.13)

Recalling that \( k_x \) is the only unknown in the expression for \( s_{22} \), it is evident that the variable \( k_x \) has been isolated. A root finding algorithm may be used to locate the \( k_x \) that satisfies this relationship. This is the de-embedded numerical dispersion of the material.
Appendix C

De-embedding reflections from an interface

Consider the situation depicted in Figure C.1. Two interfaces exist at which reflections may occur, the input port, with transmission matrix labeled $a_{ij}$, and the interface of interest with transmission matrix labeled $s_{ij}$. A reflection of either $+1$ or $-1$ will occur at the termination depending on the boundary condition chosen. If the reflection and transmission at the interface is assumed to be reciprocal, $s_{12} = s_{21}$ and $s_{11} = -s_{22}$, then the unknowns are the dispersion in each material, the reflection and transmission at the port for each material, and the reflection and transmission at the interface. The port characteristics and material dispersion can be obtained using the procedure discussed in Section B for each material in isolation. It is thus only necessary to conduct two additional simulations to isolate the interface reflection and transmission. These two cases are each

\[ l_1 \]

\[ l_2 \]

\[ a_{12} \]

\[ a_{21} \]

\[ a_{11} \]

\[ s_{12} \]

\[ s_{11} \]

\[ s_{22} \]

\[ s_{21} \]

\[ \pm 1 \]

Figure C.1: Geometry of a parallel plate waveguide, used in the investigation of numerical reflection with reflection coefficients for the various interfaces labeled
measurements of reflection from a parallel plate waveguide containing the discontinuity, one terminated with a PEC boundary condition, the other terminated with a PMC boundary. The transmission matrix method [62, pages 231–234] can be used to yield the general reflection from the structure in Figure C.1. This may be written

$$\begin{bmatrix} 1 \\ r_+ \end{bmatrix} = \begin{bmatrix} \frac{1}{a_1} & -s_{22} \\ s_1 & a_2 \end{bmatrix} \begin{bmatrix} e^{jk_1l_1} & 0 \\ 0 & e^{-jk_1l_1} \end{bmatrix} \begin{bmatrix} \frac{1}{s_1} & -s_{22} \\ s_1 & a_2 \end{bmatrix} \begin{bmatrix} e^{jk_2l_2} & 0 \\ 0 & e^{-jk_2l_2} \end{bmatrix} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \tag{C.1}$$

where $r_+$ and $r_-$ refer to reflection from the waveguide truncated with PMC and PEC respectively. This can be simplified by making the substitution

$$\begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{a_1} & -s_{22} \\ s_1 & a_2 \end{bmatrix} \begin{bmatrix} e^{jk_1l_1} & 0 \\ 0 & e^{-jk_1l_1} \end{bmatrix} \begin{bmatrix} \frac{1}{s_1} & -s_{22} \\ s_1 & a_2 \end{bmatrix} = \begin{bmatrix} \frac{e^{jk_1l_1}}{s_1} & \frac{-a_{22}e^{-jk_1l_1}}{a_2} \\ \frac{a_{12}e^{jk_1l_1}}{s_1} & \frac{a_{12}e^{-jk_1l_1}}{a_2} \end{bmatrix} \tag{C.2}$$

By making this substitution and further manipulating, Equation (C.1) may be written

$$\begin{bmatrix} D - Br_+ \pm \frac{1}{A D - BC} \frac{Ar_+ - C}{D - Br_+} \end{bmatrix} = \begin{bmatrix} \frac{e^{jk_2l_2} + (s_{22}e^{-jk_2l_2})}{s_1} \\ \frac{s_1e^{jk_2l_2} - (s_{12}s_{21} \pm s_{11}s_{22})e^{-jk_2l_2}}{s_{12}} \end{bmatrix} \tag{C.3}$$

Taking the ratio of the two elements yields

$$\frac{Ar_+ - C}{D - Br_+} = \frac{s_{11}e^{jk_2l_2} - (s_{12}s_{21} \pm s_{11}s_{22})e^{-jk_2l_2}}{s_{12}e^{jk_2l_2} + s_{12}e^{-jk_2l_2}} \tag{C.4}$$

Assuming $s_{11} = -s_{22}$, making the substitution

$$Q_\pm = \frac{Ar_+ - C}{D - Br_+} \tag{C.5}$$

and performing some further manipulation yields

$$s_{11} = \frac{(Q_+ + Q_-)e^{2jk_2l_2}}{(Q_+ - Q_-) + 2e^{2jk_2l_2}} \tag{C.6}$$

and

$$s_{12}s_{21} = Q_+e^{2jk_2l_2} - Q_+s_{22} - s_{11}e^{2jk_2l_2} + s_{11}s_{22} \tag{C.7}$$

Thus ten simulations in all are required to isolate the reflection from an interface in the finite element method, four to determine the dispersion in Region 1, four to determine the dispersion in Region 2, and two to determine the reflection from their intersection.
Appendix D

The Eigenvalue FEM in cylindrical coordinates

This section describes the reformulation of the eigenvalue finite element model in cylindrical coordinates. The derivation follows that of Section A.3. A brief discussion of conformal mapping is also presented.

To reformulate in cylindrical coordinates, \( \phi \) replaces \( z \), \( r \) replaces \( x \) and \( y \) remains. Having assumed an infinite and unvarying solution in the \( \phi \) direction, the fields can be decomposed into tangential and normal components

\[
\vec{E} = (\vec{E}_t + \vec{E}_\phi(e^{-j\gamma\phi})) e^{-j\gamma\phi}, \quad \vec{E}^+ = (\vec{E}_t - \vec{E}_\phi(e^{j\gamma\phi})) e^{j\gamma\phi}
\]

and

\[
\nabla \times \vec{E} = \frac{1}{r} \left( \frac{\partial E_x}{\partial \phi} - \frac{\partial E_\phi}{\partial z} \right) \hat{r} + \left( \frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r} \right) \hat{\phi} + \frac{1}{r} \left[ \frac{\partial (r E_\phi)}{\partial r} - \frac{\partial E_r}{\partial \phi} \right] \hat{z}.
\]

and similarly

\[
\nabla \times \vec{E}^+ = \phi \times \frac{1}{r} \left( j \gamma (\vec{E}_t + \vec{\nabla}_t (r \vec{E}_\phi)) + (\nabla_t \times \vec{E}_t) \right)
\]

Noting that

\[
\vec{E}^+ \cdot \vec{\varepsilon} \cdot \vec{E} = \vec{E}_t \cdot \vec{\varepsilon}_t \cdot \vec{E}_t - E_\phi \varepsilon_{\phi\phi} E_\phi
\]

and setting the source term to zero, Equation (A.3) can be rewritten

\[
\int_{\Omega} \left( \nabla_t \times \vec{E}_t \right) \frac{1}{\mu_{\phi\phi}} \left( \nabla_t \times \vec{E}_t \right) d\Omega - k_0^2 \int_{\Omega} \vec{E}_t \cdot \vec{\varepsilon}_t \cdot \vec{E}_t d\Omega
\]

\[
= \int_{\Omega} \left[ \phi \times (j \gamma (\vec{E}_t + \vec{\nabla}_t (r \vec{E}_\phi))) \right] \cdot \vec{\mu}_{tt}^{-1} \cdot \left[ \phi \times (j \gamma (\vec{E}_t + \vec{\nabla}_t (r \vec{E}_\phi))) \right] d\Omega
\]

\[-k_0^2 \int_{\Omega} E_\phi \varepsilon_{\phi\phi} E_\phi d\Omega \quad (D.5)
\]
If the edge basis functions are used to represent $E_t$, but the node basis functions $e_\phi$ are related to the $\phi$ polarised fields by

$$E_\phi = \frac{j\gamma}{r} e_\phi \quad \text{(D.6)}$$

then it is possible to rewrite Equation (A.19) as

$$
\int_{\Omega} \left( \nabla_t \times \overline{E}_t \right) \frac{1}{\mu_{\phi\phi}} \left( \nabla_t \times \overline{E}_t \right) \, d\Omega - k_0^2 \int_{\Omega} \overline{E}_t \cdot \overline{\varepsilon}_t \cdot \overline{E}_t \, d\Omega \\
= -\gamma^2 \int_{\Omega} \left( \phi \times \overline{E}_t \right) \cdot \frac{\mu_\mu}{r^2} \cdot \left( \phi \times \overline{E}_t \right) \, d\Omega \\
-\gamma^2 \int_{\Omega} \left( \phi \times \overline{E}_t \right) \cdot \frac{\mu_\mu}{r^2} \cdot \left( \phi \times \nabla_t e_\phi \right) \, d\Omega \\
-\gamma^2 \int_{\Omega} \left( \phi \times \nabla_t e_\phi \right) \cdot \frac{\mu_\mu}{r^2} \cdot \left( \phi \times \overline{E}_t \right) \, d\Omega \\
-\gamma^2 \int_{\Omega} \left( \phi \times \nabla_t e_\phi \right) \cdot \frac{\mu_\mu}{r^2} \cdot \left( \phi \times \nabla_t e_\phi \right) \, d\Omega - k_0^2 \int_{\Omega} e_\phi e_\phi e_\phi \, d\Omega \quad \text{(D.7)}
$$

This specifies the local matrix to be used in the eigenvalue simulation and is of almost identical form to Equation (A.20), with the exception that the material tensor $\overline{\mu}$ must be scaled by $r^2$ during integration. Thus the transformation to cylindrical coordinates can be achieved with a simple modification to the local matrix elements.
References


Publications


