BASIS FUNCTIONS WITH DIVERGENCE CONSTRAINTS FOR THE
FINITE ELEMENT METHOD

by

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Abstract

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Maxwell's equations are a system of partial differential equations of vector fields. Imposing the constitutive relations for material properties yields equations for the curl and divergence of the electric and magnetic fields. The curl and divergence equations must be solved simultaneously, which is not the same as solving three separate scalar problems in each component of the vector field.

This thesis describes a new method for solving partial differential equations of vector fields using the finite element method. New basis functions are used to solve the curl equation while allowing the divergence to be set as a constraint. The basis functions are defined on a mesh of bricks and the method is applicable for geometries that conform to a Cartesian coordinate system. The basis functions are a combination of cubic Hermite splines and second order Lagrange interpolation polynomials. The method yields a linearly independent set of constraints for the divergence, which is modelled to second order accuracy within each brick.

Mesh refinement is accomplished by dividing selected bricks into $2 \times 2 \times 2$ smaller bricks of equal size. The change in the node pattern at an interface where mesh refinement occurs necessitates a modified implementation of the divergence constraints as well as additional constraints for hanging nodes. The mesh can be refined to an arbitrary number of levels.

The basis functions can exactly model the discontinuity in the normal component of

the field at a planar interface. The method is modified to solve problems with singularities at material boundaries that form 90° edges and corners.

The primary test problem of the new basis functions is to obtain the resonant frequencies and fields of three-dimensional cavities. The new basis functions can resolve physical solutions and non-physical, spurious modes. The eigenvalues obtained with the new method are in good agreement with exact solutions and experimental values in cases where they exist. There is also good agreement with results from second-order edge elements that are obtained with the software package HFSS.

Finally, the method is modified to solve problems in cylindrical coordinates provided the domain does not contain the coordinate axis.

Dedication

To Professor Konrad and Professor Lavers, and to Michael.

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Chapter 1

Introduction

The finite element method first appeared in a paper by Courant in 1943 [1] as part of his investigations into solving equations describing flexible membranes and plates. Nearly 70 years later it has evolved into one of the most common methods for solving a wide variety of partial differential equations that arise across science and engineering. This includes Maxwell's equations, whose applicability is ubiquitous in electrical engineering.

When the finite element method is applied to solving equations for vector fields, a difficulty arises that does not exist when solving scalar equations. Essentially, it is not trivial to extend the method for scalar equations so that the curl and the divergence equations for the vector fields can be solved simultaneously. There are methods that exist for solving this problem, each with advantages and disadvantages that do not entirely overlap. A new method for solving this problem is described in this thesis. Briefly, basis functions are derived that allow the divergence of the field to be set as a constraint. The basis functions, which contain the constraint, are used to solve the curl equation.

The problems that arise from not solving the curl and the divergence equations simultaneously can be appreciated from a physical perspective. The volume charge density is related to the divergence of the electric field via Gauss' law. If the divergence is not solved accurately then the solution may contain effects of unwanted charge. Another difficulty

arises in eddy current problems, where the current density is proportional to the electric field. If the divergence of the electric field is not solved accurately then the solution may not contain a conserved current. In the context of eigenvalue problems, one effect is the occurrence of non-physical solutions, commonly referred to as spurious modes. (The term “spurious modes” is not found exclusively in the discussion of eigenvalue solutions of Maxwell’s equations using the finite element method, however, this is its only meaning in this thesis.) It is impossible to miss the presence of the spurious solutions that occur in eigenvalue problems. For this reason, eigenvalue problems are the primary test for the new method described in this thesis.

1.1 Significance of Helmholtz’s Theorem for Maxwell’s Equations

Maxwell’s equations are a mathematical description of the relationships between electric charge, electric current and the electric and magnetic fields. They can be expressed either as partial differential equations or as integral equations. (See, for example, the text by Jackson [2].) In the present discussion, it is more convenient to work with the differential form of Maxwell’s equations, which are listed below.

$$\nabla \cdot \mathbf{D} = \rho \tag{1.1}$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \tag{1.2}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{1.3}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \tag{1.4}$$

In what follows, it is assumed that the permittivity, ϵ , and permeability, μ , depend on position but not on time or frequency. It is also assumed that the polarization and magnetization of the media are linearly proportional to the electric and magnetic fields,

respectively, that is, the permittivity and the permeability do not depend on the electric and magnetic fields. Thus, $\epsilon = \epsilon(\mathbf{r})$ and $\mu = \mu(\mathbf{r})$. These assumptions imply that the electric field intensity, $\mathbf{E}$, is related to the electric flux density, $\mathbf{D}$, by the constitutive relation $\mathbf{D}(\mathbf{r}, t) = \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}, t)$. Similarly, the magnetic field intensity, $\mathbf{H}$, is related to the magnetic flux density, $\mathbf{B}$, by the constitutive relation $\mathbf{B}(\mathbf{r}, t) = \mu(\mathbf{r}) \mathbf{H}(\mathbf{r}, t)$.

The constitutive relations can be used to eliminate $\mathbf{D}$ and $\mathbf{B}$ for $\mathbf{E}$ and $\mathbf{H}$, respectively.

$$\nabla \cdot (\epsilon \mathbf{E}) = \rho \quad (1.5)$$

$$\nabla \times \mathbf{E} + \mu \frac{\partial \mathbf{H}}{\partial t} = 0 \quad (1.6)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad (1.7)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \epsilon \frac{\partial \mathbf{E}}{\partial t} \quad (1.8)$$

This substitution was performed explicitly to illustrate that Maxwell's equations contain a curl equation and a divergence equation for each field $\mathbf{E}$ and $\mathbf{H}$. Helmholtz's theorem states that a vector field, such as the electric or magnetic field, is uniquely determined from its curl, divergence and appropriate boundary conditions [5, 6]. Thus, the electric field, $\mathbf{E}$, and the magnetic field, $\mathbf{H}$, are uniquely determined from Maxwell's equations provided appropriate boundary conditions are included. (This is unchanged using any combination of either $\mathbf{D}$ or $\mathbf{E}$ and either $\mathbf{B}$ or $\mathbf{H}$.)

The curl equations and the divergence equations are independent: the divergence of the fields cannot be derived from the curl of the fields. For example, Faraday's law cannot be used to uniquely determine the divergence of the magnetic flux density $\mathbf{B}$. To illustrate, the divergence operator is applied to equation (1.2).

$$\nabla \cdot \left(\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} \right) = 0 \quad (1.9)$$

$$\nabla \cdot \nabla \times \mathbf{E} + \nabla \cdot \frac{\partial \mathbf{B}}{\partial t} = 0 \quad (1.10)$$

$$\frac{\partial}{\partial t} \nabla \cdot \mathbf{B} = 0 \quad (1.11)$$

This implies only that $\nabla \cdot \mathbf{B}$ does not depend explicitly on time, that is, $\nabla \cdot \mathbf{B} = f(\mathbf{r})$, where $f(\mathbf{r})$ is an arbitrary function of position. Specifically, $f(\mathbf{r})$ is not necessarily zero everywhere: the divergence of the field needs to be stated independently. A similar argument holds for the electric flux density if the divergence operator is applied to (1.4).

In general, it is not possible to obtain exact solutions of Maxwell's equations. Nonetheless, in many cases, an approximate solution with sufficient accuracy can be obtained. Commonly used approximation techniques are the finite element method [7–9], the method of moments [10, 11] and the finite difference time domain method [12]. These methods have a point in common which is that they convert, in one way or another, differential equations or integral equations that depend on the continuous variables $\mathbf{r}$ and possibly t into a finite number of algebraic equations with a finite number of unknowns. Increasing the number of unknowns will usually improve the approximation. Since this involves more arithmetic, these methods are implemented on a computer, although, in principle, the calculations could be carried out by hand.

1.2 Eigenvalue Problems and Spurious Modes

Consider the problem of solving for the resonant frequencies and the corresponding fields inside of a cavity with perfectly conducting walls. The permittivity and permeability inside of the cavity are linear and may be inhomogeneous. There is no charge or current inside of the cavity although, in general, both are found on the cavity walls. By assuming that the fields oscillate sinusoidally with angular frequency ω , the time harmonic form of Maxwell's equations are obtained. In what follows, $\mathbf{E}(\mathbf{r}, t) = \text{Re}\{\mathbf{E}(\mathbf{r})e^{j\omega t}\}$, where $\mathbf{E}(\mathbf{r})$ can be, in general, complex and the complex conjugate is denoted by $\mathbf{E}(\mathbf{r})^*$. Similar relations hold for the magnetic field $\mathbf{H}$.

$$\nabla \cdot (\epsilon \mathbf{E}) = 0 \tag{1.12}$$

$$\nabla \times \mathbf{E} + j\omega\mu\mathbf{H} = 0 \quad (1.13)$$

$$\nabla \cdot (\mu\mathbf{H}) = 0 \quad (1.14)$$

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E} \quad (1.15)$$

It is worth noting that if ϵ , μ and ω are real then $\mathbf{E}(\mathbf{r})^*$ and $\mathbf{H}(\mathbf{r})^*$ satisfy the same set of equations as $\mathbf{E}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r})$.

The curl equations can be combined to eliminate $\mathbf{H}$ so that there is only a curl-curl equation and a divergence equation for $\mathbf{E}$.

$$\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} = 0 \quad (1.16)$$

$$\nabla \cdot (\epsilon \mathbf{E}) = 0 \quad (1.17)$$

The cavity walls are perfect conductors and so the tangential component of electric field vanishes on the surface of the cavity wall. This is equivalent to stating that $\mathbf{n} \times \mathbf{E} = 0$ at the boundary, where $\mathbf{n}$ is a unit vector perpendicular to the surface pointing out of the cavity.

For reasons that are discussed in chapter 2, formulation of the cavity problem for the finite element method involves solving only the curl-curl equation with the boundary conditions. In most cases, the divergence equation for $\mathbf{E}$ is not solved with the curl-curl equation. In the case of eigenvalue problems, this results in extra solutions, called spurious modes. It is useful to see a simple example before proceeding with a general discussion.

Consider a two-dimensional cavity in the shape of a square with walls that are perfect electric conductors. Each side of the square has unit length. This problem can be solved exactly: the electric and magnetic fields are standing waves with eigenvalues given by $k^2 = \pi^2(m^2 + n^2)$, where m and n are non-negative integers and at least one of them is greater than zero. The derivation of the eigenvalue is similar to the three-dimensional

case found, for example, in the text by Wangsness [45]. Here, $k^2 = \omega^2/c^2$, where ω is the angular frequency of the standing wave and c is the speed of light. (Since $c = 299792458$ m/s, which is a very large number, it is numerically more stable to use k instead of ω because for the problems under consideration, $k^2 \sim 10$.)

Figure 1.1: Simple meshes for two-dimensional square cavity. Left: 1×1 mesh. Right: 2×1 mesh.

The units for k^2 are $(\text{length})^{-2}$, which will be denoted by L^{-2} . If the two-dimensional cavity is $1 \text{ m} \times 1 \text{ m}$ then the units of k^2 are m^{-2} , or if the cavity is $1 \text{ cm} \times 1 \text{ cm}$ then the units of k^2 are cm^{-2} . Also, if the cavity is $5 \text{ cm} \times 5 \text{ cm}$ then the units are $1/25 \text{ cm}^{-2}$ because the eigenvalue scales according to L^{-2} . The units of k^2 are L^{-2} for three-dimensional problems as well. The frequency f is related to k^2 by

$$f = \frac{c\sqrt{k^2}}{2\pi} \quad (1.18)$$

where c is the speed of light in units of L/second . If the unit of length in the speed c is the same as the unit of length used to describe the dimensions of the cavity then the unit of frequency is hertz, Hz.

The two-dimensional cavity is solved with the finite element method on two different meshes and using two different sets of basis functions. The meshes are shown in figure 1.1. In the first two calculations, the basis functions for each field component E_x and E_y are a product of second order Lagrange interpolation polynomials, $L_i(x)L_j(y)$, which

Table 1.1: Eigenvalues, k^2 , in units of L^{-2} , of two-dimensional square cavity with sides of unit length. Multiplicity in parentheses. There are no divergence constraints.

Exact	1×1 mesh	2×1 mesh	FEM mode classification
	0.0000 (1)	0.0000 (2)	spurious
		4.2455 (1)	spurious
9.8696 (2)	10.0000 (4)	9.9438 (2), 10.0000 (2)	physical
19.7392 (1)	20.0000 (1)	19.9261 (1)	physical
39.4784 (2)		40.0000 (2)	physical
49.3480 (2)		50.0000 (1)	physical
78.9568 (1)			
88.8264 (2)			
98.6960 (2)			
128.3049 (2)		128.7228 (2), 134.4951 (1)	physical

are defined in section 2.1. The divergence equation is ignored, only the curl equation is solved. The results for the eigenvalues are found in table 1.1. It can be seen that some of the eigenvalues are close approximations to the exact solutions. In the calculation on the 1×1 mesh, the spurious modes have an eigenvalue of $0.0000 L^{-2}$. However, in the calculation on the 2×1 mesh, there are two spurious modes with an eigenvalue of $0.0000 L^{-2}$ but also a spurious mode with an eigenvalue of $4.2455 L^{-2}$. All of the physical modes have eigenvalues that are greater than zero. It would be possible to classify the modes by their eigenvalues if all of the spurious modes had eigenvalues that are zero. The problem is that there are also spurious modes with eigenvalues greater than zero.

In this simple example, the eigenvalues of the spurious modes are below the lowest eigenvalue of the physical modes, but this is not always the case. In general, it is not possible to establish a cutoff frequency with the property that all of the spurious modes lie below this frequency and all of the physical modes are found above it. Another feature that can be observed in the table is that the multiplicity is not always correct. This is observed in other calculations later in the thesis and even with commercial software

Table 1.2: Eigenvalues, k^2 , in units of L^{-2} , of two-dimensional square cavity with sides of unit length. Multiplicity in parentheses. Trivial divergence constraints: $E_x = E_x(y)$ and $E_y = E_y(x)$.

Exact	1×1 mesh	2×1 mesh	FEM mode classification
9.8696 (2)	10.0000 (2)	9.9438 (1), 10.0000 (2)	physical
19.7392 (1)			
39.4784 (2)		40.0000 (1)	physical
49.3480 (2)			
78.9568 (1)			
88.8264 (2)			
98.6960 (2)			
128.3049 (2)		128.7228 (1)	physical

packages such as HFSS [46], as seen later. It can also be seen from the table that some of the lower modes, for example, $k^2 = 78.9568 L^{-2}$, are missed with the 2×1 calculation, but there are higher modes, for example, $k^2 = 128.7228 L^{-2}$ that are present. This is because the basis functions and the mesh do not have enough flexibility to model the oscillations in the field for the missing modes. However, those modes will be present with a finer mesh or higher order basis functions. Finally, the largest eigenvalue, $k^2 = 134.4951 L^{-2}$, does not agree well with any of the exact solutions, but it is likely a poor approximation to one of the lower lying modes.

The basis functions in the preceding example can be modified to solve the divergence equation in a trivial way by letting $E_x = E_x(y)$ and $E_y = E_y(x)$. The results are found in table 1.2. There are no spurious modes, at $k^2 = 0$ or otherwise. These basis functions are too inflexible to solve most problems (including this one) because, in general, $E_x = E_x(x, y)$ and $E_y = E_y(x, y)$. However, the example serves to illustrate that solving only the curl equation allows extra solutions, the spurious modes, and that they are not present if the divergence equation is solved with the curl equation.

More general information on the effect of omitting the divergence equation when solv-

ing eigenvalue problems can be gained by applying the divergence operator to equation (1.16).

$$\nabla \cdot \left(\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} \right) = 0 \quad (1.19)$$

$$\nabla \cdot \left(\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) \right) - \omega^2 \nabla \cdot (\epsilon \mathbf{E}) = 0 \quad (1.20)$$

$$\omega^2 \nabla \cdot (\epsilon \mathbf{E}) = 0 \quad (1.21)$$

There are three categories of solutions of equation (1.21), each with a different physical meaning.

1. $\nabla \cdot \epsilon \mathbf{E} = 0$ and $\omega^2 \neq 0$
2. $\nabla \cdot \epsilon \mathbf{E} \neq 0$ and $\omega^2 = 0$
3. $\nabla \cdot \epsilon \mathbf{E} = 0$ and $\omega^2 = 0$

Physical solutions of the eigenvalue equation must satisfy $\nabla \cdot \epsilon \mathbf{E} = 0$ because there is no charge inside of the cavity. This means that solutions in the first and last categories are physically admissible. Solutions for which $\omega^2 = 0$ are static, so the last two categories correspond to electrostatic fields inside of the cavity.

Solutions in the third category are now considered in greater detail. Since $\omega^2 = 0$ then $\nabla \times \mathbf{E} = 0$ and so $\mathbf{E} = -\nabla \phi$. Apply the divergence operator to the quantity $\phi \epsilon \nabla \phi$:

$$\nabla \cdot (\phi \epsilon \nabla \phi) = \phi \nabla \cdot (\epsilon \nabla \phi) + \epsilon \nabla \phi \cdot \nabla \phi \quad (1.22)$$

$$= \epsilon |\nabla \phi|^2 \quad (1.23)$$

The last line follows as $\nabla \cdot (\epsilon \nabla \phi) = 0$ because $\nabla \cdot (\epsilon \mathbf{E}) = 0$. Now integrate over the

volume of the cavity and use the divergence theorem.

$$\iiint \epsilon |\nabla \phi|^2 dV = \iint \phi \epsilon \nabla \phi \cdot \mathbf{n} dS \quad (1.24)$$

$$= \phi \iint \epsilon \nabla \phi \cdot \mathbf{n} dS \quad (1.25)$$

$$= -\phi \iint \mathbf{D} \cdot \mathbf{n} dS \quad (1.26)$$

$$= -\phi Q_{inside} \quad (1.27)$$

$$= 0 \quad (1.28)$$

Since the cavity walls are perfect conductors then they are an equipotential surface, that is, ϕ is a constant on the surface, which is why ϕ can be factored out of the surface integral in the second line. The third line follows from the integral form of Gauss' law, which can be obtained by applying the divergence theorem to equation (1.1), where the charge inside the cavity, denoted by Q_{inside} , is zero. Since $\epsilon > 0$ and $|\nabla \phi|^2 \geq 0$ then $\iiint \epsilon |\nabla \phi|^2 dV = 0$ implies that $|\nabla \phi| = 0$, or $|\mathbf{E}| = 0$, which implies that $\mathbf{E} = 0$. Thus, the only solution in the third category is $\mathbf{E} = 0$, which is a trivial solution to the eigenvalue equation. This proof is similar to what is found in Jackson [3] to prove the uniqueness of the solution for Poisson's equations. The modified version above is included in the present discussion to clarify the nature of all possible solutions to the eigenvalue problem.

Solutions in the first category have the correct divergence. They are the physically correct solutions for that reason and therefore they are the sought after cavity modes. The eigenvalues are non-zero.

Solutions of equation (1.21) that fall into the second category do not have the correct divergence. For that reason they are not physically correct solutions and are labelled as spurious modes. Since $\omega^2 = 0$, the spurious modes are static solutions. It follows from Faraday's law that they are irrotational, that is, $\nabla \times \mathbf{E} = 0$ since $\omega = 0$. From a physical point of view, the spurious modes describe non-zero electrostatic solutions whose source is electric charge inside of the cavity. These modes satisfy the equations $\nabla \times \mathbf{E} = 0$ and

$\nabla \cdot \epsilon \mathbf{E} = \rho$, although ρ is not specified, which is similar to the discussion of equations (1.9) – (1.11).

Since the spurious modes are static and the physical modes are not, then it may seem reasonable to solve the eigenvalue problem in equation (1.16) and classify the solutions according to their eigenvalue. However, it turns out that this is not always possible, as seen in the simple example. In the same way that the eigenvalues of equation (1.16) corresponding to the physical solutions are approximate values, so are the eigenvalues corresponding to the spurious modes, that is, the eigenvalues of the spurious modes are not exactly zero. Furthermore, there is not even a cutoff value in the eigenvalue spectrum for which it is possible to say that all eigenvalues below the cutoff are spurious and those above the cutoff are physical. The only way to determine if the eigenvalues are physical solutions is to evaluate the divergence of the eigenvector and ascertain whether it is acceptably close to zero.

In summary, it is necessary to solve the curl and divergence equations in order to determine a vector field. This is true whether the equations can be solved exactly or whether the finite element method is used to obtain an approximate solution. This becomes very clear in eigenvalue problems: it is not simply that the solutions have a limited amount of inaccuracy if the divergence equation is not satisfied, it is possible that there are solutions that do not have any physical meaning at all!

In the discussion above, spurious modes arose in the context of a resonant cavity. From a historical perspective, Cendes and Silvester first noticed the existence of spurious modes in 1970 while calculating dispersion relations of inhomogeneous waveguides [13], which are also eigenvalue problems. While spurious modes are often discussed in high frequency eigenvalue problems, they also occur at low frequencies in the modal analysis of eddy current problems [22, 25]. This analysis indicates that spurious modes can affect the solution of driven problems as well, that is, ordinary problems in the time domain or frequency domain that are not even eigenvalue problems.

Any numerical method must certainly resolve or avoid the problem of spurious modes. There are several methods for doing this, however, in each method compromises are made that introduce other difficulties or inaccuracies. The existing methods are discussed on a case-by-case basis in the next section.

1.3 Survey of existing methods for tackling the spurious modes problem

Several finite element methods have been developed for vector fields that eliminate spurious modes or ensure a simple classification of spurious modes or physical modes. Each method has strengths and weaknesses that do not overlap entirely, and there is more than one method in use at the present time.

1.3.1 Adding a penalty term to the functional

One of the earliest methods employed for dealing with the existence of spurious modes is known as the penalty method or the penalty function method. This method has been applied by several authors to cavity problems and waveguide problems [14–16]. For a cavity problem, the lowest resonant frequencies and the corresponding fields are of interest. These modes lie above, and are surrounded by, spurious modes, which have a non-zero divergence, as discussed in the previous section. Thus, a penalty term containing the divergence of the field can be added to the functional (1.29) in an effort to push the spurious modes above the lowest physical modes. For example, in ref. [16], the modes of an empty rectangular cavity and a rectangular cavity with a dielectric post are obtained by minimizing the following functional of the magnetic field. (This is discussed further in chapter 2.)

$$\mathcal{F}(\mathbf{H}) = \iiint \left[\frac{1}{\epsilon_r} (\nabla \times \mathbf{H}^*) \cdot (\nabla \times \mathbf{H}) - k^2 \mathbf{H}^* \cdot \mathbf{H} \right] dV \quad (1.29)$$

The magnetic field is used since it is continuous throughout the domain, whereas the normal component of the electric field is discontinuous where the permittivity is discontinuous. The continuity of the magnetic field is simple to enforce with nodal basis functions. This functional is modified by adding a penalty term involving the divergence of the field.

$$\mathcal{F}_\lambda(\mathbf{H}) = \mathcal{F}(\mathbf{H}) + \lambda \iiint |\nabla \cdot \mathbf{H}|^2 dV \quad (1.30)$$

The parameter λ is chosen to push the spurious modes above the low-lying physical modes of interest. A difficulty with this method is that it is not known *a priori* what value to assign to λ : if the value is too low then the eigenvalues of the spurious modes are not pushed above the physical modes but if the value is too high then the computed eigenvalues are inaccurate since the divergence equation is solved at great expense to the curl-curl equation.

The authors of references [14–16] have obtained the modes for a wide range of values of the parameter λ . The spurious modes are observed to depend on λ while the physical modes are much less dependent on λ . This suggests another classification method for the solutions but a major drawback is that the problem needs to be solved many times for different values of λ .

In practice, the method produces mostly physical solutions with a small number of spurious modes that are classified by evaluating the divergence [17]. The method has advantages and disadvantages but it works and is still in use for optics problems [18]. It is interesting to note that Courant considered the inclusion of a penalty term in his original paper [1] in order to improve the accuracy of the derivatives of the approximate solution.

1.3.2 Imposing constraints for the divergence

Several methods have been developed for directly implementing divergence constraints [19–23]. Konrad [19] has derived a method for imposing divergence constraints for a curvilinear brick. The basis functions are a product of second order Lagrange interpolation polynomials for each of the field components. The matrices corresponding to the curl equation are reduced in size by eliminating coefficients so that the divergence equation is satisfied exactly throughout the brick. As a result, there are no spurious modes in the eigenvalue spectrum. The method is difficult to implement for a general mesh with more than one curvilinear brick but it clearly demonstrates that the origin of spurious modes is due to the divergence equation not being satisfied. It is also observed that spurious modes can occur if the principal boundary conditions are not imposed. This point is discussed further in another paper [20].

Kobelansky and Webb [21] provide a method for deriving global basis functions that are divergence free. The global basis functions are a subset of the eigenvectors of a related symmetric eigenvalue problem. Since the matrices are symmetric then the basis functions (eigenvectors) can be made orthogonal. The matrices resulting from the curl equation are projected orthogonally into the subspace of the global basis functions and as a result, the spurious modes are eliminated. The drawbacks of this method are that many basis functions need to be calculated and the basis functions are not sparse so the projected curl matrices are not sparse either. Thus, the memory required is no longer linearly proportional to the number of basis functions and the calculation takes more time. However, the advantages of this method are that the divergence equations and the curl equations are satisfied for a general mesh and it is another clear demonstration that the origin of the spurious modes is due to the divergence equation not being satisfied.

Wong and Cendes [22, 23] use basis functions of the form $\mathbf{V} = \nabla \times \mathbf{A}$ so that the divergence of $\mathbf{V}$ is automatically zero, thus eliminating spurious modes. For this to be possible, the basis functions $\mathbf{A}$ must be smooth across the mesh interfaces so that

$\mathbf{V}$ is continuous. This is not possible with an arbitrary mesh. However, the authors demonstrate that a mesh that allows for smooth interpolation of random data is adequate and they develop a procedure to construct such a mesh. They are also able to show that using the standard Lagrange interpolation basis functions [7] on a smooth mesh without imposing the divergence constraints ensures that the eigenvalues of the spurious modes are exactly zero. This method is another clear demonstration that spurious modes are eliminated if both the curl equations and the divergence equations are satisfied. It is not clear how easy it is to construct a smooth mesh in general cases and the authors do not appear to have continued with this work in spite of the fact that, on the surface at least, this method seems promising.

1.3.3 Using covariant projection elements as basis functions

Crowley, Silvester and Hurwitz have derived mixed order curvilinear elements that correctly model the null space of the curl operator [24]. Recalling the discussion in section 1.2, spurious modes, if solved exactly, are static, have non-zero divergence and are irrotational (the curl is zero). Thus, the physical solutions can be distinguished from the spurious solutions by ensuring that the physical solutions are orthogonal to all irrotational functions. The solutions obtained from the finite element method are approximations to the exact solutions, including the spurious solutions. Although the exact spurious solutions are irrotational, the curl of the approximate solutions may not be exactly zero. This is the origin of the non-zero eigenvalue for the spurious modes obtained with the finite element method. The authors derive basis functions that ensure that finite element approximations of irrotational solutions are irrotational, which implies these solutions have an eigenvalue of zero. Using this method, the modes with non-zero eigenvalues are physical solutions and the modes with zero eigenvalues are spurious solutions, and thus, the solutions can be classified by their eigenvalues. The authors have applied this method to a waveguide problem and a two-dimensional eddy current problem. In another paper,

Table 1.3: Eigenvalues, k^2 , in units of L^{-2} , of two-dimensional square cavity with sides of unit length. Multiplicity in parentheses. The basis functions are covariant projection elements.

Exact	1×1 mesh	2×1 mesh	FEM mode classification
	0.0000 (1)	0.0000 (2)	spurious
9.8696 (2)	10.0000 (2)	9.9438 (1), 10.0000 (1)	physical
19.7392 (1)	20.0000 (1)	19.8774 (1)	physical
39.4784 (2)		40.0000 (1)	physical
49.3480 (2)		50.0000 (1)	physical
78.9568 (1)			
88.8264 (2)			
98.6960 (2)			
128.3049 (2)		128.7228 (1), 128.7892 (1)	physical

the contribution of spurious modes to driven vector diffusion problems is made clear through eddy current modal analysis [25]. It is worth noting that the basis functions are nodal basis functions for the different field components and that the mesh is divided into curvilinear quadrilaterals.

The simple example problem that was solved in section 1.2 is solved again using the basis functions derived by these authors. The results are found in table 1.3. The spurious modes are still present, however, $k^2 = 0 L^{-2}$. The eigenvalues of the physical modes are greater than zero, and so the solutions can be classified by their eigenvalue.

1.3.4 Using edge elements as basis functions

Edge elements are used as basis functions in finite element method software packages that solve vector problems in electromagnetics, such as HFSS [46], Maxwell [47] and Comsol Multiphysics [48]. At the present time, this is the most common method for solving the curl and the divergence simultaneously.

Edge elements were derived by Nedelec in 1980 [26]. Bossavit and Vrit applied edge

elements to solve three-dimensional eddy current problems in 1982 [27]. The idea has been applied and developed further by many authors ever since then. (See, for example, references [28–31].)

Similar to covariant projection elements described previously, edge elements ensure that the eigenvalues of the spurious modes are zero. This method does not constrain the divergence of the field, but rather ensures that the null space of the curl operator is modelled accurately, similar to the covariant projection elements. Again, spurious modes are not eliminated but they are identified by their eigenvalue.

Tangential continuity conditions at tetrahedra boundaries are explicitly enforced but normal continuity conditions are not. A major advantage of edge elements is that they are used on arbitrary tetrahedral meshes. The normal component of the field is not constrained to be continuous but rather it converges as the size of the tetrahedra decrease [28]. This is a source of inaccuracy that also has a physical description when the boundary conditions of the fields are considered. For example, when edge elements are applied to problems where the electric field is solved, the discontinuity of the normal component of the field implies a surface charge density on the interface of adjacent tetrahedra. This occurs at all frequencies, static or otherwise. In eddy current problems, a discontinuity in the normal component of the field means that the current flowing from one tetrahedron to the next is not conserved. Advantages and disadvantages of edge elements are discussed further by other authors [32–34].

1.3.5 Formulations specifically for waveguide problems

There are several methods for eliminating spurious modes specifically for waveguides [35–37]. The permittivity of the waveguide is, in general, inhomogeneous and the walls can be perfect conductors or not, as in the case of an optical fibre. Since the material is non-magnetic (the permeability is μ_0), the magnetic field $\mathbf{H}$ is continuous. The field is

assumed to have the form

$$\mathbf{H}(x, y, z, t) = \mathbf{h}(x, y)e^{j(\omega t - k_z z)} \quad (1.31)$$

and so the divergence condition yields

$$h_z = -\frac{1}{jk_z} \left(\frac{\partial h_x}{\partial x} + \frac{\partial h_y}{\partial y} \right). \quad (1.32)$$

This is used to eliminate h_z from the curl equations so that the equations to be solved contain the divergence constraint. Since these equations contain $h_x(x, y)$ and $h_y(x, y)$, which are both continuous, the magnetic field formulation with nodal basis functions is used. There are no spurious modes.

1.3.6 Other methods for solving Maxwell's equations

This subsection contains brief descriptions of other methods for solving Maxwell's equations that are not finite element methods. The methods to be discussed are the finite difference time domain method [12] and the plane wave method [38]. The curl and divergence equations are solved simultaneously in both methods, although the methods are not completely general.

Finite difference time domain method

In the finite difference time domain method [12], both $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$ are used as variables in the calculation. They are updated one after the other in a leap frog scheme using finite difference formulae for the curl equations. The divergence equations are not solved explicitly, however, the type of calculations that can be performed are restricted. Calculations are commonly performed with the initial condition $\mathbf{E}(\mathbf{r}, t) = 0$ and $\mathbf{H}(\mathbf{r}, t) = 0$, after which the system is excited by a pulse. The fields are zero at the beginning of the simulation, which means that the $\nabla \cdot \mathbf{D}(\mathbf{r}, 0) = 0$ and $\nabla \cdot \mathbf{B}(\mathbf{r}, 0) = 0$. As seen

from equations (1.9)–(1.11), Faraday’s law does not allow for the divergence to change in time, so if $\nabla \cdot \mathbf{B} = 0$ in the beginning, the time evolution from Faraday’s law does not change that. The situation is not as simple for the electric field, because it is possible that $\nabla \cdot \mathbf{J} \neq 0$, which means that the divergence of the electric field will change because the charge density is not zero anymore. Thus, the method cannot be used in cases where the divergence is not zero.

Plane wave method

A method using plane waves to solve problems involving photonic crystals has been developed more recently by Johnson and Joannopoulos [38]. In these problems, the permittivity is periodic and the object is to obtain the dispersion relations for the crystal using the fast Fourier transform. The curl and the divergence equations are solved simultaneously and consequently there are no spurious modes. The normal component of the electric field is discontinuous where the permittivity is discontinuous, and yet the plane waves are continuous functions. The authors use a smoothed approximation for the permittivity at discontinuities so that the continuous plane wave basis functions can be used.

1.4 Thesis objectives and contributions

A general remark can be made about all of the methods used to address the issue of spurious modes described in section 1.3: there are always compromises! All of the methods have advantages and disadvantages that do not completely overlap with each other, and none of the methods works on every kind of problem.

The purpose of the present work is to develop a finite element method that can simultaneously solve the curl and divergence equations for a vector field. The curl equations are solved using basis functions that allow for the divergence of the field to be set as a

constraint. The basis functions are a product of cubic Hermite splines and second order Lagrange interpolation polynomials. This is the first time that such a method has been proposed.

The method must be able to satisfy boundary conditions for the different field components at an interface between two different media. In addition to planar interfaces, the method must also work where the interface forms an edge or corner. The method is tested on eigenvalue problems, specifically, resonant cavities, to verify that spurious modes are not present.

The main contribution in this thesis is a set of basis functions to model vector fields possessing the important property that the divergence is set as a constraint. Once the constraint has been set, the basis functions are used to solve the curl equations. This means that both the curl and divergence equations are solved, at least approximately, and it follows that there are no spurious modes for eigenvalue problems. The basis functions are valid for a mesh of bricks. It is not necessary that all of the bricks be the same size, but the faces of adjacent bricks must occur in common planes. The method is extended to incorporate mesh refinement and specific constraints are derived for solving problems with singular fields that arise where the material boundaries form edges and corners. The new basis functions are tested by solving for the resonant frequencies and fields of three-dimensional cavities. The results obtained with the new basis functions are compared with exact solutions when they exist, measurements that have been made, and with values obtained using the software package HFSS [46].

1.5 Thesis outline

The thesis describes a new method for solving Maxwell's equations with the finite element method using basis functions with the divergence set as a constraint to solve the curl equations. The new basis functions are defined in chapter 2. The simple example de-

scribed in chapter 1 is solved using the new basis functions to show that spurious modes are eliminated and to show explicitly how the divergence constraints are implemented. The test problem for the new basis functions is to determine the frequencies and fields of resonant cavities. This problem can be solved using the electric field formulation or the magnetic field formulation, as described in this chapter. There are several examples of resonant cavities, including some where either exact solutions are known or experimental measurements have been made. These problems are used to determine the accuracy of the method.

Chapter 3 contains the description of a mesh refinement procedure. The method consists of dividing a selected brick into $2 \times 2 \times 2$ smaller bricks of equal size. Each smaller brick can be refined further. In principal, the process of refinement can continue *ad infinitum*. As a result of this division, the divergence constraints need to be modified. There are additional constraints to ensure that the field is continuous at an interface where the level of mesh refinement changes, which are referred to as hanging node constraints. The modified divergence constraints and the hanging node constraints are described in detail. The examples that are solved in chapter 2 are solved again using refined meshes to test the method.

Chapter 4 contains a description for using the new basis functions to solve problems where the field is singular at edges and corners of material boundaries. There is a procedure for solving problems containing edges and corners of perfect conductors. This procedure utilizes the mesh refinement method of chapter 3. There are two methods for solving problems with electric fields that are singular at dielectric edges and corners. They are equally applicable to solving problems with magnetic fields that are singular where the boundaries of magnetic materials form edges and corners. Several examples of resonant cavities with singular fields are solved with the new basis functions and with the software package HFSS [46] for comparison. There is agreement between the eigenvalues obtained with the new basis functions and with HFSS.

The final chapter contains a brief summary of the thesis work and an outline of projects considered for future work. Results for cylindrical coordinates are found in Appendix C.

Chapter 2

Basis Functions With Inbuilt Divergence Constraints

Finite element methods that are used for solving scalar equations cannot be trivially extended to solve problems involving vector fields. A particular difficulty is the occurrence of non-physical solutions of eigenvalue problems called spurious modes, as discussed in chapter 1. The curl and divergence equations must be satisfied simultaneously so that the vector field is uniquely determined, as stated in Helmholtz's theorem [5,6]. It is the inability to solve the curl and divergence equations simultaneously that is the source of the spurious modes. The variational formulation contains only the curl equation, shown explicitly in section 2.4, and so the divergence equation is not satisfied. Nodal basis functions are used when the finite element method is used to solve scalar problems. These functions do not have a continuous derivative in the direction that is perpendicular to the boundary of the triangle or tetrahedron, and so it is not possible to impose divergence constraints while preserving the sparsity of the matrices.

This chapter contains a description of basis functions that are used for solving differential equations of vector fields with the finite element method. The most important property of the new basis functions is that the divergence of the field is set as a constraint.

Once the divergence is set, the basis functions are used to solve the curl equations. The definition of the new basis functions is given in section 2.1. The divergence constraints are derived in section 2.2. In section 2.3, the simple 2-dimensional example that was solved in chapter 1 is solved using the new basis functions. A detailed derivation of the Rayleigh-Ritz formulation for a cavity problem is given in section 2.4 since this is the main test for the new basis functions. Section 2.5 contains example calculations that are chosen because the results can be compared either to exact solutions or experimental data. In these examples, the field is continuous. The basis functions can be used to solve problems where either or both the permittivity and permeability change discontinuously at a planar interface, as discussed in section 2.6. The new basis functions yield matrices with favourable convergence properties when an iterative projection method such as the Lanczos algorithm is used, which is discussed in section 2.7. The results are summarized at the end of the chapter.

2.1 Definition of basis functions for divergence constraints

In many cases, the divergence of the field is a continuous function, including the specific case where the divergence is zero everywhere. The divergence is the flux per unit volume, which, in Cartesian coordinates, can be expressed by the formula

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} \quad (2.1)$$

provided the partial derivatives are continuous. One way to guarantee that the finite element approximation of the divergence will be a continuous function is to require that $\partial E_x/\partial x$, $\partial E_y/\partial y$ and $\partial E_z/\partial z$ are each continuous functions. A difficulty with using the Lagrange interpolation polynomials is that it is easy to impose continuity of the field

(a) Second order Lagrange interpolation polynomials

(b) Cubic Hermite splines

Figure 2.1: Piecewise polynomials on $[0, 1]$ and $[1, 2]$.

Table 2.1: Properties of cubic Hermite splines.

	$f(0)$	$f'(0)$	$f(1)$	$f'(1)$
$H_0(x)$	1	0	0	0
$H_1(x)$	0	1	0	0
$H_2(x)$	0	0	1	0
$H_3(x)$	0	0	0	1

between adjacent subdomains in the mesh but it is not easy to impose continuity of the derivatives. To be more precise, imposing continuity will result in sparse matrices but the sparsity will be lost if continuity of the derivatives is imposed. However, it is easy to impose continuity of the field and the first derivative using cubic Hermite polynomials. This is illustrated graphically in figure 2.1, which shows the second order Lagrange polynomials and the cubic Hermite splines plotted piecewise on $[0, 1]$ and $[1, 2]$. The cubic Hermite splines are listed below and some relevant properties are found in table 2.1.

$$H_0(x) = 1 - 3x^2 + 2x^3 \quad (2.2)$$

$$H_1(x) = x - 2x^2 + x^3 \quad (2.3)$$

$$H_2(x) = 3x^2 - 2x^3 \quad (2.4)$$

$$H_3(x) = -x^2 + x^3 \quad (2.5)$$

Similarly, the second order Lagrange interpolation polynomials are also listed below and some relevant properties are contained in table 2.2.

$$L_0(x) = 1 - 3x + 2x^2 \quad (2.6)$$

$$L_1(x) = 4x - 4x^2 \quad (2.7)$$

$$L_2(x) = -x + 2x^2 \quad (2.8)$$

Table 2.2: Properties of second order Lagrange interpolation polynomials.

	$f(0)$	$f(0.5)$	$f(1)$
$L_0(x)$	1	0	0
$L_1(x)$	0	1	0
$L_2(x)$	0	0	1

Consider a mesh of bricks. For a particular brick, $x_0 \leq x \leq x_1$, $y_0 \leq y \leq y_1$ and $z_0 \leq z \leq z_1$. The lengths of the sides of the brick are $\delta_x = x_1 - x_0$, $\delta_y = y_1 - y_0$ and $\delta_z = z_1 - z_0$. For each particular brick, local coordinates, denoted by (x', y', z') , are defined such that $0 \leq x' \leq 1$, $0 \leq y' \leq 1$ and $0 \leq z' \leq 1$, and are given by

$$x' = (x - x_0)/\delta_x \quad (2.9)$$

$$y' = (y - y_0)/\delta_y \quad (2.10)$$

$$z' = (z - z_0)/\delta_z. \quad (2.11)$$

Partial derivatives with respect to the global coordinates can be expressed in terms of the local coordinates using the chain rule.

$$\frac{\partial f}{\partial x}(x, y, z) = \frac{dx'}{dx} \frac{\partial f}{\partial x'}(x', y', z') \quad (2.12)$$

$$= \frac{1}{\delta_x} \frac{\partial f}{\partial x'}(x', y', z') \quad (2.13)$$

The local coordinates are used almost exclusively in the remainder of the thesis. It is convenient to drop the “prime” notation when there is no ambiguity and use it only when there is a possibility for confusion.

The basis functions for the Cartesian components of the field $\mathbf{E}$ are defined as a product of cubic Hermite splines and second order Lagrange interpolation polynomials.

$$E_x(x, y, z) = \sum_{i=0}^3 \sum_{j=0}^2 \sum_{k=0}^2 c_{ijk}^x \Delta_{xi} H_i(x) L_j(y) L_k(z) \quad (2.14)$$

$$E_y(x, y, z) = \sum_{i=0}^2 \sum_{j=0}^3 \sum_{k=0}^2 c_{ijk}^y \Delta_{yj} L_i(x) H_j(y) L_k(z) \quad (2.15)$$

$$E_z(x, y, z) = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^3 c_{ijk}^z \Delta_{zk} L_i(x) L_j(y) H_k(z) \quad (2.16)$$

The coefficients c_{ijk}^x , c_{ijk}^y and c_{ijk}^z are the unknowns. Different field components have nodes that are located in different positions, as shown in figure 2.2. Each node in the figure corresponds to a value of the field component and a value of its derivative. The factor Δ_{xi} is equal to δ_x if $i = 1$ or $i = 3$ and it is unity if $i = 0$ or $i = 2$. The other factors Δ_{yj} and Δ_{zk} are defined similarly.

Figure 2.2: Field component nodes

To illustrate that $\partial E_x / \partial x$ is continuous using these basis functions, consider its continuity across each face of a brick. For points that are on the surfaces $x = 0$ and $x = 1$,

$$\frac{\partial E_x}{\partial x}(0, y, z) = \sum_{j=0}^2 \sum_{k=0}^2 c_{1jk}^x L_j(y) L_k(z) \quad (2.17)$$

and

$$\frac{\partial E_x}{\partial x}(1, y, z) = \sum_{j=0}^2 \sum_{k=0}^2 c_{3jk}^x L_j(y) L_k(z), \quad (2.18)$$

respectively. Thus, continuity of $\partial E_x/\partial x$ can be enforced explicitly by equating c_{1jk}^x and c_{3jk}^x from adjacent bricks. (Note that $\Delta_{x,1} = \Delta_{x,3} = \delta_x$, which cancels with the factor $1/\delta_x$ due to the chain rule. Thus, the factors Δ_{xi} , Δ_{yj} and Δ_{zk} lead to simpler conditions for the continuity of the derivatives if adjacent bricks are not the same size and they also result in simpler divergence constraints if the brick is not a cube.)

On each of the other four faces, $\partial/\partial x$ is a derivative that is tangential to each face and so continuity of $\partial E_x/\partial x$ is automatically satisfied if E_x is continuous everywhere on each face. This does not depend on using Hermite splines and it is also true using the standard nodal basis functions for tetrahedra [8]. Similar arguments hold for establishing the continuity of $\partial E_y/\partial y$ and $\partial E_z/\partial z$. Note that using the basis functions in equations (2.14)–(2.16), $\partial E_x/\partial y$, for example, is not guaranteed to be continuous across the face $y = 0$.

The matrix elements S_{ij} and T_{ij} are defined in Appendix D.

2.2 Divergence constraints

The derivatives of cubic Hermite splines can be expressed as a linear combination of second order Lagrange polynomials.

$$\frac{dH_0}{dx}(x) = -\frac{3}{2}L_1(x) \quad (2.19)$$

$$\frac{dH_1}{dx}(x) = L_0(x) - \frac{1}{4}L_1(x) \quad (2.20)$$

$$\frac{dH_2}{dx}(x) = \frac{3}{2}L_1(x) \quad (2.21)$$

$$\frac{dH_3}{dx}(x) = L_2(x) - \frac{1}{4}L_1(x) \quad (2.22)$$

Thus it is possible to expand the divergence of the field within a given brick using only second order Lagrange polynomials.

$$\nabla \cdot \mathbf{E}(x, y, z) = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^2 d_{ijk} L_i(x) L_j(y) L_k(z) \quad (2.23)$$

The divergence equation yields 27 linearly independent constraints per brick. A relatively simple set of constraints is obtained if (2.23) is evaluated at the nodes of the Lagrange polynomials. The utility of the method is due to the fact that it is easy to identify a linearly independent set of constraints for the entire mesh (not only within a particular brick) and because the equations are easy to solve, involving relatively few operations and preserving sparsity. A list of all of the divergence constraints is found in Appendix A, as well as figures containing the node locations for all of the coefficients of the basis functions. The constraints can be classified by the location of the node of the divergence equation (2.23): at a corner of the brick, at the midpoint of an edge, at the centre of a face or at the centre of the brick.

By evaluating the divergence (2.23) at the corner $(1, 0, 1)$ it follows that

$$d_{202} = c_{302}^x + c_{212}^y + c_{203}^z \quad (2.24)$$

The coefficients are those of the derivative terms with nodes occurring only at the corner $(1, 0, 1)$ as shown in figure 2.3(a). The constraints at other corners have the same form as the one above, that is, they involve only coefficients corresponding to derivative nodes at the given corner. If a corner is common to multiple bricks then there will be as many constraints as bricks for this corner, however, all of the constraints are identical once the continuity and smoothness conditions between adjacent bricks have been imposed. Thus, each corner in the mesh has only one constraint that is as simple as the one given above. This would not occur if a mixture of second and third order Lagrange polynomials were used in place of the basis functions in equations (2.14)–(2.16). The constraint can be

 (a) Nodes appearing in corner constraint at $(1, 0, 1)$.

 (b) Nodes appearing in edge constraint at $(1, 0, \frac{1}{2})$.

 (c) Nodes appearing in face constraint at $(1, \frac{1}{2}, \frac{1}{2})$.

 (d) Nodes appearing in centre constraint at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

Figure 2.3: Nodes for divergence constraints.

imposed by using equation (2.24) to eliminate one of the three coefficients in the curl-curl equations. For example, if $\nabla \cdot \mathbf{E} = 0$ then c_{302}^x can be eliminated using $c_{302}^x = -c_{212}^y - c_{203}^z$.

Evaluating the divergence (2.23) at $(1, 0, \frac{1}{2})$, which is the midpoint of an edge, results in the following constraint.

$$d_{201} = c_{301}^x + c_{211}^y - \frac{3}{2\delta_z} c_{200}^z - \frac{1}{4} c_{201}^z + \frac{3}{2\delta_z} c_{202}^z - \frac{1}{4} c_{203}^z \quad (2.25)$$

The nodes with coefficients in this constraint are shown in figure 2.3(b). While this constraint is not as simple as equation (2.24), it still contains only nodes occurring on the edge whose midpoint is $(1, 0, \frac{1}{2})$. This edge is common to adjacent bricks but again the constraints arising from different bricks are identical once continuity and smoothness are imposed. The constraint can be enforced by eliminating either c_{301}^x or c_{211}^y . Note that the coefficient c_{203}^z occurs both in the corner constraint (2.24) and in the edge constraint (2.25). Thus, to reduce the S and T matrices efficiently, the edge constraints are applied before the corner constraints.

If the divergence is evaluated at the centre of a face, for example $(1, \frac{1}{2}, \frac{1}{2})$ then, again, only coefficients corresponding to nodes on this face occur, as shown in figure 2.3(c).

$$\begin{aligned} d_{211} = & c_{311}^x - \frac{3}{2\delta_y} c_{201}^y - \frac{1}{4} c_{211}^y + \frac{3}{2\delta_y} c_{221}^y - \frac{1}{4} c_{231}^y \\ & - \frac{3}{2\delta_z} c_{210}^z - \frac{1}{4} c_{211}^z + \frac{3}{2\delta_z} c_{212}^z - \frac{1}{4} c_{213}^z \end{aligned} \quad (2.26)$$

The coefficient c_{311}^x can be eliminated from the S and T matrices to implement this constraint. Note that since the coefficient c_{211}^y occurs in this constraint and since it may have been eliminated to implement the edge constraint (2.25), then the constraints can be imposed efficiently by applying the edge constraints after the face constraints.

The constraint that occurs at the centre of the brick is given below and the nodes involved in the constraint are shown in figure 2.3(d).

$$\begin{aligned}
 d_{111} = & -\frac{3}{2\delta_x}c_{011}^x - \frac{1}{4}c_{111}^x + \frac{3}{2\delta_x}c_{211}^x - \frac{1}{4}c_{311}^x \\
 & -\frac{3}{2\delta_y}c_{101}^y - \frac{1}{4}c_{111}^y + \frac{3}{2\delta_y}c_{121}^y - \frac{1}{4}c_{131}^y \\
 & -\frac{3}{2\delta_z}c_{110}^z - \frac{1}{4}c_{111}^z + \frac{3}{2\delta_z}c_{112}^z - \frac{1}{4}c_{113}^z
 \end{aligned} \tag{2.27}$$

In this constraint, the nodes occur in six adjacent bricks, which makes it more difficult to implement than the face, edge or corner constraints. Suppose that c_{211}^x is eliminated in one brick and then the same thing is attempted in the next brick in the direction of increasing x . The coefficient c_{011}^x in the next brick is related to the coefficient c_{211}^x of the previous brick by the continuity (or discontinuity, as the case may be) of the normal component of the field. Thus, as the coefficients c_{211}^x are eliminated by stepping through the mesh they are related to previous bricks through c_{011}^x and this reduces the sparsity. Note also that the coefficient c_{311}^x occurs in equation (2.27) and in equation (2.26) and so the constraints at the centre of each brick must be eliminated before the face constraints. For example, if the permittivity, ϵ , is constant and $\nabla \cdot \mathbf{E} = 0$ then $d_{111} = 0$ and $c_{011,i}^x = c_{211,i-1}^x$, where the subscript i refers to the brick number from the boundary $x = x_{min}$. The constraint for the i^{th} brick can be expressed as a linear combination of coefficients in the bricks before it.

$$\begin{aligned}
 c_{211,i}^x = & \sum_{n=1}^i \delta_{x,n} \left(\frac{1}{6}c_{111,n}^x + \frac{1}{6}c_{311,n}^x + \frac{1}{\delta_{y,n}}c_{101,n}^y + \frac{1}{6}c_{111,n}^y - \frac{1}{\delta_{y,n}}c_{121,n}^y + \frac{1}{6}c_{131,n}^y \right. \\
 & \left. + \frac{1}{\delta_{z,n}}c_{110,n}^z + \frac{1}{6}c_{111,n}^z - \frac{1}{\delta_{z,n}}c_{112,n}^z + \frac{1}{6}c_{113,n}^z \right) + c_{011,1}^x
 \end{aligned} \tag{2.28}$$

The divergence constraints at the centre of each brick are implemented by moving in a straight line from one end of the mesh to the other. This reduces the sparsity by creating non-zero off-diagonal elements between nodes occurring in the string of bricks.

Unfortunately it is not possible to implement the constraints by moving around in a rectangle and thus creating a “super” brick with sets of four bricks having reduced sparsity rather than an entire string of bricks. The reason this is not possible is because the constraints are not linearly independent on the four interior nodes to be eliminated, rather, only three of the interior nodes can be eliminated. The 4×4 matrix that results from the four interior nodes has a rank of 3 and so an exterior node must be eliminated to guarantee that all four constraints are implemented. This reduces the sparsity, and an equation similar to equation (2.28) will result as the exterior node of the “super” brick is eliminated throughout the mesh.

To summarize, each brick has 27 linearly independent divergence constraints, but once the continuity and smoothness of the field have been imposed then there is only one constraint for each corner, edge and face in the mesh, as well as one for the centre of each brick. The constraints can be used to reduce the size of the S and T matrices resulting from the curl-curl equations. This is done efficiently if the constraints at the centre of each brick (2.27) are imposed first, followed by the face constraints (2.26), the edge constraints (2.25) and, lastly, the corner constraints (2.24). It is possible to perform this reduction with matrix multiplication.

$$S' = D_{corner}^T D_{edge}^T D_{face}^T D_{centre}^T S D_{centre} D_{face} D_{edge} D_{corner} \quad (2.29)$$

The matrices D_{face} , D_{edge} and D_{corner} arise from the constraints for the faces, edges and corners, respectively, and D_{centre} arises from the constraints at the centre of each brick. Once the divergence constraints have been imposed, the total number of non-zero elements in the S and T matrices increases by approximately a factor of two. This reduction in sparsity is due to the divergence constraint at the centre of each brick, equation (2.27).

There is one node eliminated for each constraint that is imposed. Thus, the matrices

containing constraints should be rectangular and successively reduce the size of the S and T matrices. However, it is also possible to use square matrices with columns whose elements are zero for the eliminated nodes. The matrix size is reduced by removing the nodes from the divergence constraints and the nodes for the boundary conditions altogether as the last step before the eigenvalue solver is called. This method was found to be faster using the software package Matlab [55] because the array sizes change only once, which means that memory allocation and data movement are minimized.

If all of the divergence constraints are contained in a square matrix D such that

$$D = D_{centre}D_{face}D_{edge}D_{corner} \quad (2.30)$$

then D is idempotent, that is, $D^2 = D$.

It is also possible to implement the constraints for each brick during the global matrix assembly. In this case, the total number of basis functions in each brick is reduced from 108 to 81. The matrix assembly is not done this way because there are many more terms in the intermediate steps as a result of the constraints occurring at the centre of each brick in equation (2.28).

2.3 Simple example illustrating implementation of divergence constraints

The simple example that was solved in chapter 1 is solved here using the new basis functions on a 2×1 mesh to show how the divergence constraints are implemented. Since the problem is two dimensional, there are only three types of constraints – those at the corners, at the midpoint of each edge and in the centre of the rectangles. The nodes for the different field components are shown in figure 2.4. The basis functions and the functional for the curl-curl equation (2.36) are used to set up the S and T matrices

Figure 2.4: Field component nodes for the simple example. Each node has two coefficients, one is for the field (the top number) and one is for the derivative of the field (the bottom number).

in the usual way. It is simplest to impose the divergence constraints after the S and T matrices have been formed. The boundary conditions are imposed after the divergence constraints are imposed. Since the divergence constraints are the main contribution in this thesis, a listing of Matlab [55] code for their implementation to solve the simple example in chapter 1 is given below.

```
dx = 0.5;    % length of each brick in x-direction
dy = 1;      % length of each brick in y-direction

D_centre = speye(38); % initialize matrix containing centre constraints
D_edge = speye(38);   % initialize matrix containing edge constraints
D_corner = eye(38);   % initialize matrix containing corner constraints

% The first row of cen contains the nodes for the centre constraint of
% the left brick, while the second row contains the nodes for the
% centre constraint of the right brick. The coefficients of the centre
% constraint are found in the third row.
cen = [ 4  3 10    9    14    17    20    23;      % nodes
       26 4 29    10    31    33    35    37;      % nodes
       0  1 1/6*dx 1/6*dx dx*dy -dx*dy 1/6*dx 1/6*dx];

% Impose the centre constraint for the left brick, then the right brick.
D_centre( cen(1,1), cen(1,:) ) = cen(3,:);
D_centre( cen(2,1), cen(2,:) ) = cen(3,:);
```

```
% Node 4 occurs in the centre constraint for the right brick, but it is
% eliminated to impose the centre constraint of the left brick. The
% constraint of the right brick is modified so that node 4 is replaced
% by its value from the centre constraint of the left brick.
```

```
D_centre( cen(2,1), cen(2,2) ) = 0;
D_centre( cen(2,1), : ) = D_centre( cen(2,1), : ) ...
    + D_centre( cen(2,2), : );
```

```
% The first three rows of edge_x contain the nodes that are used in the
% edge constraints for edges parallel to the y-axis, which are nodes
% corresponding to values of Ex. The fourth line contains the
% coefficients of the constraints.
```

```
edge_x = [ 9 13 16 19 22; % nodes
           10 15 18 21 24; % nodes
           29 32 34 36 38; % nodes
           0 1.5/dy -1.5/dy 0.25 0.25];
```

```
% The first four rows of edge_y contain the nodes that are used in the
% edge constraints for edges parallel to the x-axis, which are nodes
% corresponding to values of Ey. The fifth line contains the
% coefficients of the constraints.
```

```
edge_y = [ 20 1 2 7 8; % nodes
           23 5 6 11 12; % nodes
           35 2 25 8 28; % nodes
           37 6 27 12 30; % nodes
           0 1.5/dx -1.5/dx 0.25 0.25];
```

```
% Modify the matrix D_edge so that it contains the edge constraints.
```

```
for ii=1:3
    D_edge( edge_x(ii,1), edge_x(ii,:) ) = edge_x(4,:);
end
for ii=1:4
    D_edge( edge_y(ii,1), edge_y(ii,:) ) = edge_y(5,:);
end
```

```
% The first six rows of corner contain the nodes that are used in the
% corner constraints. The seventh line contains the coefficients of
% the constraints.
```

```
corner = [ 7 19; % nodes
           8 21; % nodes
           11 22; % nodes
           12 24; % nodes
           28 36; % nodes
           30 38; % nodes
           0 -1];
```

```

% Modify the matrix D_corner so that it contains the corner constraints.
for ii=1:6
    D_corner( corner(ii,1), corner(ii,:) ) = corner(7,:);
end

% Nodes that are eliminated to impose the corner constraints are found
% in the edge constraints. Similarly, nodes that are eliminated to
% impose the edge constraints are found in the centre constraints.
D = D_centre * D_edge * D_corner;

% The S and T matrices are defined in another part of the code.
% SD and TD are modified versions that contain the divergence
% constraints.
SD = D' * S * D;
TD = D' * T * D;

```

Observe that the constraint at the midpoint of the edge where node 10 is eliminated involves nodes 2, 6, 8 and 12. The constraint occurs for the left brick and the right brick but it is the same linear combination of the same nodes in both cases, and so it only needs to be implemented once. This preserves the sparsity of the S and T matrices. The same is true at the corner of each brick. For example the coefficient for node 8 is replaced by the negative of the coefficient of node 21. This constraint occurs for both bricks but it is the same for each.

In the example, the constraint at the centre of the left brick was imposed by eliminating node 4, which occurs in the constraint at the centre of the brick on the right so it had to be replaced there as well. If the mesh was 3×1 then node 26 would have to be replaced in the constraint at the centre of the third brick. In general, the procedure is repeated until the end of the mesh is reached. It is this process that reduces the sparsity of the reduced S and T matrices. The sparsity is greatest if the nodes are eliminated in the direction with the least amount of bricks in the mesh because the sum in equation (2.28) will then contain the least number of terms. In the simple example, this would mean implementing the centre constraints by moving in the y -direction. In that case, the sum in equation (2.28) involves only 1 brick. Instead, the centre constraints were

Table 2.3: Eigenvalues, k^2 , of two dimensional square cavity with sides of unit length. Multiplicity in parentheses.

Exact	Without divergence constraints	With divergence constraints	Classification of FEM modes
	0.0733 (1)		spurious
	0.1878 (1)		spurious
	2.6327 (1)		spurious
9.8696 (2)	9.9438 (1), 10.0000 (1)	9.9438 (1), 10.0000 (1)	physical
19.7392 (1)	19.8529 (1)	19.8498 (1)	physical
39.4784 (2)	40.0000 (1)	40.0000 (1)	physical
49.3480 (2)	49.8122 (1)	49.8118 (1)	physical
78.9568 (1)			
88.8264 (2)			
98.6960 (2)			
128.3049 (2)	128.7228 (1), 136.1078 (1)	128.7228 (1), 135.3372(1)	physical

imposed by moving in the x -direction because there are 2 bricks in that direction. As a result, the sum in equation (2.28) has more terms, which is what happens if the mesh is larger, that is, not 2×1 .

After the divergence constraints and the boundary conditions are imposed, the matrices are 7×7 . The results of the calculation are shown in table 2.3, and indicate that the divergence constraints eliminate the spurious modes.

It is interesting to note that the eigenvalues that are computed using the 2×1 mesh are not the lowest possible values. This is caused by limited flexibility of the basis functions arising from the unsymmetric, coarse mesh. There is greater flexibility in the x -direction than the y -direction. Consequentially, modes that oscillate more rapidly along the y -direction are absent from the spectrum.

2.4 Cavity problem

The main test problem for the basis functions in this thesis is to calculate the resonant frequencies and fields for a cavity. This is because spurious modes will occur if the divergence is not solved simultaneously with the curl equation, as discussed in chapter 1. The functionals used in the Rayleigh-Ritz formulation of this problem were given by Berk in 1956 [39]. Some of the details are repeated here to emphasize that the divergence equation does not emerge from varying the functional and also to discuss the boundary conditions.

Either the electric field $\mathbf{E}$ or the magnetic field $\mathbf{H}$ can be used for the calculation. The boundary conditions for each field are different and there are situations where it is more advantageous to use one than the other, so each are discussed separately. The physical interpretation of the functional is discussed in Appendix B.

2.4.1 Electric Field Formulation

Recall that the time-harmonic form of the electric field $\mathbf{E}(\mathbf{r})$ is defined such that $\mathbf{E}(\mathbf{r}, t) = \text{Re}\{\mathbf{E}(\mathbf{r})e^{j\omega t}\}$, where $\text{Re}\{\cdot\}$ indicates the real part of the expression in brackets. Note that, in general, $\mathbf{E}(\mathbf{r})$ is complex. The eigenvalue equation for time-harmonic form of the electric field is derived from the curl equations below.

$$\frac{1}{\mu} \nabla \times \mathbf{E} - j\omega \mathbf{H} = 0 \quad (2.31)$$

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) - j\omega \nabla \times \mathbf{H} = 0 \quad (2.32)$$

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) - \omega^2 \epsilon \mathbf{E} = 0 \quad (2.33)$$

In the last step above, Ampere's law with the Maxwell displacement term was used with the current density $\mathbf{J}$ set to zero. If ϵ and μ (as well as ω) are real then $\mathbf{E}(\mathbf{r})^*$ also satisfies equation (2.33), which can be shown by taking the complex conjugate of each

term in that equation. The volume charge density inside of the cavity is zero and so the divergence equation for the electric field is given by

$$\nabla \cdot (\epsilon \mathbf{E}) = 0. \quad (2.34)$$

If ϵ is real then $\mathbf{E}(\mathbf{r})^*$ satisfies the same divergence equation. Since the walls of the cavity are perfectly conducting then the tangential component of the electric field at the boundary is zero. This is equivalent to

$$\mathbf{n} \times \mathbf{E} = 0 \quad (2.35)$$

where $\mathbf{n}$ is the unit normal vector pointing out of the cavity. Note that $\mathbf{E}(\mathbf{r})^*$ satisfies the same boundary conditions as $\mathbf{E}(\mathbf{r})$.

If ϵ and μ are real then the following functional has stationary functions $\mathbf{E}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})^*$ that satisfy the eigenvalue equation (2.33) and the boundary condition (2.35), although nothing is implied about the divergence of the field.

$$F(\mathbf{E}) = \iiint \left[\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \mathbf{E} \right] dV \quad (2.36)$$

The stationary functions can be found by evaluating F at $\mathbf{E} + \delta \mathbf{E}$ and requiring that the terms that are linear in $\delta \mathbf{E}$ and $\delta \mathbf{E}^*$, called the first variation, are set to zero. (The analogy with a function of one real variable $f(x)$ is that if there is a stationary point at x_0 , that is, if $df/dx = 0$ at $x = x_0$, then the first order term in the Taylor series expansion of $f(x_0 + \alpha)$ about x_0 vanishes. For more details on the calculus of variations, the reader may consult the text by Courant and Hilbert, volume 1, chapter 4 [40].)

$$\begin{aligned} F(\mathbf{E} + \delta \mathbf{E}) = & \iiint \frac{1}{\mu} (\nabla \times (\mathbf{E}^* + \delta \mathbf{E}^*)) \cdot (\nabla \times (\mathbf{E} + \delta \mathbf{E})) \\ & - \omega^2 \epsilon (\mathbf{E}^* + \delta \mathbf{E}^*) \cdot (\mathbf{E} + \delta \mathbf{E}) dV \end{aligned} \quad (2.37)$$

$$\begin{aligned}
&= \iiint \left[\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \mathbf{E} \right] dV \\
&+ \iiint \left[\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \delta \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \delta \mathbf{E} \right] dV \\
&+ \iiint \left[\frac{1}{\mu} (\nabla \times \delta \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \delta \mathbf{E}^* \cdot \mathbf{E} \right] dV \\
&+ \iiint \left[\frac{1}{\mu} (\nabla \times \delta \mathbf{E}^*) \cdot (\nabla \times \delta \mathbf{E}) - \omega^2 \epsilon \delta \mathbf{E}^* \cdot \delta \mathbf{E} \right] dV \quad (2.38) \\
&= F(\mathbf{E}) + \delta F + F(\delta \mathbf{E}) \quad (2.39)
\end{aligned}$$

The first variation δF , containing the terms that are linear in $\delta \mathbf{E}$ and $\delta \mathbf{E}^*$, can be manipulated further.

$$\begin{aligned}
\delta F &= \iiint \left[\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \delta \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \delta \mathbf{E} \right] dV \\
&+ \iiint \left[\frac{1}{\mu} (\nabla \times \delta \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \delta \mathbf{E}^* \cdot \mathbf{E} \right] dV \quad (2.40)
\end{aligned}$$

$$\begin{aligned}
&= \iiint \nabla \cdot \left[\delta \mathbf{E} \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) \right] dV \\
&+ \iiint \left[\delta \mathbf{E} \cdot \nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) - \omega^2 \epsilon \mathbf{E}^* \cdot \delta \mathbf{E} \right] dV \\
&+ \iiint \nabla \cdot \left[\delta \mathbf{E}^* \times \frac{1}{\mu} (\nabla \times \mathbf{E}) \right] dV \\
&+ \iiint \left[\delta \mathbf{E}^* \cdot \nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} \cdot \delta \mathbf{E}^* \right] dV \quad (2.41)
\end{aligned}$$

$$\begin{aligned}
&= \iint \left[\delta \mathbf{E} \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) \right] \cdot \mathbf{n} dS \\
&+ \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) - \omega^2 \epsilon \mathbf{E}^* \right] \cdot \delta \mathbf{E} dV \\
&+ \iint \left[\delta \mathbf{E}^* \times \frac{1}{\mu} (\nabla \times \mathbf{E}) \right] \cdot \mathbf{n} dS \\
&+ \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} \right] \cdot \delta \mathbf{E}^* dV \quad (2.42)
\end{aligned}$$

$$\begin{aligned}
 &= \iint (\mathbf{n} \times \delta \mathbf{E}) \cdot \frac{1}{\mu} (\nabla \times \mathbf{E}^*) dS \\
 &+ \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) - \omega^2 \epsilon \mathbf{E}^* \right] \cdot \delta \mathbf{E} dV \\
 &+ \iint (\mathbf{n} \times \delta \mathbf{E}^*) \cdot \frac{1}{\mu} (\nabla \times \mathbf{E}) dS \\
 &+ \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} \right] \cdot \delta \mathbf{E}^* dV
 \end{aligned} \tag{2.43}$$

Equation (2.41) follows from equation (2.40) using the vector identity $\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B})$. The divergence theorem is used in between equation (2.41) and equation (2.42). The order of the vectors in the vector triple product occurring in the integrand of the surface integral is cycled to arrive at equation (2.43).

If the tangential component of the electric field is fixed on the boundary then that quantity does not vary and so $\mathbf{n} \times \delta \mathbf{E} = 0$. In this problem, $\mathbf{n} \times \mathbf{E} = 0$ and $\mathbf{n} \times \mathbf{E}^* = 0$, that is, the tangential component of the electric field is set to a constant (which happens to be zero) and thus the tangential component is fixed. This means that the surface integrals in equation (2.43) are zero and so the first variation can be simplified further.

$$\begin{aligned}
 \delta F &= \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) - \omega^2 \epsilon \mathbf{E}^* \right] \cdot \delta \mathbf{E} dV \\
 &+ \iiint \left[\nabla \times \frac{1}{\mu} (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E} \right] \cdot \delta \mathbf{E}^* dV
 \end{aligned} \tag{2.44}$$

If the first variation is zero for all variations $\delta \mathbf{E}$ and $\delta \mathbf{E}^*$ then, from the fundamental lemma of the calculus of variations [40], the eigenvalue equation (2.33) is obtained for *both* $\mathbf{E}$ and $\mathbf{E}^*$. This is why it is necessary that ϵ and μ be real, because otherwise $\mathbf{E}^*$ would not satisfy equation (2.33). However, in this procedure nothing is required of the divergence of the electric field or $\nabla \cdot (\epsilon \mathbf{E})$. Unless this is accounted for separately, for example, as a constraint, then there will be spurious modes as discussed in chapter 1.

Since $\epsilon_0 \approx 8.854 \times 10^{-12}$ F/m and $\mu_0 = 4\pi \times 10^{-7}$ N/A² then the two terms in the functional (2.36) are approximately 17 orders of magnitude different for the lowest

frequency modes. The large disparity of the two terms in the eigenvalue equation causes inaccuracy in the eigenvalue solver. To remedy this, the functional is multiplied by μ_0 and the eigenvalue is changed to the square of the magnitude of the wavevector $k^2 = \omega^2/c^2$, where $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light. The rescaled functional in terms of the relative permeability μ_r and the relative permittivity ϵ_r is given below and it is the one used in the numerical calculations.

$$F(\mathbf{E}) = \iiint \left[\frac{1}{\mu_r} |\nabla \times \mathbf{E}|^2 - k^2 \epsilon_r |\mathbf{E}|^2 \right] dV \quad (2.45)$$

Note that for the lowest eigenvalues, $k^2 \approx (2\pi/d)^2$ where d is an estimate of the size (length) of the cavity.

If the coefficients of the basis functions are contained in the column matrix x then, in the electric field formulation, the S matrix is defined by

$$x^T S x = \iiint \frac{1}{\mu_r} |\nabla \times \mathbf{E}|^2 dV \quad (2.46)$$

and the T matrix is defined by

$$x^T T x = \iiint \epsilon_r |\mathbf{E}|^2 dV. \quad (2.47)$$

In the electric field formulation, the nodes for the derivatives that occur in the basis functions (2.14)–(2.16) are zero on the surface of a perfect conductor. It is easiest to see why with a specific example. If the boundary is a plane for which the Cartesian coordinate z is a constant then $E_x = 0$ and $E_y = 0$ for all (x, y) in the plane. Since the values of E_x and E_y are fixed in the plane then their derivatives in the directions tangential to the plane are also zero, that is, $\partial E_x/\partial x = 0$, $\partial E_x/\partial y = 0$, $\partial E_y/\partial x = 0$ and $\partial E_y/\partial y = 0$. Since $\partial E_x/\partial x = 0$ and $\partial E_y/\partial y = 0$ then $\nabla \cdot \mathbf{E} = 0$ implies that $\partial E_z/\partial z = 0$.

The differential equations of a variational problem are called the Euler equations [40]. Rather than perform the variation of the functional to derive the Euler equations and then solve them approximately, the functional itself is first approximated, in this case, by requiring the function $\mathbf{E}$ to be a linear combination of piecewise continuous polynomials, and then choosing the coefficients to make the approximation of the functional stationary. The functional becomes an ordinary function of the coefficients x ,

$$F(x) = x^T S x - k^2 x^T T x \quad (2.48)$$

and the partial derivatives with respect to the different coefficients are required to vanish. This is a special case of the Rayleigh-Ritz method. (In general, the Rayleigh-Ritz method is not restricted to a linear combination of piecewise continuous polynomials.)

2.4.2 Magnetic Field Formulation

The resonant frequencies of a cavity can also be calculated using the magnetic field formulation. The derivation is similar to that for the electric field and so it is not given in detail. The eigenvalue equation and the divergence equation are listed below.

$$\nabla \times \left(\frac{1}{\epsilon} \nabla \times \mathbf{H} \right) - \omega^2 \mu \mathbf{H} = 0 \quad (2.49)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad (2.50)$$

The boundary condition for the magnetic field is different than that for the electric field. If the tangential component of the electric field is zero at the surface of a perfect conductor, then Faraday's law implies that $\omega \mathbf{H} \cdot \mathbf{n} = 0$ for a time-harmonic field, that is, if $\omega \neq 0$ then $\mathbf{H} \cdot \mathbf{n} = 0$. (Note that, in general, $\mathbf{H} \cdot \mathbf{n} \neq 0$ for a static field.) As a specific example, let the boundary lie in a plane where the Cartesian coordinate z is a constant. This means that $E_x = 0$ and $E_y = 0$ for all (x, y) in the plane, and so also that $\partial E_x / \partial y = 0$

and $\partial E_y / \partial x = 0$. However, from Faraday's law, $\partial E_y / \partial x - \partial E_x / \partial y = -j\omega\mu H_z$ and so $j\omega\mu H_z = 0$. Thus, if $\omega \neq 0$ then $H_z = 0$.

The functional for the magnetic field is

$$F(\mathbf{H}) = \iiint \left[\frac{1}{\epsilon} |\nabla \times \mathbf{H}|^2 - \omega^2 \mu |\mathbf{H}|^2 \right] dV. \quad (2.51)$$

The first variation results in terms that are similar to equation (2.43) for the electric field.

$$\begin{aligned} \delta F &= \iint (\mathbf{n} \times \delta \mathbf{H}) \cdot \frac{1}{\epsilon} (\nabla \times \mathbf{H}^*) dS \\ &+ \iiint \left[\nabla \times \frac{1}{\epsilon} (\nabla \times \mathbf{H}^*) - \omega^2 \mu \mathbf{H}^* \right] \cdot \delta \mathbf{H} dV \\ &+ \iint (\mathbf{n} \times \delta \mathbf{H}^*) \cdot \frac{1}{\epsilon} (\nabla \times \mathbf{H}) dS \\ &+ \iiint \left[\nabla \times \frac{1}{\epsilon} (\nabla \times \mathbf{H}) - \omega^2 \mu \mathbf{H} \right] \cdot \delta \mathbf{H}^* dV \end{aligned} \quad (2.52)$$

The boundary condition is $\mathbf{H} \cdot \mathbf{n} = 0$, which does *not* imply that $\mathbf{n} \times \delta \mathbf{H} = 0$. However, $\nabla \times \mathbf{H} = j\omega\epsilon \mathbf{E}$ and so the integrand of the first surface integral can be expressed as $j\omega(\mathbf{n} \times \mathbf{E}^*) \cdot \delta \mathbf{H}$ and the integrand of the second surface integral can be expressed as $-j\omega(\mathbf{n} \times \mathbf{E}) \cdot \delta \mathbf{H}^*$. The integrands of the surface integrals are zero because $\mathbf{n} \times \mathbf{E} = 0$ on the boundary, however, this does not result from setting $\mathbf{H} \cdot \mathbf{n} = 0$ on the boundary. Instead, this is part of the solution of the variational problem: the integrands of the surface integrals of the approximate solution will be close to zero in the same way that the integrand of the volume integral, which is the differential equation itself, is close to zero. This is called a natural boundary condition. In the case of the magnetic field formulation, the natural boundary condition is $\mathbf{n} \times \frac{1}{\epsilon} (\nabla \times \mathbf{H}) = 0$. If the surface integral is zero as a result of constraining the basis functions on the boundary, for example, setting $\mathbf{n} \times \mathbf{E} = 0$ in the electric field formulation, then the boundary condition is referred to as fixed, artificial or rigid, as in Courant's original FEM paper [1], or essential or principal,

as, for example, in the text by Silvester and Ferrari [9].

The functional is rescaled in the same way as the functional for the electric field formulation.

$$F(\mathbf{H}) = \iiint \left[\frac{1}{\epsilon_r} |\nabla \times \mathbf{H}|^2 - k^2 \mu_r |\mathbf{H}|^2 \right] dV \quad (2.53)$$

If the coefficients of the basis functions are contained in the column matrix x then, in the magnetic field formulation, the S matrix is defined by

$$x^T S x = \iiint \frac{1}{\epsilon_r} |\nabla \times \mathbf{H}|^2 dV \quad (2.54)$$

and the T matrix is defined by

$$x^T T x = \iiint \mu_r |\mathbf{H}|^2 dV. \quad (2.55)$$

Whereas in the case of the electric field formulation the derivative terms that occur in the basis functions are set to zero on the boundary, there are no such constraints for the magnetic field formulation.

The coefficient c_{211}^x is eliminated to implement the divergence constraint at the node in the centre of the brick, equation (2.27). However, this is also one of the coefficients that needs to be set to zero in the case where the boundary of a perfect conductor is in the plane where x is a constant. Should the coefficient c_{211}^x be eliminated to satisfy the divergence constraint or the boundary condition? If the divergence constraints are not implemented then there are spurious modes. If the boundary conditions are not implemented, then there are also spurious modes [20].

The boundary condition $\mathbf{H} \cdot \mathbf{n} = 0$ is derived from the condition that $\mathbf{n} \times \mathbf{E} = 0$. Another way to accomplish this is to set $\mathbf{n} \times (\nabla \times \mathbf{H}) = 0$, since this is proportional to the tangential component of the electric field through the curl equation (1.15). Notice that this is also the natural boundary condition that occurs in the surface integral of the

first variation, equation (2.52). Consider the component $(\nabla \times \mathbf{H})_z = \partial H_y / \partial x - \partial H_x / \partial y$ on a boundary where x is a constant. For a given brick, there are 9 nodes of the component H_x on the boundary and all 9 of the coefficients should be set to zero, which would imply that $H_x = 0$ and so $\partial H_x / \partial y = 0$ and $\partial H_x / \partial z = 0$ on that face of the brick. If that were true of the derivative terms, then the natural boundary condition would reduce to $\partial H_y / \partial x = 0$ on the boundary. Since it *should* be true, as $H_x = 0$ for the correct solution, then it can be set to zero as a principal boundary condition. The natural boundary condition reduces to $\partial H_x / \partial y = 0$ with $\partial H_y / \partial x = 0$ as a principal boundary condition. Similarly, the component $(\nabla \times \mathbf{H})_y = \partial H_z / \partial x - \partial H_x / \partial z$ occurs in the natural boundary condition, and so setting $\partial H_z / \partial x = 0$ as a principal boundary condition reduces the natural boundary condition to $\partial H_x / \partial z = 0$. Now the natural boundary condition is $\partial H_x / \partial y = 0$ and $\partial H_x / \partial z = 0$ and when this is combined with the fact that $H_x = 0$ is set explicitly for 8 out of the 9 nodes on the boundary, then the combination of boundary conditions implies that $H_x = 0$ on the entire surface.

As noted by Konrad [20], if the boundary condition $\mathbf{H} \cdot \mathbf{n} = 0$ is not satisfied then there will be spurious modes. What was entirely a principal boundary condition, $H_x = 0$, now occurs as a combination of principal boundary conditions and natural boundary conditions. Natural boundary conditions will not be satisfied exactly, in the same way that the Euler equation is not satisfied exactly. Consequently, there are still some spurious modes with this method, although they occur higher in the spectrum. An example considered below is a cubic cavity with a $12 \times 12 \times 12$ mesh. In that case, without the principal boundary conditions $\partial H_y / \partial x = 0$ and $\partial H_z / \partial x = 0$, the lowest frequency spurious modes occur as the 12th and 13th modes but with the principal boundary conditions already mentioned, the lowest frequency spurious modes are pushed up to the 86th and 87th lowest modes. This is discussed in further detail in subsection 2.5.1, as well as techniques for identifying spurious modes that arise in this manner. To be clear, the additional principal constraints that are discussed above do not eliminate the spurious modes but

the result is that they are pushed higher into the spectrum.

The derivation of the constraint $\partial H_y / \partial x = 0$ is done using the notation where the global coordinates are labeled by (x, y, z) and the local coordinates for a particular brick are labeled by (x', y', z') . The boundary under consideration lies in the plane $x' = 1$ and where x is a maximum for given values of y and z . Since

$$H_y(x', y', z') = \sum_{i=0}^2 \sum_{j=0}^3 \sum_{k=0}^2 c_{ijk}^y \Delta_{yj} L_i(x') H_j(y') L_k(z') \quad (2.56)$$

then

$$\frac{\partial H_y}{\partial x}(x, y, z) = \frac{1}{\delta_x} \frac{\partial H_y}{\partial x'}(x', y', z') \quad (2.57)$$

$$= \sum_{i=0}^2 \sum_{j=0}^3 \sum_{k=0}^2 c_{ijk}^y \Delta_{yj} \frac{1}{\delta_x} \frac{dL_i}{dx'}(x') H_j(y') L_k(z') \quad (2.58)$$

$$= 0 \quad (2.59)$$

at $x' = 1$ for all (y', z') within the particular brick. Since this is true for all (y', z') then

$$0 = \sum_{i=0}^2 c_{ijk}^y \frac{\Delta_{yj}}{\delta_x} \frac{dL_i}{dx'}(1) \quad (2.60)$$

$$= \frac{\Delta_{yj}}{\delta_x} (c_{0jk}^y - 4c_{1jk}^y + 3c_{2jk}^y) \quad (2.61)$$

which can be implemented by requiring that

$$c_{2jk}^y = \frac{4}{3}c_{1jk}^y - \frac{1}{3}c_{0jk}^y. \quad (2.62)$$

Similarly, the constraint $\partial H_z / \partial x = 0$ on the boundary can be implemented by requiring that

$$c_{2jk}^z = \frac{4}{3}c_{1jk}^z - \frac{1}{3}c_{0jk}^z. \quad (2.63)$$

Note that c_{111}^y , c_{131}^y , c_{111}^z and c_{113}^z are replaced with the divergence constraints that occur

on the centre of each face. The coefficients c_{110}^y , c_{112}^y , c_{130}^y and c_{132}^y are replaced to implement divergence constraints at the midpoints of each edge. The constraints (2.62) and (2.63) must be modified so that those coefficients are replaced by the appropriate divergence constraints, which is not difficult.

2.4.3 Choice of field formulation

If the permittivity ϵ is discontinuous then so is the normal component of the electric field $\mathbf{E}$, although the tangential components are continuous. The basis functions can accomodate this discontinuity in $\mathbf{E}$ at a planar interface, as discussed in section 2.6. However, the situation is worse if the discontinuity forms an edge or a corner. If the permittivity (permeability) is discontinuous at an edge, the electric (magnetic) field is infinite and varies rapidly in direction [57]. This behaviour is impossible to model using polynomials. However, it is possible that only the permittivity is discontinuous, including at edges, while the permeability is continuous throughout the domain. In this case, the magnetic field is continuous, and moreover, its magnitude is finite, in spite of the fact that the electric field is infinite. Situations such as these occur in optics (see, for example, the article by Kejalakshmy *et. al.* [18], where the penalty method is used) and in radio frequency applications (see, for example, the resonators developed by Zhang and Mansour [51–53]).

Finally, it is worth noting that the Rayleigh-Ritz formulation of the problem is equivalent to the discretization of the weak formulation of the problem in cases where the operator is self-adjoint and the test functions are identical to the basis functions.

2.5 Resonant cavity examples with continuous field

In this section, the resonant frequencies for several different cavities are calculated and compared with exact solutions in cases where they exist. All of the cavities are rectangular

boxes with walls that are perfect conductors. In the first example, which is an empty cavity, both the electric and magnetic field formulations are used because they are both continuous. Subsequent examples contain dielectric materials of different shapes. In this section, only the magnetic field formulation is used for these problems, since $\mathbf{H}$ is continuous whereas $\mathbf{E}$ is not.

2.5.1 Empty cubic cavity

The first example is a cavity in the shape of an empty cube. This problem can be solved exactly using separation of variables. (See, for example, the text by Wangsness [45].) If the cube has sides of unit length, then the eigenvalues are

$$k^2 = \pi^2 (n_x^2 + n_y^2 + n_z^2) \quad (2.64)$$

where n_x , n_y and n_z are non-negative integers and more than one of them is non-zero. The eigenvalue k^2 is degenerate because different combinations of n_x , n_y and n_z produce the same eigenvalue. The eigenvalues obtained using the electric field formulation with a $12 \times 12 \times 12$ mesh and 25921 unknowns are shown in table 2.4 along with the exact values. There are no spurious modes. The multiplicity of some of the eigenvalues is not correct. For example, $k^2 = 29.6089 \text{ L}^{-2}$ occurs twice instead of once. This occurred using both the Lanczos algorithm and the Jacobi-Davidson algorithm [41,44] and it even occurred using HFSS, version 11 [46], which uses edge elements.

The calculation is also performed with the magnetic field formulation on a $12 \times 12 \times 12$ mesh. In the first calculation, the constraint for the partial derivatives on the boundary $x = 1$ is *not* imposed. (See the discussion at the end of subsection 2.4.2.) There are 29519 unknowns, which is greater than the number of unknowns using the electric field because there are fewer coefficients set to zero with the boundary condition for the magnetic field. The lowest 23 eigenvalues are found in table 2.5. The eigenvalues corresponding

Table 2.4: Eigenvalues, k^2 , in units of L^{-2} , of cubic cavity using electric field formulation. Multiplicity in parentheses. $12 \times 12 \times 12$ mesh with 25921 unknowns.

Analytical	FEM	FEM Error (%)
19.7392(3)	19.7393(3)	0.0005
29.6088(1)	29.6089(2)	0.0004
49.3480(6)	49.3521(6)	0.008
59.2176(3)	59.2204(3), 59.2218(3)	0.005, 0.007
78.9568(3)	78.9650(3)	0.01
88.8264(3)	88.8306(3), 88.8341(3)	0.005, 0.009
98.6960(6)	98.7416(6)	0.05

to physical modes agree well with the exact values but there are spurious modes present because the boundary condition $H_x = 0$ cannot be imposed on the surface $x = 1$, as discussed in subsection 2.4.2. However, the spurious modes can be identified and discarded using two techniques discussed next.

Two methods for classifying the modes as physical or spurious are considered here. As discussed in subsection 2.4.2, the difficulty is that c_{211}^x is eliminated to impose a divergence constraint and so it cannot be set to zero to satisfy the boundary condition $\mathbf{H} \cdot \mathbf{n} = 0$. There are two methods used to classify the modes. The first is to use the root mean square of the coefficients c_{211}^x that occur on the boundary.

$$\langle c_{211}^x \rangle_{RMS} = \sqrt{\sum_{n=1}^N \frac{(c_{211,n}^x)^2}{N}} \quad (2.65)$$

The sum is over all of the bricks that are against the boundary where x is a maximum, in this example, the surface $x = 1$, and N is the number of bricks against that boundary. As seen in table 2.5, the value of $\langle c_{211}^x \rangle_{RMS}$ is close to 1 for the spurious modes and the value for the physical modes is at least 4 orders of magnitude lower. The spurious modes have much greater values of $\langle c_{211}^x \rangle_{RMS}$ because the spurious modes originate

due to the fact that the boundary condition $H_x = 0$ cannot be imposed on the surface $x = 1$.

The second method to classify the modes is to evaluate the flux of the Poynting vector, $\mathbf{S} = \mathbf{E} \times \mathbf{H}^*/2$, through the boundary. The flux of the Poynting vector is related to the natural boundary condition, as discussed in the previous section. The quantity

$$P = -j\omega \iint (\mathbf{E} \times \mathbf{H}^*) \cdot \mathbf{n} dS \quad (2.66)$$

is evaluated and included in the tables. The spurious modes have surface integrals that are approximately 5 orders of magnitude greater than the physical modes. The fluxes through the individual faces of the cube are omitted for brevity. However, it is observed that the flux through the surface $x = 1$ is the greatest contributor to the total. This is because the boundary condition $H_x = 0$ cannot be imposed on the surface $x = 1$, which is the cause of the spurious modes.

To confirm that the spurious modes are caused by the conflicting demands of the coefficient c_{211}^x , the boundary condition $H_y = 0$ on the surface $y = 1$ is relaxed such that $c_{121}^y = 0$ is not imposed. (This is analogous to $c_{211}^x = 0$ not being imposed on the surface $x = 1$.) The lowest 26 eigenvalues are listed in table 2.6. Spurious modes are observed at even lower frequencies in the spectrum. The flux of the Poynting vector is much greater for the spurious modes than for the physical modes by approximately 5 orders of magnitude, with dominant contributions coming from both surfaces where the principal boundary conditions are not enforced. The root mean square quantity is modified to include contributions of c_{121}^y from the surface $y = 1$.

$$< c^{xy} >_{RMS} = \sqrt{\frac{\sum_{n=1}^{N_x} (c_{211,n}^x)^2 + \sum_{n=1}^{N_y} (c_{121,n}^y)^2}{N_x + N_y}} \quad (2.67)$$

The first sum is over the number of bricks N_x bricks on the surface $x = 1$ and the second

Table 2.5: Eigenvalues, k^2 , in units of L^{-2} , of cubic cavity using magnetic field formulation. Multiplicity in parentheses. $12 \times 12 \times 12$ mesh with 29519 unknowns. No derivative constraints on boundary $x = 1$. P is defined in equation (2.66) and $\langle c_{211}^x \rangle_{RMS}$ is defined in equation (2.65).

Analytical	FEM	FEM Error (%)	P	$\langle c_{211}^x \rangle_{RMS}$
19.73921(3)	19.739273	0.00001	2.6×10^{-2}	5.3×10^{-8}
19.73921(3)	19.739273	0.00001	2.7×10^{-2}	6.6×10^{-8}
19.73921(3)	19.739273	0.00001	2.6×10^{-2}	7.8×10^{-8}
29.60881(1)	29.608942	0.0002	3.5×10^{-2}	3.8×10^{-8}
29.60881(1)	29.608942	0.0002	3.5×10^{-2}	7.6×10^{-8}
49.34802(6)	49.351291	0.006	1.2×10^{-1}	9.8×10^{-6}
49.34802(6)	49.351291	0.006	1.2×10^{-1}	9.8×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	7.7×10^{-7}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	7.7×10^{-7}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	5.6×10^{-7}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	5.6×10^{-7}
	55.929655	spurious	$2.6 \times 10^{+4}$	5.3×10^{-1}
	55.929655	spurious	$2.6 \times 10^{+4}$	5.3×10^{-1}
59.21762(3)	59.220430	0.005	9.0×10^{-2}	1.0×10^{-5}
59.21762(3)	59.220430	0.005	1.1×10^{-1}	3.1×10^{-6}
59.21762(3)	59.220430	0.005	1.1×10^{-1}	3.1×10^{-6}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	7.5×10^{-8}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	4.2×10^{-9}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	7.5×10^{-8}
	78.824871	spurious	$2.8 \times 10^{+4}$	5.3×10^{-1}
78.95683(3)	78.960924	0.005	1.6×10^{-1}	3.6×10^{-6}
78.95683(3)	78.960924	0.005	1.6×10^{-1}	3.6×10^{-6}
78.95683(3)	78.960924	0.005	1.7×10^{-1}	5.1×10^{-9}

sum is over the number of bricks N_y on the surface $y = 1$. The value of $\langle c^{xy} \rangle_{RMS}$ is close to 1 for the spurious modes and the value for the physical modes is at least 4 orders of magnitude lower.

The principal boundary conditions for the derivatives, $\partial H_y / \partial x = 0$ and $\partial H_z / \partial x = 0$ on the boundary $x = 1$, are imposed with the result that $H_x = 0$ is a combination of principal and natural boundary conditions, as discussed in subsection 2.4.2. The lowest 20 eigenvalues are listed in table 2.7. The eigenvalues of the spurious modes have increased and are not found below 78.95683, which is the greatest eigenvalue in the table. For the physical modes shown in the table, the quantities $\langle c_{211}^x \rangle_{RMS}$ are much less than 1. The lowest frequency spurious modes occur at mode numbers 86 and 87 and the quantity $\langle c_{211}^x \rangle_{RMS}$ is 2.9×10^{-1} , which is 3 orders of magnitude greater than for all of the physical modes up to mode number 100. The flux of the Poynting vector is relatively small compared to the values for the spurious modes found in table 2.5 and table 2.6, and its magnitude is comparable for all of the physical modes. The flux of the Poynting vector is 2.3×10^2 for both spurious modes 86 and 87, which is 3 orders of magnitude greater than for all of the physical modes up to mode number 100.

2.5.2 Cavity with dielectric post

The next example is a rectangular dielectric box or post mounted inside of a rectangular box that has perfectly conducting walls. The relative permittivity of the dielectric post is $\epsilon_r = 2.05$. The dimensions of the cavity are shown in figure 2.5. This geometry does not allow for separation of variables and an exact solution for the resonant frequencies does not exist at this point in time. This example is chosen because it has been analyzed previously by Lee and Mittra in 1992 using edge elements [50] and by Albani and Bernardi in 1974 using a finite difference method for an integral equation [49]. The paper by Albani and Bernardi also contains an experimental measurement, which is exceptionally valuable because it creates a test problem with a non-trivial geometry. The experimental

Table 2.6: Eigenvalues, k^2 , in units of L^{-2} , of cubic cavity using magnetic field formulation. Multiplicity in parentheses. $12 \times 12 \times 12$ mesh with 29663 unknowns. No derivative constraints on boundary $x = 1$ and c_{121}^y not set to zero on boundary $y = 1$. P is defined in equation (2.66) and $\langle c^{xy} \rangle_{RMS}$ is defined in equation (2.67).

Analytical	FEM	FEM Error (%)	P	$\langle c^{xy} \rangle_{RMS}$
19.73921(3)	19.739273	0.00001	2.6×10^{-2}	5.2×10^{-8}
19.73921(3)	19.739273	0.00001	2.6×10^{-2}	7.5×10^{-8}
19.73921(3)	19.739273	0.00001	2.6×10^{-2}	7.5×10^{-8}
29.60881(1)	29.608942	0.0002	3.5×10^{-2}	8.1×10^{-8}
29.60881(1)	29.608942	0.0002	3.5×10^{-2}	6.7×10^{-8}
	36.664159	spurious	$2.1 \times 10^{+4}$	3.9×10^{-1}
	39.386198	spurious	$2.0 \times 10^{+4}$	3.9×10^{-1}
	41.692555	spurious	$2.4 \times 10^{+4}$	3.7×10^{-1}
49.34802(6)	49.351291	0.006	1.3×10^{-1}	2.8×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	1.3×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	6.7×10^{-7}
49.34802(6)	49.351291	0.006	1.3×10^{-1}	2.8×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	2.8×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	3.6×10^{-6}
59.21762(3)	59.220429	0.005	9.6×10^{-2}	1.9×10^{-5}
59.21762(3)	59.220429	0.005	9.2×10^{-2}	8.9×10^{-6}
59.21762(3)	59.220430	0.005	1.2×10^{-1}	7.8×10^{-6}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	6.2×10^{-8}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	6.9×10^{-8}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	8.2×10^{-8}
	65.208591	spurious	$2.4 \times 10^{+4}$	3.8×10^{-1}
	66.974561	spurious	$2.6 \times 10^{+4}$	3.7×10^{-1}
	70.284228	spurious	$1.7 \times 10^{+4}$	4.1×10^{-1}
78.95683(3)	78.960924	0.005	1.6×10^{-1}	4.2×10^{-6}
78.95683(3)	78.960924	0.005	1.6×10^{-1}	2.1×10^{-6}
78.95683(3)	78.960924	0.005	1.7×10^{-1}	4.5×10^{-6}

Table 2.7: Eigenvalues, k^2 , in units of L^{-2} , of cubic cavity using magnetic field formulation. Multiplicity in parentheses. $12 \times 12 \times 12$ mesh with 28319 unknowns. Derivative constraints on boundary $x = 1$. P is defined in equation (2.66) and $\langle c_{211}^x \rangle_{RMS}$ is defined in equation (2.65).

Analytical	FEM	FEM Error (%)	P	$\langle c_{211}^x \rangle_{RMS}$
19.73921(3)	19.739273	0.00001	2.7×10^{-2}	1.4×10^{-11}
19.73921(3)	19.739273	0.00001	2.0×10^{-2}	1.1×10^{-6}
19.73921(3)	19.739273	0.00001	2.0×10^{-2}	1.1×10^{-6}
29.60881(1)	29.608942	0.0002	3.2×10^{-2}	1.0×10^{-6}
29.60881(1)	29.608942	0.0002	2.7×10^{-2}	4.1×10^{-12}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	1.1×10^{-7}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	1.1×10^{-7}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	1.0×10^{-6}
49.34802(6)	49.351291	0.006	1.4×10^{-1}	1.0×10^{-6}
49.34802(6)	49.351319	0.006	7.1×10^{-2}	1.6×10^{-5}
49.34802(6)	49.351319	0.006	7.1×10^{-2}	1.6×10^{-5}
59.21762(3)	59.220430	0.005	1.0×10^{-1}	1.1×10^{-6}
59.21762(3)	59.220430	0.005	1.0×10^{-1}	1.1×10^{-6}
59.21762(3)	59.220454	0.005	6.2×10^{-2}	1.8×10^{-5}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	6.4×10^{-7}
59.21762(3)	59.221754	0.007	1.5×10^{-1}	6.4×10^{-7}
59.21762(3)	59.221790	0.007	7.9×10^{-2}	1.7×10^{-14}
78.95683(3)	78.960924	0.005	1.7×10^{-1}	7.2×10^{-13}
78.95683(3)	78.960943	0.005	1.2×10^{-1}	1.9×10^{-5}
78.95683(3)	78.960943	0.005	1.2×10^{-1}	1.9×10^{-5}

Figure 2.5: Cavity with dielectric post.

measurement for the lowest frequency mode is $k^2 = 27.2 \text{ L}^{-2}$ and the computed value by the same authors is $k^2 = 30.8 \text{ L}^{-2}$, while Lee and Mittra obtained $k^2 = 26.62 \text{ L}^{-2}$.

The problem is solved with the new basis functions (2.14)–(2.16) using the magnetic field formulation. Results obtained with an $8 \times 10 \times 12$ mesh are listed in table 2.8. There were 16663 unknowns. None of the eigenvalues are degenerate due to a lack of symmetry. The principal boundary conditions for the derivatives were not used. There is one spurious mode among the 10 lowest frequency modes, which is easily identified by the flux of the Poynting vector and $\langle c_{211}^x \rangle_{RMS}$.

The lowest resonant frequency is also computed for several other meshes and the results are listed in table 2.9. This problem was also solved using HFSS [46] for several meshes, with the adaptive mesh refinement feature turned *off*. The reason for turning off the adaptive mesh refinement is that adaptive mesh refinement is not used with the new basis functions either. Results were obtained from HFSS using first and second order edge elements. They are plotted together with the results from the new basis functions in figure 2.6.

This example brings attention to the accuracy of different numerical methods as well

Table 2.8: Eigenvalues, k^2 , in units of L^{-2} , of cavity with dielectric post with $8 \times 10 \times 12$ and 16663 unknowns. P is defined in equation (2.66) and $\langle c_{211}^x \rangle_{RMS}$ is defined in equation (2.65).

Eigenvalue	P	$\langle c_{211}^x \rangle_{RMS}$
30.9385	1.2×10^{-1}	2.3×10^{-6}
49.6728	1.6×10^{-1}	7.5×10^{-6}
53.0827	$1.3 \times 10^{+5}$	6.9×10^{-1}
56.3392	2.6×10^{-1}	9.8×10^{-6}
62.6955	5.0×10^{-1}	1.5×10^{-5}
78.0231	3.3×10^{-1}	1.9×10^{-5}
79.8877	2.7×10^{-1}	6.2×10^{-6}
85.4794	1.7×10^{-1}	6.4×10^{-6}
101.3371	7.0×10^{-1}	1.2×10^{-5}
103.3675	1.5×10^{-2}	1.1×10^{-4}

Table 2.9: Lowest eigenvalue, k^2 , in units of L^{-2} , of cavity with dielectric post.

Mesh	Unknowns	Eigenvalue
$2 \times 3 \times 3$	380	31.1329
$8 \times 10 \times 8$	11215	30.9415
$8 \times 10 \times 16$	22111	30.9376
$8 \times 10 \times 20$	27559	30.9372
$16 \times 10 \times 20$	54119	30.9363

Figure 2.6: Cavity with dielectric post.

as the comparison with experimental measurements. In table 2.9, the lowest eigenvalue computed with the new basis functions and a $16 \times 10 \times 20$ mesh is 30.936 L^{-2} while the value obtained with the greatest number of unknowns using HFSS is 30.933 L^{-2} , a difference of only 0.01%. The value $k^2 = 30.8 \text{ L}^{-2}$ computed by Albani and Bernardi using a finite difference approximation for an integral equation differs from the previous two results by only 0.3%. However, the measured value is $k^2 = 27.2 \text{ L}^{-2}$, which is lower than all three methods by about 10%. (The experimental error was not given by Albani and Bernardi [49].) The value obtained by Lee and Mittra using edge elements is $k^2 = 26.62 \text{ L}^{-2}$, which, although differing from the measurement by only 2%, differs from the commercial software package HFSS, which *also uses edge elements*, by about 15%. Additionally, the dimensions of the constructed cavity are not exactly the same as

those given, including, for example, the fact that the metal walls and the faces of the dielectric post have been assumed to be parallel or perpendicular to each other. The dielectric constant of the post, made out of teflon, is also not exactly 2.05 and it may not be uniform throughout the post, specifically near the edges and corners.

2.5.3 Dielectric resonator filter

Examples with more complicated geometry occur, for instance, in the dielectric resonators developed by Zhang and Mansour [51–53]. These resonators consist of a high-K ceramic

Figure 2.7: Dielectric resonator filter. (Not to scale.)

Table 2.10: Eigenvalues, k^2 , in units of L^{-2} , of dielectric resonator filter with $9 \times 24 \times 30$ and 109223 unknowns. P is defined in equation (2.66) and $\langle c_{211}^x \rangle_{RMS}$ is defined in equation (2.65).

New basis functions	P	$\langle c_{211}^x \rangle_{RMS}$	HFSS	Difference
3.5385	2.7×10^{-2}	5.3×10^{-5}	3.5250	0.4%
3.6971	2.2×10^{-2}	4.5×10^{-5}	3.6668	0.8%
3.9523	2.3×10^{-2}	5.5×10^{-5}	3.9122	1.0%
4.7869	2.8×10^{-2}	5.2×10^{-5}	4.7257	1.3%
4.8528	3.3×10^{-2}	6.3×10^{-5}	4.8081	0.9%
4.9269	3.5×10^{-2}	6.1×10^{-5}	4.8765	1.0%
5.8712	4.4×10^{-2}	7.9×10^{-5}	5.8211	0.9%
6.5705	3.5×10^{-2}	6.8×10^{-5}	6.4765	1.4%
6.6893	2.8×10^{-2}	5.3×10^{-5}	6.6378	0.8%
6.7525	5.0×10^{-2}	8.6×10^{-5}	6.6588	1.4%

supported by teflon inside of a rectangular box. The filters that they have described can be modeled using bricks, with the exception of one example where they have cut a circular hole through the high-K ceramic. A diagram of one of the resonators is given in figure 2.7.

The resonant frequencies and fields are solved with the new basis functions using the magnetic field formulation. The magnetic field is continuous because the dielectric materials are non-magnetic. The results obtained with a $9 \times 24 \times 30$ mesh and 109223 unknowns are shown in table 2.10, along side the values obtained with HFSS. There are no spurious modes among the 10 lowest frequency eigenvalues with this mesh. The lowest frequency eigenvalues differ by 0.4% and the 10th lowest eigenvalues differ by 1.4%.

In table 2.11 the eigenvalues for the lowest frequency mode is listed for different meshes and different numbers of unknowns. There is a spurious mode among the lowest 10 modes for the $9 \times 8 \times 15$ mesh and the $18 \times 8 \times 15$ mesh. The eigenvalue of the spurious mode increases as the mesh is refined, which is the same phenomenon that occurs with the

spurious modes that occur with the cubic cavity and the cavity with the dielectric post. Qualitatively, it is because a finer mesh has more degrees of freedom resulting in trial functions with greater flexibility to solve the Euler equation and the natural boundary condition.

Table 2.11: Lowest eigenvalue, k^2 , in units of L^{-2} , of dielectric resonator filter.

Mesh	Unknowns	Eigenvalue
$9 \times 8 \times 15$	18707	3.6083
$18 \times 8 \times 15$	36815	3.6056
$9 \times 16 \times 15$	36875	3.5865
$9 \times 16 \times 30$	73175	3.5412
$9 \times 24 \times 30$	109223	3.5385

Zhang and Mansour used HFSS to simulate the frequency response of their filters and they have plotted these results with their experimental measurements. In one of their papers [52] they have noted that they use tuning screws to compensate for the tolerance of the dielectric constant of the high-K ceramic as stated by the manufacturer (38.6 ± 1) and the tolerance for the dimensions as a result of the machining process. A rough estimate from viewing the plots of the S-parameters indicates that, after tuning, the agreement in frequency of the measurements with the HFSS simulation is approximately 0.5%, while in decibels it is much worse. There are multiple sources of experimental error, including, but not limited to, the fact that the surfaces are not perfectly flat, the walls do not intersect at exactly 90° and the dielectrics do not align perfectly with each other and the cavity walls. The point of this discussion is to remark that, from an engineering perspective, it is pointless to simulate these results to an accuracy of less than 0.1%, and 1% is not unreasonable.

2.6 Solving problems with discontinuous fields at planar interfaces

The new basis functions can be used to solve problems where the field is discontinuous at an interface. The interface conditions for the different fields can be found, for example, in the text by Jackson [2]. Suppose that the unit normal is $\mathbf{n} = \mathbf{x}$, where $\mathbf{x}$ is the unit vector parallel to the x -axis. The subscripts 1 and 2 denote field components on either side of the interface such that $\mathbf{n}$ points in the direction from 1 to 2. Since the tangential component of the electric field is continuous, then $E_{y,1} = E_{y,2}$ and $E_{z,1} = E_{z,2}$, which can be imposed with the new basis functions by equating coefficients on either side of the interface. The normal component for the electric flux density satisfies $D_{x,2} - D_{x,1} = \rho_s$, where ρ_s is the free surface charge density on the interface. In terms of the electric field component, $E_{x,2} = (\epsilon_1 E_{x,1} + \rho_s) / \epsilon_2$, and in particular, if $\rho_s = 0$ then $E_{x,2} = (\epsilon_{r,1} / \epsilon_{r,2}) E_{x,1}$. This can be implemented exactly with the new basis functions, for example, $c_{0jk,2}^x = (\epsilon_{r,1} / \epsilon_{r,2}) c_{2jk,1}^x$. Note that this interface condition cannot be imposed using edge elements, even in the case where the electric field is continuous. Rather, the normal components converge to $E_{x,2} = (\epsilon_{r,1} / \epsilon_{r,2}) E_{x,1}$ as the mesh is refined further and further, specifically as the area of that face of the tetrahedron goes to zero [28].

The new basis functions also contain derivative terms that have nodes on the interface. Since E_y and E_z are continuous at all points in the plane then $\partial E_y / \partial y$ and $\partial E_z / \partial z$ are also continuous. Since E_x is discontinuous across the interface then it is not defined at the interface and therefore $\partial E_x / \partial x$ is not defined at the interface either. However, as the interface is approached from either side, limiting values of the partial derivative exist. If the permittivity is constant on either side of the interface then $\nabla \cdot \mathbf{E}_1 = \rho_1 / \epsilon_1$ and $\nabla \cdot \mathbf{E}_2 = \rho_2 / \epsilon_2$, where ρ denotes the volume charge density. Since $\partial E_{y,1} / \partial y = \partial E_{y,2} / \partial y$

and $\partial E_{z,1}/\partial z = \partial E_{z,2}/\partial z$, then upon subtracting the divergence equations, the result

$$\frac{\partial E_{x,2}}{\partial x} = \frac{\partial E_{x,1}}{\partial x} + \frac{\rho_2}{\epsilon_2} - \frac{\rho_1}{\epsilon_1} \quad (2.68)$$

is obtained. If $\rho_1 = 0$ and $\rho_2 = 0$, then $\partial E_{x,1}/\partial x = \partial E_{x,2}/\partial x$. If the permittivity is not piecewise constant then $\partial E_y/\partial y$ and $\partial E_z/\partial z$ are still continuous and although the discontinuity in $\partial E_x/\partial x$ is more complicated, it can be derived in a straight-forward manner.

2.6.1 Example: Cavity with dielectric slab

The problem of a rectangular cavity containing a dielectric slab can be solved using the electric field formulation. The relative permittivity ϵ_r is 16 and the dimensions are given in figure 2.8. This is the same as one of the examples found in the paper by Lee and Mittra [50]. The discontinuity of the normal component of the electric field is implemented exactly during the assembly of the S and T matrices, as is the continuity of the tangential components and the derivative terms.

Figure 2.8: Cavity with dielectric slab.

The problem can be solved by separation of variables. The solutions can be separated into two categories: solutions for which the electric field component that is normal to the

dielectric surface is zero and solutions for which the corresponding magnetic field component is zero. The former set of solutions are called longitudinal-section electric modes, or LSE modes, and the latter set of solutions are called longitudinal-section magnetic modes, or LSM modes. The LSE modes can be further divided according to whether the electric field is symmetric or anti-symmetric about the plane passing through the centre of the dielectric slab, parallel to the interfaces. An identical classification results for the LSM modes. The lowest resonant modes are oscillatory inside the dielectric and evanescent (decaying) in the empty region. In the dielectric slab the field is proportional to $\sin(lx)$ or $\cos(lx)$ and in the empty region the field is proportional to $\sinh(hx)$ or $\cosh(hx)$ where x is the coordinate perpendicular to the interface. The eigenvalues are obtained by simultaneously solving the first equation below and one of the four equations that follow, depending on the type of solution.

$$l^2 = -\epsilon_r h^2 + (\epsilon_r - 1) \left(\frac{n_y^2 \pi^2}{b^2} + \frac{n_z^2 \pi^2}{c^2} \right) \quad (2.69)$$

$$h \coth(hd) = l \tan\left(\frac{lt}{2}\right) \quad \text{for symmetric LSE modes} \quad (2.70)$$

$$l \tanh(hd) = -h \tan\left(\frac{lt}{2}\right) \quad \text{for anti-symmetric LSE modes} \quad (2.71)$$

$$h \tanh(hd) = \frac{l}{\epsilon_r} \tan\left(\frac{lt}{2}\right) \quad \text{for symmetric LSM modes} \quad (2.72)$$

$$h \tanh(hd) = -\frac{l}{\epsilon_r} \cot\left(\frac{lt}{2}\right) \quad \text{for symmetric LSM modes} \quad (2.73)$$

For the LSM modes, n_y and n_z are both integers that are greater than zero, while for the LSE modes, only one of the integers must be greater than zero. These solutions are similar to what is found in the text by Collin [54] for a waveguide with a dielectric slab.

The lowest eigenvalues for a uniform $16 \times 8 \times 6$ mesh with 11201 unknowns are given in table 2.12 and are compared with the solutions of the transcendental equations. There are no spurious modes since the divergence equation and the boundary conditions are satisfied.

Table 2.12: Eigenvalues, k^2 , in units of L^{-2} , of cavity with dielectric slab using electric field formulation. Eigenvalue multiplicity is 1 for all solutions. Symmetric modes are labelled (s) and anti-symmetric modes are labelled (a). $16 \times 8 \times 6$ mesh with 11201 unknowns.

Transcendental	FEM	FEM Error (%)	Type
6.6713	6.6716	0.005	LSE (s)
10.3141	10.3152	0.01	LSE (s)
14.7208	14.7221	0.009	LSE (s)
19.3486	19.3611	0.07	LSE (a)
19.8241	19.8282	0.02	LSM (s)
19.9036	19.9137	0.05	LSE (s)
24.1438	24.1615	0.07	LSE (a)
27.2405	27.2495	0.03	LSE (s)
29.5749	29.5973	0.08	LSE (a)
31.6194	31.6344	0.05	LSM (s)

This problem is solved with several different meshes. The relative errors of the ten lowest eigenvalues are plotted against the number of unknowns in the eigenvalue equation in figure 2.9. The results obtained with the commercial software package HFSS [46] using first and second order edge elements are plotted with the data from the new basis functions. Adaptive mesh refinement is disabled in the HFSS calculations because the mesh is not refined adaptively with the new basis functions either. Relative error is plotted as a function of matrix size instead of computing time. HFSS is a professional package that has been under continuous development for more than 20 years, whereas the code for the new basis functions has been written in MATLAB [55], which is an interpreted language, and is inherently much slower.

The plots indicate that the new basis functions have a convergence rate similar to the second order edge elements. This is consistent with the fact that the product of cubic Hermite and second order Lagrange interpolation polynomials contains all of the

(a) Comparison with first order edge elements.

(b) Comparison with second order edge elements.

Figure 2.9: Comparison of relative error of 10 lowest eigenvalues using new basis functions and using edge elements via HFSS without adaptive mesh refinement. The relative error is plotted against the number of unknowns in the matrix eigenvalue equation. The relative error is $r = |k_{FEM}^2 - k_{trans}^2| / 0.5(k_{FEM}^2 + k_{trans}^2)$, where the subscript “trans” denotes solutions of the transcendental equations (2.69)–(2.73).

monomials in x , y and z up to second order. There are higher order terms that occur, (for example, E_x contains the term $x^3y^2z^2$) but not all of the higher order monomials are present. This is a general property of quadrilateral and hexahedral elements, in contradistinction to triangular and tetrahedral nodal basis functions which do not have extra higher order terms, making the latter type more efficient in terms of the number of unknowns. In spite of the extra terms that arise using a product basis for bricks, the error for the new basis functions is comparable to that for the second order tetrahedral edge elements. However, it should be noted that the S and T matrices with the new basis functions are less sparse due to the divergence constraint at the centre of the brick 2.27. In cases where the mesh is cubic, the total number of non-zero matrix elements (the sum for the S and T matrices) increases by a factor of approximately 4.2. In the above case, where the mesh is $16 \times 8 \times 6$, the constraints in the centre of the bricks can be implemented in the direction with the fewest number of bricks, that is, in the direction with only 6 bricks, which amounts to a rotation of the coordinate system so that the x -axis is in the shortest direction. In this case, the total number of non-zero matrix elements increases by a factor of approximately 2.4.

2.7 Rate of convergence of eigenvalue solver

The examples given are perfectly conducting cavities with domains that are simply connected. In such cases, the static electric field is zero, as discussed in section 1.2. Since there are no static modes then the resonant angular frequencies, ω , are non-zero, and thus $k^2 = \omega^2/c^2 > 0$. The T matrix is defined by the integral

$$x^T T x = \iiint \epsilon(\mathbf{r}) |\mathbf{E}(\mathbf{r})|^2 dV \quad (2.74)$$

and therefore it is positive definite, that is, $x^T T x > 0$ for all $x \neq 0$. Since

$$x^T S x = k^2 x^T T x \quad (2.75)$$

and since $k^2 > 0$ and $x^T T x > 0$ for all $x \neq 0$, then $x^T S x > 0$ for all $x \neq 0$, that is, the S matrix is also positive definite.

For the Lanczos algorithm to be used in a generalized eigenvalue problem, where the equation is of the form $Ax = \lambda Bx$, the matrix B must be positive definite [42]. In the case where $A = S$, $B = T$ and $\lambda = k^2$, the lowest frequency modes correspond to the lowest eigenvalues. However, the Lanczos algorithm converges faster if the greatest eigenvalues are sought after. Since the S matrix is also positive definite, then it is possible to solve the eigenvalue equation in the case where $A = T$, $B = S$ and $\lambda = 1/k^2$. In the test calculations described in this thesis, there are sometimes more than 300 iterations required for convergence when the problem is set up with $\lambda = k^2$, while there are only between 8 and 30 iterations required for convergence when $\lambda = 1/k^2$. (The code for all of the calculations was written in Matlab [55]. The eigenvalues were calculated with an implementation of the Lanczos algorithm called in Matlab by the function `eigs`, which is based on the software package Arpack [56].)

Parenthetically, when using edge elements the eigenvalue $k^2 = 0$ occurs many times. Thus, the S matrix is not positive definite. The iterative projective methods, such as the Lanczos algorithm and the Jacobi-Davidson algorithm, obtain approximations for eigenvalues that lie at the extremities of the eigenvalue spectrum, that is, the greatest or least eigenvalues. After finding the greatest or least eigenvalue, the next greatest or least eigenvalue can be obtained by requiring that the new eigenvector be orthogonal to the previous eigenvector. This process continues until the desired number of eigenvalues are found. In order to avoid computation of all of the eigenvectors for which $k^2 = 0$, a shift-and-invert scheme is employed [43]. In that case, a lower estimate for the

lowest sought after eigenvalue is required. It has been observed that the default estimate provided by HFSS can be greater than the lowest non-zero eigenvalue, and consequently this eigenvalue and its eigenvector are not obtained in the solution. The estimate is a parameter that can be changed by the user, and so it is recommended by this author that the user lower this parameter several times by, for example, a factor of 2 in order to avoid missing any solutions.

The matrices arising from the new basis functions are less sparse than those arising from edge elements. However, the matrices arising from the new basis functions are positive definite and, consequently, a shift-and-invert scheme is not required to obtain the lowest resonant frequencies. Both of these facts require consideration when making a comparison of the computational efficiency of the new basis functions with edge elements.

2.8 Summary

A combination of cubic Hermite splines and second order Lagrange interpolation polynomials are used to construct basis functions for a vector field. The divergence equation is satisfied to second order in x , y and z (by construction of the basis functions) and the curl equation is solved by the finite element method. The basis functions can be used only if the geometry of the problem conforms to a Cartesian coordinate system. The domain is divided into bricks by level surfaces for the different Cartesian coordinates. The bricks are not required to be the same size. The number of basis functions per brick is initially 108 and then reduced to 81 when the 27 divergence constraints are implemented. The S and T matrices have more non-zero elements after the divergence constraints are imposed because the divergence constraint corresponding to the node at the centre of each brick involves nodes of non-adjacent bricks. A simple 2-dimensional example is given to illustrate the method for imposing the divergence constraints, which is not difficult.

The primary test problem for the new basis functions is determining the resonant

frequencies of a 3-dimensional cavity. The variational formulation for this problem is described using both the electric field and the magnetic field. This formulation does not determine the divergence of the field, which is why it is set as a constraint. When the electric field formulation is used, there are no spurious modes because by using the basis functions in equations (2.14)–(2.16), the divergence equation and boundary conditions are both satisfied. (Spurious modes are caused by not satisfying either one or both of the divergence equation and the boundary conditions, as discussed in sections 1.2 and 1.3.)

When using the magnetic field formulation, one of the nodes required to meet the principal boundary condition $\mathbf{H} \cdot \mathbf{n} = 0$ is also required to meet one of the divergence constraints. This leads to spurious modes in the low frequency part of the eigenvalue spectrum, however, they are identified by evaluating the flux of the Poynting vector and also by checking how closely those coefficients are to zero. The number of spurious modes in the low frequency part of the spectrum are less than the number of physical modes, and the frequency of the spurious modes increases as the mesh is refined, as seen in the examples in section 2.5.

The resonant frequencies of several different cavities are calculated using the new basis functions. There is good agreement with exact values in cases where they exist. In other cases, the agreement with experimental measurements and other numerical methods, notably with edge elements via the commercial software package HFSS, is good.

An interesting feature is that in cases where there are no non-trivial static solutions then the S matrix is positive definite. Thus, the generalized eigenvalue problem can be solved for the largest eigenvalues, $\lambda = 1/k^2$, which, in general, converges faster than when solving for the smallest eigenvalues. For comparison, when using edge elements, the matrices contain many eigenvalues for which $k^2 = 0$ and so a shift-and-invert technique is used for finding the lowest non-zero eigenvalues without first finding all of the eigenvalues that are zero.

Chapter 3

Mesh Refinement

The previous chapter described divergence constraints for a uniform mesh of bricks. In this case, the flexibility of the trial functions is the same everywhere as a result of the degrees of freedom being distributed uniformly throughout the domain. However, in some cases the solution may change more rapidly in certain parts of the domain than others. Greater flexibility in specific regions can be provided to the trial functions by using a finer mesh, which is the topic of this chapter.

A brief description of the mesh refinement method developed for this thesis is found in section 3.1. The prescription for ensuring continuity of the field and the relevant partial derivatives is discussed in section 3.2. The implementation of the divergence constraints needs to be modified for a refined mesh, which is detailed in section 3.3. The example calculations in chapter 2 are performed again, but this time with refined meshes. These examples are chosen because either there are exact solutions or experimental data that are used for verifying the accuracy of the new method in this thesis. The results are contained in section 3.4.

This chapter contains the linear algebra necessary to implement the divergence constraints for a refined mesh. Readers who are not interested in the mathematical details can skip sections 3.2 and 3.3. The remainder of the chapter and the subsequent chapter

can be understood independent of the material in those sections.

3.1 Overview of the mesh refinement method

The purpose of mesh refinement is to provide more degrees of freedom in regions of the domain where the field varies more rapidly, while simultaneously providing less degrees of freedom in regions of the domain where the field varies less rapidly. In the mesh refinement method described here, selected bricks are divided into smaller bricks. In the literature, the method of reducing the brick size or tetrahedron size in a given region is generally referred to as *h*-refinement. In contrast, with *p*-refinement the degree of the polynomials are increased within specific bricks or tetrahedra.

There are many ways to cut a given brick into smaller bricks. The method chosen here is to cut a given brick into eight smaller bricks of equal size arranged $2 \times 2 \times 2$. Each of the smaller bricks can be refined further. In principle, the process of division can continue *ad infinitum*. In practice, a finite amount of memory and computing speed limit the amount of mesh refinement since it increases the matrix size. In this particular implementation, the level of mesh refinement can only change by one at a given interface, that is, a larger brick can only form an interface with four smaller bricks. An example is shown in 2-dimensions in figure 3.1. (A 2-dimensional diagram is used for simplicity, but all of the results are 3-dimensional.)

Figure 3.2 is a plot of the node positions for E_x and E_y in a 2-dimensional 3×3 mesh with one level of refinement in the centre square. There are nodes in the fine bricks that do not have a corresponding node in the coarse brick. In this thesis, these are referred to as hanging nodes. The value of the field is fixed at the hanging nodes to ensure continuity across the interface. This is discussed in detail in section 3.2. In other cases, nodes may occupy different positions in the larger bricks compared to the positions in the smaller bricks. For example, the nodes located at the corner in a fine brick may be located at

Figure 3.1: Example of a 2-dimensional mesh with refinement. At a given interface, the mesh changes by at most one level of refinement.

either the corner, midpoint of an edge or centre of a face in an adjacent coarse brick. The divergence constraints for nodes at the corners are not the same as constraints at the midpoint of an edge or the centre of a face. Thus, the implementation of the divergence constraints needs to be modified, which is the subject of section 3.3.

Figure 3.2: Nodes for field components in 2 dimensions with refined mesh. Node 1 is a corner node for the coarse bricks and the fine brick. Nodes 2 and 3 are nodes that occur in the fine bricks but not in the coarse brick. They are referred to as hanging nodes. Node 4 is a corner node for the fine bricks and an edge or face node for the coarse brick.

Figure 3.3: Nodes of E_x at an interface where $x = 1$ in the local coordinate system of the large brick and $x = 0$ in the local coordinate systems of the small bricks. The nodes for the partial derivative $\partial E_x / \partial x$ are obtained by changing C_{2jk}^x to C_{3jk}^x and $c_{0jk,q}^x$ to $c_{1jk,q}^x$.

3.2 Hanging nodes

The coefficients of the hanging nodes are fixed to ensure that the field is continuous across the interface where the mesh refinement level changes. The same is true for the partial derivatives that occur explicitly in the basis functions. This is described in detail for the component E_x across a boundary perpendicular to the x -axis and across a boundary perpendicular to the y -axis. In the former case, the field component is perpendicular to the interface and in the latter case the field component is parallel to the interface. In section 3.3, it is shown that continuity of the relevant partial derivatives ensures that the divergence is continuous as well.

Consider the continuity of the component of the field parallel to the x -axis, E_x , across an interface lying in a plane where x is a constant. In this example, the interface lies in

the plane $x = 1$ of the local coordinate for the large brick and in the plane $x = 0$ of the local coordinates for the small bricks, so the small bricks lie more towards greater x . The nodes are shown in figure 3.3. They are denoted by C_{2jk}^x for the large brick and $c_{0jk,q}^x$ for the small bricks, where the subscript q is used to label each of the four small bricks. For the derivative terms, the coefficients are C_{3jk}^x and $c_{1jk,q}^x$. The results can be applied to E_y in a plane where y is a constant and E_z in a plane where z is a constant by cyclic permutation of the indices.

The value of E_x at any point in the plane $x = 1$ for the large brick is uniquely determined by the nine coefficients C_{2jk}^x . The value of E_x at any point in the plane $x = 0$ for the small bricks is uniquely determined by the nine coefficients $c_{0jk,q}^x$ for each of the four bricks labelled by q . Thus, continuity of E_x can be ensured by expressing the coefficients $c_{0jk,q}^x$ as appropriate linear combinations of the coefficients C_{2jk}^x . This is easy when the nodes for the smaller bricks coincide with the nodes for the larger brick.

$$C_{200}^x = c_{000,1}^x \quad (3.1)$$

$$C_{210}^x = c_{020,1}^x = c_{000,2}^x \quad (3.2)$$

$$C_{220}^x = c_{020,2}^x \quad (3.3)$$

$$C_{201}^x = c_{002,1}^x = c_{000,3}^x \quad (3.4)$$

$$C_{211}^x = c_{022,1}^x = c_{002,2}^x = c_{020,3}^x = c_{000,4}^x \quad (3.5)$$

$$C_{221}^x = c_{022,2}^x = c_{020,4}^x \quad (3.6)$$

$$C_{202}^x = c_{002,3}^x \quad (3.7)$$

$$C_{212}^x = c_{022,3}^x = c_{002,4}^x \quad (3.8)$$

$$C_{222}^x = c_{022,4}^x \quad (3.9)$$

The coefficients for the hanging nodes are determined by evaluating the basis functions for the large brick at the position of the hanging node. For example, $c_{010,1}^x$ is fixed so that

it is equal to the value of the basis functions for the large brick at the point $(1, 1/4, 0)$ in the local coordinate system of the large brick.

$$E_x(1, 1/4, 0) = \sum_{i=0}^3 \sum_{j=0}^2 \sum_{k=0}^2 C_{ijk}^x \Delta_{xi} H_i(1) L_j(1/4) L_k(0) \quad (3.10)$$

$$= \sum_{j=0}^2 C_{2j0}^x L_j(1/4) \quad (3.11)$$

$$= \frac{3}{8} C_{200}^x + \frac{3}{4} C_{210}^x - \frac{1}{8} C_{220}^x \quad (3.12)$$

For the small bricks, the value of E_x at this point is $c_{010,1}^x$ and so setting

$$c_{010,1}^x = \frac{3}{8} C_{200}^x + \frac{3}{4} C_{210}^x - \frac{1}{8} C_{220}^x \quad (3.13)$$

ensures that E_x is continuous at that point in the mesh. There are 12 hanging nodes that lie on an edge of at least one of the small bricks, including the example in equations (3.10)–(3.13). The constraints for those hanging nodes are listed below, beside the position in the local coordinate system of the large brick where they occur.

$$\left(1, \frac{1}{4}, 0\right) \quad c_{010,1}^x = \frac{3}{8} C_{200}^x + \frac{3}{4} C_{210}^x - \frac{1}{8} C_{220}^x \quad (3.14)$$

$$\left(1, \frac{3}{4}, 0\right) \quad c_{010,2}^x = -\frac{1}{8} C_{200}^x + \frac{3}{4} C_{210}^x + \frac{3}{8} C_{220}^x \quad (3.15)$$

$$\left(1, \frac{1}{4}, 1\right) \quad c_{012,3}^x = \frac{3}{8} C_{202}^x + \frac{3}{4} C_{212}^x - \frac{1}{8} C_{222}^x \quad (3.16)$$

$$\left(1, \frac{3}{4}, 1\right) \quad c_{012,4}^x = -\frac{1}{8} C_{202}^x + \frac{3}{4} C_{212}^x + \frac{3}{8} C_{222}^x \quad (3.17)$$

$$\left(1, 0, \frac{1}{4}\right) \quad c_{001,1}^x = \frac{3}{8} C_{200}^x + \frac{3}{4} C_{201}^x - \frac{1}{8} C_{202}^x \quad (3.18)$$

$$\left(1, 0, \frac{3}{4}\right) \quad c_{001,3}^x = -\frac{1}{8} C_{200}^x + \frac{3}{4} C_{201}^x + \frac{3}{8} C_{202}^x \quad (3.19)$$

$$\left(1, 1, \frac{1}{4}\right) \quad c_{021,2}^x = \frac{3}{8} C_{220}^x + \frac{3}{4} C_{221}^x - \frac{1}{8} C_{222}^x \quad (3.20)$$

$$\left(1, 1, \frac{3}{4}\right) \quad c_{021,4}^x = -\frac{1}{8} C_{220}^x + \frac{3}{4} C_{221}^x + \frac{3}{8} C_{222}^x \quad (3.21)$$

$$\left(1, \frac{1}{4}, \frac{1}{2}\right) \quad c_{012,1}^x = c_{010,3}^x = \frac{3}{8}C_{201}^x + \frac{3}{4}C_{211}^x - \frac{1}{8}C_{221}^x \quad (3.22)$$

$$\left(1, \frac{3}{4}, \frac{1}{2}\right) \quad c_{012,2}^x = c_{010,4}^x = -\frac{1}{8}C_{201}^x + \frac{3}{4}C_{211}^x + \frac{3}{8}C_{221}^x \quad (3.23)$$

$$\left(1, \frac{1}{2}, \frac{1}{4}\right) \quad c_{021,1}^x = c_{001,2}^x = \frac{3}{8}C_{210}^x + \frac{3}{4}C_{211}^x - \frac{1}{8}C_{212}^x \quad (3.24)$$

$$\left(1, \frac{1}{2}, \frac{3}{4}\right) \quad c_{021,3}^x = c_{001,4}^x = -\frac{1}{8}C_{210}^x + \frac{3}{4}C_{211}^x + \frac{3}{8}C_{212}^x \quad (3.25)$$

The constraints for the hanging nodes that are at the centre of the face of a small brick involve more terms from the large brick.

$$\begin{aligned} \left(1, \frac{1}{4}, \frac{1}{4}\right) \quad c_{011,1}^x = & \frac{9}{64}C_{200}^x + \frac{9}{32}C_{210}^x - \frac{3}{64}C_{220}^x \\ & + \frac{9}{32}C_{201}^x + \frac{9}{16}C_{211}^x - \frac{3}{32}C_{221}^x \\ & - \frac{3}{64}C_{202}^x - \frac{3}{32}C_{212}^x + \frac{1}{64}C_{222}^x \end{aligned} \quad (3.26)$$

$$\begin{aligned} \left(1, \frac{3}{4}, \frac{1}{4}\right) \quad c_{011,2}^x = & -\frac{3}{64}C_{200}^x + \frac{9}{32}C_{210}^x + \frac{9}{64}C_{220}^x \\ & - \frac{3}{32}C_{201}^x + \frac{9}{16}C_{211}^x + \frac{9}{32}C_{221}^x \\ & + \frac{1}{64}C_{202}^x - \frac{3}{32}C_{212}^x - \frac{3}{64}C_{222}^x \end{aligned} \quad (3.27)$$

$$\begin{aligned} \left(1, \frac{1}{4}, \frac{3}{4}\right) \quad c_{011,3}^x = & -\frac{3}{64}C_{200}^x - \frac{3}{32}C_{210}^x + \frac{1}{64}C_{220}^x \\ & + \frac{9}{32}C_{201}^x + \frac{9}{16}C_{211}^x - \frac{3}{32}C_{221}^x \\ & + \frac{9}{64}C_{202}^x + \frac{3}{32}C_{212}^x - \frac{3}{64}C_{222}^x \end{aligned} \quad (3.28)$$

$$\begin{aligned} \left(1, \frac{3}{4}, \frac{3}{4}\right) \quad c_{011,4}^x = & \frac{1}{64}C_{200}^x - \frac{3}{32}C_{210}^x - \frac{3}{64}C_{220}^x \\ & - \frac{3}{32}C_{201}^x + \frac{9}{16}C_{211}^x + \frac{9}{32}C_{221}^x \\ & - \frac{3}{64}C_{202}^x + \frac{9}{32}C_{212}^x + \frac{9}{64}C_{222}^x \end{aligned} \quad (3.29)$$

Equations (3.1)–(3.9) and (3.14)–(3.29) enforce the continuity of E_x across the boundary $x = 1$ in the local coordinate system of the large brick. The same equations can be used to enforce the continuity of $\partial E_x / \partial x$ continuous provided C_{2jk}^x is changed to C_{3jk}^x and

$c_{0jk,q}^x$ is changed to $c_{1jk,q}^x$.

In equations (3.1)–(3.29), the large brick is positioned towards $-\infty$ and the smaller bricks are positioned towards $+\infty$. If the situation is reversed, so that the large brick is positioned towards increasing x and the small bricks are positioned towards decreasing x , then the same relations hold provided

$$C_{2jk}^x \longrightarrow C_{0jk}^x \quad (3.30)$$

$$C_{3jk}^x \longrightarrow C_{1jk}^x \quad (3.31)$$

$$c_{0jk,q}^x \longrightarrow c_{2jk,q}^x \quad (3.32)$$

$$c_{1jk,q}^x \longrightarrow c_{3jk,q}^x . \quad (3.33)$$

In this example, the equations describe constraints for hanging nodes of the component E_x at an interface where x is a constant. The equations for the hanging nodes for the component E_y at an interface where y is a constant can be derived from those above by cyclic permutation of the indices.

$$C_{ijk}^x \longrightarrow C_{kij}^y \quad (3.34)$$

$$c_{ijk,q}^x \longrightarrow c_{kij,q}^y \quad (3.35)$$

The index q is numbered from the cyclic permutation of the axes in figure 3.3, that is, the y -axis becomes the z -axis and the z -axis becomes the x -axis. A similar transformation can be applied to obtain the constraints for the hanging nodes of the component E_z in a plane where z is a constant.

$$C_{ijk}^x \longrightarrow C_{jki}^z \quad (3.36)$$

$$c_{ijk,q}^x \longrightarrow c_{jki,q}^z \quad (3.37)$$

In this case, the numbering of the index q follows from figure 3.3 if the y -axis becomes

Figure 3.4: Nodes of E_x at an interface where $y = 1$ in the local coordinate system of the large brick and $y = 0$ in the local coordinate systems of the small bricks. The nodes for the partial derivative $\partial E_x / \partial x$ are obtained by changing the first subscript from 0 to 1 or 2 to 3.

the x -axis and the z -axis becomes the y -axis.

Now consider the hanging nodes of the component E_x at an interface that lies in the plane $y = 1$ of the local coordinate system of the large brick and in the plane $y = 0$ of the local coordinate system of the small bricks. The nodes are labelled in figure 3.4. Continuity of the field is easy to establish for nodes that are common to the large brick and the small bricks.

$$C_{020}^x = c_{000,1}^x \quad (3.38)$$

$$C_{220}^x = c_{200,2}^x \quad (3.39)$$

$$C_{022}^x = c_{002,3}^x \quad (3.40)$$

$$C_{222}^x = c_{202,4}^x \quad (3.41)$$

$$C_{021}^x = c_{002,1}^x = c_{000,3}^x \quad (3.42)$$

$$C_{221}^x = c_{202,2}^x = c_{200,4}^x \quad (3.43)$$

The relations for the partial derivatives are the same if

$$C_{020}^x \longrightarrow C_{120}^x \quad (3.44)$$

$$C_{020}^x \longrightarrow C_{320}^x \quad (3.45)$$

$$c_{020,q}^x \longrightarrow c_{120,q}^x \quad (3.46)$$

$$c_{020,q}^x \longrightarrow c_{320,q}^x . \quad (3.47)$$

The constraints for the hanging nodes that lie in the planes $x = 0$ and $x = 1$ of the large brick are the same as those found above, but they are included here for completeness.

$$\left(0, 1, \frac{1}{4}\right) \quad c_{221,2}^x = \frac{3}{8}C_{020}^x + \frac{3}{4}C_{021}^x - \frac{1}{8}C_{022}^x \quad (3.48)$$

$$\left(0, 1, \frac{3}{4}\right) \quad c_{221,4}^x = -\frac{1}{8}C_{020}^x + \frac{3}{4}C_{021}^x + \frac{3}{8}C_{022}^x \quad (3.49)$$

$$\left(1, 1, \frac{1}{4}\right) \quad c_{021,2}^x = \frac{3}{8}C_{220}^x + \frac{3}{4}C_{221}^x - \frac{1}{8}C_{222}^x \quad (3.50)$$

$$\left(1, 1, \frac{3}{4}\right) \quad c_{021,4}^x = -\frac{1}{8}C_{220}^x + \frac{3}{4}C_{221}^x + \frac{3}{8}C_{222}^x \quad (3.51)$$

The constraints for the nodes of $\partial E_x / \partial x$ can be obtained using equations (3.44)–(3.47).

The hanging nodes that lie in the plane $x = 1/2$ in the local coordinate system of the large brick mix the nodes of E_x and $\partial E_x / \partial x$.

$$\begin{aligned} \left(\frac{1}{2}, 1, 0\right) \quad c_{200,1}^x &= c_{000,2}^x \\ &= \frac{1}{2}C_{020}^x + \frac{1}{8}\delta_x C_{120}^x + \frac{1}{2}C_{220}^x - \frac{1}{8}\delta_x C_{320}^x \end{aligned} \quad (3.52)$$

$$\begin{aligned} \left(\frac{1}{2}, 1, \frac{1}{2}\right) \quad c_{202,1}^x &= c_{002,2}^x = c_{200,3}^x = c_{000,4}^x \\ &= \frac{1}{2}C_{021}^x + \frac{1}{8}\delta_x C_{121}^x + \frac{1}{2}C_{221}^x - \frac{1}{8}\delta_x C_{321}^x \end{aligned} \quad (3.53)$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, 1\right) \quad c_{202,3}^x &= c_{002,4}^x \\
&= \frac{1}{2}C_{022}^x + \frac{1}{8}\delta_x C_{122}^x + \frac{1}{2}C_{222}^x - \frac{1}{8}\delta_x C_{322}^x
\end{aligned} \tag{3.54}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, \frac{1}{4}\right) \quad c_{201,1}^x &= c_{001,2}^x \\
&= \frac{3}{16}C_{020}^x + \frac{3}{64}\delta_x C_{120}^x + \frac{3}{16}C_{220}^x - \frac{3}{64}\delta_x C_{320}^x \\
&\quad + \frac{3}{8}C_{021}^x + \frac{3}{32}\delta_x C_{121}^x + \frac{3}{8}C_{221}^x - \frac{3}{32}\delta_x C_{321}^x \\
&\quad - \frac{1}{16}C_{022}^x - \frac{1}{64}\delta_x C_{122}^x - \frac{1}{16}C_{222}^x + \frac{1}{64}\delta_x C_{322}^x
\end{aligned} \tag{3.55}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, \frac{3}{4}\right) \quad c_{201,3}^x &= c_{001,4}^x \\
&= -\frac{1}{16}C_{020}^x - \frac{1}{64}\delta_x C_{120}^x - \frac{1}{16}C_{220}^x + \frac{1}{64}\delta_x C_{320}^x \\
&\quad + \frac{3}{8}C_{021}^x + \frac{3}{32}\delta_x C_{121}^x + \frac{3}{8}C_{221}^x - \frac{3}{32}\delta_x C_{321}^x \\
&\quad + \frac{3}{16}C_{022}^x + \frac{3}{64}\delta_x C_{122}^x + \frac{3}{16}C_{222}^x - \frac{3}{64}\delta_x C_{322}^x
\end{aligned} \tag{3.56}$$

The length δ_x is a dimension of the large brick. The constraints for the nodes of the partial derivative $\partial E_x / \partial x$ that lie in the plane $x = 1/2$ of the large brick are *not* obtained with a simple transformation but rather with straight-forward differentiation of the Hermite splines and then evaluating them at $x = 1/2$.

$$\begin{aligned}
\left(\frac{1}{2}, 1, 0\right) \quad c_{300,1}^x &= c_{100,2}^x \\
&= -\frac{3}{2\delta_x}C_{020}^x - \frac{1}{4}C_{120}^x + \frac{3}{2\delta_x}C_{220}^x - \frac{1}{4}C_{320}^x
\end{aligned} \tag{3.57}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, \frac{1}{4}\right) \quad c_{301,1}^x &= c_{101,2}^x \\
&= -\frac{9}{8\delta_x}C_{020}^x - \frac{3}{32}C_{120}^x + \frac{9}{16\delta_x}C_{220}^x - \frac{3}{32}C_{320}^x \\
&\quad - \frac{9}{8\delta_x}C_{021}^x - \frac{3}{16}C_{121}^x + \frac{9}{8\delta_x}C_{221}^x - \frac{3}{16}C_{321}^x \\
&\quad + \frac{3}{16\delta_x}C_{022}^x + \frac{1}{32}C_{122}^x - \frac{3}{16\delta_x}C_{222}^x + \frac{1}{32}C_{322}^x
\end{aligned} \tag{3.58}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, \frac{1}{2}\right) \quad c_{302,1}^x &= c_{102,2}^x = c_{300,3}^x = c_{100,4}^x \\
&= -\frac{3}{2\delta_x} C_{021}^x - \frac{1}{4} C_{121}^x + \frac{3}{2\delta_x} C_{221}^x - \frac{1}{4} C_{321}^x
\end{aligned} \tag{3.59}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, \frac{3}{4}\right) \quad c_{301,3}^x &= c_{101,4}^x \\
&= \frac{3}{16\delta_x} C_{020}^x + \frac{1}{32} C_{120}^x - \frac{3}{16\delta_x} C_{220}^x + \frac{1}{32} C_{320}^x \\
&\quad - \frac{9}{8\delta_x} C_{021}^x - \frac{3}{16} C_{121}^x + \frac{9}{8\delta_x} C_{221}^x - \frac{3}{16} C_{321}^x \\
&\quad - \frac{9}{16\delta_x} C_{022}^x - \frac{3}{32} C_{122}^x + \frac{9}{16\delta_x} C_{222}^x - \frac{3}{32} C_{322}^x
\end{aligned} \tag{3.60}$$

$$\begin{aligned}
\left(\frac{1}{2}, 1, 1\right) \quad c_{302,3}^x &= c_{102,4}^x \\
&= -\frac{3}{2\delta_x} C_{022}^x - \frac{1}{4} C_{122}^x + \frac{3}{2\delta_x} C_{222}^x - \frac{1}{4} C_{322}^x
\end{aligned} \tag{3.61}$$

In these equations also, the length δ_x is a dimension of the large brick.

Equations (3.38)–(3.61) enforce the continuity of E_x and $\partial E_x / \partial x$ across an interface in the plane $y = 1$ in the local coordinate system of the large brick and in the plane $y = 0$ in the local coordinates system of the small bricks. If the bricks are reflected in the interface then the equations are the same provided

$$C_{i2k}^x \longrightarrow C_{i0k}^x \tag{3.62}$$

$$C_{i3k}^x \longrightarrow C_{i1k}^x \tag{3.63}$$

$$c_{i0k}^x \longrightarrow c_{i2k}^x \tag{3.64}$$

$$c_{i1k}^x \longrightarrow c_{i3k}^x. \tag{3.65}$$

If the interface is in a plane where z is a constant then the constraints for the hanging nodes are obtained by changing C_{ijk}^x to C_{ikj}^x and c_{ijk}^x to c_{ikj}^x . The constraints for the field components E_y and E_z for cases where the interface is parallel to the field component are obtained by cyclic permutations of the indices in the equations where the interface is parallel to E_x .

3.3 Modified divergence constraints

The implementation of the divergence constraints needs to be modified at an interface where the level of mesh refinement changes. This is because the relative positions of the nodes in the small bricks are not always the same as in the large bricks, including the occurrence of hanging nodes. The required adjustments are divided into four categories listed below.

1. Divergence constraints at nodes inside of the small bricks that are dependent on hanging nodes.
2. On the interface where the level of mesh refinement changes, the nodes at the corners of the small bricks, which also occur in the large brick, are used in the hanging node constraints. For example, in figure 3.3, the node $c_{122,1}^x$, which occurs at the same position as $c_{022,1}^x$, is at the corner of brick 1, which is a small brick, and it is at the centre of the face of the large brick. The hanging node constraints depend on this coefficient.
3. On the interface where the level of mesh refinement changes, the face and edge constraints of the small bricks are imposed by eliminating a hanging node. For example, in figure 3.3, the node $c_{111,1}^x$, which occurs at the same position as $c_{011,1}^x$, is a hanging node, but it is also the node that is eliminated to impose a face constraint.
4. The constraint that results from the node of the divergence equation at the centre of each brick is imposed by eliminating the coefficient c_{211}^x . If the adjacent brick in the $+x$ -direction has less refinement or none at all then the coefficient c_{211}^x of the current brick is a hanging node, which means that it has already been eliminated to impose the continuity of the field across the interface. Thus, another node must be eliminated to implement the divergence constraint.

The constraints are contained in two matrices, H and D . Initially, the matrix H contains all of the constraints for the hanging nodes described in section 3.2. It is the identity matrix modified such that if node n is a hanging node then $H_{n,n} = 0$ and the other elements in row n contain the coefficients for the hanging node constraints. The matrix H needs to be updated when a divergence constraint is imposed by eliminating a node that occurs in the hanging node constraints. The matrix D is initially equal to the identity matrix and is updated as the divergence constraints are implemented. The divergence constraints are stored in the matrix D in the same way that the hanging node constraints are stored in matrix H . Note that $H^2 = H$ and $D^2 = D$, which means they are idempotent, although neither matrix is orthogonal.

The first category concerns divergence constraints that are imposed by eliminating nodes that do not lie on an interface where the mesh refinement level changes, yet the eliminated node is a linear combination of some nodes that lie on the interface and are hanging nodes. The matrix D is updated to include the divergence constraint as it occurs for a uniform mesh. The hanging node constraints are incorporated using matrix multiplication: $D \rightarrow D \times H$.

The second category of adjustments concerns nodes of the divergence equation that lie at the corners of the small bricks. These are not hanging nodes. With regards to the large brick, a node such as this may be located at one of the corners, the midpoint of an edge, or the centre of a face. The coefficients that are eliminated to implement these constraints occur in the hanging node constraints, so the matrix H must be updated. The matrix H is updated by matrix multiplication once D has been updated: $H \rightarrow H \times D$. Also, even though the nodes are in different locations for the large and small bricks, the divergence equations will be the same once the hanging node constraints are implemented. For example, in figure 3.3, the coefficient C_{210}^x for the big brick is at an edge whereas it occurs at the corners for the smaller bricks. The constraints at an edge and a corner are different but this works out once the hanging node constraints are considered. The

constraint at this corner for brick 1 is

$$c_{120,1}^x + c_{030,1}^y + c_{021,1}^z = 0 . \quad (3.66)$$

Recall that the last index denotes brick 1. Continuity of the partial derivatives that occur explicitly in the basis functions implies that

$$c_{120,1}^x = C_{310}^x \quad (3.67)$$

and

$$c_{021,1}^z = C_{211}^z \quad (3.68)$$

as well as the hanging node constraint

$$c_{030,1}^y = -\frac{3}{2\delta_y}C_{200}^y - \frac{1}{4}C_{210}^y + \frac{3}{2\delta_y}C_{220}^y - \frac{1}{4}C_{230}^y . \quad (3.69)$$

which is similar to equation (3.57). Upon substituting equations (3.67)–(3.69) into equation (3.66), the edge constraint for the large brick emerges from the corner constraint of the small brick.

$$c_{120,1}^x + c_{030,1}^y + c_{021,1}^z = C_{310}^x + C_{211}^z - \frac{3}{2\delta_y}C_{200}^y - \frac{1}{4}C_{210}^y + \frac{3}{2\delta_y}C_{220}^y - \frac{1}{4}C_{230}^y \quad (3.70)$$

This is the same as equation (A.34), which is the edge constraint at $(1, 1/2, 0)$. Similar proofs hold for the other nodes in the third category of adjustments.

The third category of adjustments concerns divergence constraints that occur at the corners of the small bricks on the interface where the mesh refinement changes. These nodes occur in the large brick on the other side of the interface, however the location may be different, that is, they may be at the corner, midpoint of an edge or centre of a face. The divergence constraints of the large brick impose the correct divergence of the field

on the large brick side of the interface and the hanging node constraints make the field and the relevant partial derivatives continuous, so the divergence is continuous across the interface. The proofs are similar to the one above that results in equation (3.70).

The fourth category of adjustments concerns the implementation of the divergence constraints at the centre of the small bricks. For a uniform mesh, the node that is eliminated is c_{211}^x , which is in the plane $x = 1$ in the local coordinate system. If the brick adjacent to this plane is less refined, then the node c_{211}^x is a hanging node. Another node must be chosen to enforce the constraint since c_{211}^x has been eliminated to enforce the continuity of the field. To emphasize, a modification needs to be made if, in relation to the interface, the small bricks lie towards the $-x$ -direction and the large brick lies towards the $+x$ -direction. There is no adjustment necessary if the small bricks lie towards the $+x$ -direction and the large brick lies towards the $-x$ -direction.

To refine the mesh, a given brick is cut into $2 \times 2 \times 2$ bricks of equal size. At an interface where the mesh refinement changes, there are four small bricks arranged 2×2 and one large brick on the other side of the interface. All four divergence constraints at the centre of the four small bricks are imposed simultaneously. The nodes to eliminate are $c_{121,1}^y = c_{101,2}^y$, $c_{112,1}^z = c_{110,3}^z$, $c_{112,2}^z = c_{112,4}^z$ and $C_{011}^x = c_{222,1}^x = c_{202,2}^x = c_{220,3}^x = c_{200,4}^x$. The extra index in the lower case coefficients denotes the brick number, as in figure 3.3. The constraint in brick 1 involves $c_{121,1}^y$ and $c_{112,1}^z$ directly and C_{011}^x via a hanging node constraint. Similarly, the constraint in brick 2 involves $c_{101,2}^y$ and $c_{112,2}^z$ directly and C_{011}^x via a hanging node constraint. The constraint in brick 3 involves $c_{220,3}^x$ and C_{011}^x while the constraint in brick 4 involves $c_{112,4}^z$ and C_{011}^x . Thus, all four constraints must be solved simultaneously. It is not possible to choose nodes to impose the constraints for each brick individually or in pairs.

The four equations are linearly independent on the variables mentioned in the paragraph above. If C_{011}^x is replaced with $c_{121,3}^y = c_{101,4}^y$ then all of the nodes are in the centre of each of the faces dividing the four small bricks. However, the four equations are not

Figure 3.5: Locations of nodes that are used to impose divergence constraints at the centre of all four bricks, plus the face constraints and the edge constraint between the bricks. The coefficients x_i are defined in equations (3.71)–(3.79).

linearly independent on these four variables: the rank is only 3. Thus these four nodes cannot be used to impose the four divergence equations at the centre of each brick. If it were possible to use these nodes then this would mean that the four bricks could be combined into a “super brick”. The “super brick” could be used to impose the divergence constraints at the centre of the brick for any four adjacent bricks in the mesh and obviate the need for the method that links the bricks straight across the mesh. Unfortunately, this is not true.

The coefficient C_{011}^x appears in five other constraints of the four small bricks. It appears explicitly in the constraint of the edge that is common to all four small bricks. Through the hanging node constraints, it appears in the constraints of the four faces that divide the four small bricks from each other. For a uniform mesh, the face and edge constraints do not contain C_{011}^x and so the face and edge constraints are imposed after the constraint at the centre of the brick. However, this is not true for a refined mesh. The nine constraints are implemented simultaneously by solving a linear system of equations.

The nodes are labelled in the diagram in figure 3.5. There are only nine coefficients so they are plotted on one diagram instead of three. For the purpose of explaining the

algorithm for eliminating the coefficients, the variables are labelled by x_i where i is an integer and $1 \leq i \leq 9$.

$$x_1 = c_{121,1}^y = c_{101,2}^y \quad (3.71)$$

$$x_2 = c_{112,1}^z = c_{110,3}^z \quad (3.72)$$

$$x_3 = c_{112,2}^z = c_{110,4}^z \quad (3.73)$$

$$x_4 = c_{131,1}^y = c_{111,2}^y \quad (3.74)$$

$$x_5 = c_{113,1}^z = c_{111,3}^z \quad (3.75)$$

$$x_6 = c_{131,3}^y = c_{111,4}^y \quad (3.76)$$

$$x_7 = c_{113,2}^z = c_{111,4}^z \quad (3.77)$$

$$x_8 = c_{132,1}^y = c_{112,2}^y = c_{130,3}^y = c_{110,4}^y \quad (3.78)$$

$$x_9 = c_{222,1}^x = c_{202,2}^x = c_{220,3}^x = c_{200,4}^x = C_{011}^x \quad (3.79)$$

These nine coefficients must be eliminated simultaneously from the nine equations described above. The nine constraints can be expressed in terms of the x_i , augmented with terms from the other variables in the equations. For example, the first constraint is the node in the divergence at the centre of brick 1.

$$\begin{aligned} 0 = & -\frac{3}{2\delta_x} c_{011,1}^x - \frac{1}{4} c_{111,1}^x + \frac{3}{2\delta_x} c_{211,1}^x - \frac{1}{4} c_{311,1}^x \\ & -\frac{3}{2\delta_y} c_{101,1}^y - \frac{1}{4} c_{111,1}^y + \frac{3}{2\delta_y} c_{121,1}^y - \frac{1}{4} c_{131,1}^y \\ & -\frac{3}{2\delta_z} c_{110,1}^z - \frac{1}{4} c_{111,1}^z + \frac{3}{2\delta_z} c_{112,1}^z - \frac{1}{4} c_{113,1}^z \end{aligned} \quad (3.80)$$

The variables x_1 , x_2 , x_4 and x_5 occur explicitly in the equation, while the variable x_9 occurs through the hanging node constraint for $c_{211,1}^x$. The coefficient of x_9 is

$$\frac{3}{2\delta_x} L_1\left(\frac{1}{4}\right) L_1\left(\frac{1}{4}\right) = \frac{27}{32\delta_x}. \quad (3.81)$$

The coefficient $c_{011,1}^x$ is already eliminated from the divergence constraint at the centre of the brick adjacent to it in the $-x$ -direction, and so that introduces more terms in the equation. If the brick in the $-y$ -direction is larger, then the coefficients $c_{101,1}^y$ and $c_{111,1}^y$ are hanging nodes and so there would be more terms entering via those constraints. Similarly, if the brick in the $-z$ -direction is larger, then the coefficients $c_{110,1}^z$ and $c_{111,1}^z$ are hanging nodes and so there would be more terms entering via those constraints as well. In terms of the variables x_i , the equation is

$$\frac{3}{2\delta_y}x_1 + \frac{3}{2\delta_z}x_2 - \frac{1}{4}x_4 - \frac{1}{4}x_5 + \frac{27}{32\delta_x}x_9 + (\text{other terms}) = 0 . \quad (3.82)$$

The nine equations produce a 9×9 matrix, A , which is augmented by another matrix, B , containing the terms for the other variables. The augmented matrix $[A|B]$ is converted to reduced row echelon form $[I_9|C]$ where I_9 is the 9×9 identity matrix and C results from B via the elementary row operations. The matrix A is shown below.

$$A = \begin{bmatrix} \frac{3}{2\delta_y} & \frac{3}{2\delta_z} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 & \frac{27}{32\delta_x} \\ -\frac{3}{2\delta_y} & 0 & \frac{3}{2\delta_z} & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & \frac{27}{32\delta_x} \\ 0 & -\frac{3}{2\delta_z} & 0 & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2\delta_z} & 0 & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{1}{4} & \frac{9}{8\delta_x} \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \frac{9}{8\delta_x} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\frac{1}{4} & \frac{9}{8\delta_x} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \frac{9}{8\delta_x} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \frac{3}{2\delta_x} \end{bmatrix} \quad (3.83)$$

The algorithm to row reduce the augmented matrix is given in Matlab notation. Only the operations on A are shown. To begin, solve for x_9 .

```

A(9,:) = A(9,:) + 4*( A(1,:) + A(2,:) + A(3,:) + A(4,:) ) ...
              + 2*( A(5,:) + A(6,:) + A(7,:) + A(8,:) )
A(9,:) = A(9,:) / A(9,9)

```

Eliminate x_9 in the first eight rows.

```

for i = 1:8
    A(i,:) = A(i,:) - A(i,9) * A(9,:)
end

```

The resulting matrix is shown below.

$$\begin{bmatrix}
 \frac{3}{2\delta_y} & \frac{3}{2\delta_z} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 & 0 \\
 -\frac{3}{2\delta_y} & 0 & \frac{3}{2\delta_z} & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 \\
 0 & -\frac{3}{2\delta_z} & 0 & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 \\
 0 & 0 & -\frac{3}{2\delta_z} & 0 & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{1}{4} & 0 \\
 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\frac{1}{4} & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
 \end{bmatrix} \tag{3.84}$$

The upper-left 8×8 block still needs to be solved.

```

for i = 2:8
    A(i,:) = A(i,:) + A(i-1,:)
end

```

Now the matrix is in upper triangular form, shown below.

$$\begin{bmatrix} \frac{3}{2\delta_y} & \frac{3}{2\delta_z} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2\delta_z} & \frac{3}{2\delta_z} & -\frac{1}{2} & -\frac{1}{4} & 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{3}{2\delta_z} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \quad (3.85)$$

Set the diagonal elements to 1

```
for i = 1:8
    A(i,:) = A(i,:) / A(i,i)
end
```

and eliminate the remaining non-diagonal coefficients.

```
for j = 8 : -1 : 2
    for i = j-1 : -1 : 1
        A(i,:) = A(i,:) - A(i,j) * A(j,:)
    end
end
```

The variables x_i can be eliminated to impose the divergence constraints.

3.4 Resonant cavity examples with mesh refinement

In chapter 2, resonant frequencies of cavities were calculated with uniform meshes. Examples with either exact solutions or experimental data were chosen so that the accuracy

of the new basis functions could be verified. In this section, the same examples are used to test the accuracy of the mesh refinement method described in this chapter. In particular, the meshes are refined inside of the dielectrics since, for a given frequency, the wavelength of the field is shorter in regions where the permittivity is greater.

3.4.1 Cavity with dielectric slab

In section 2.6.1, the resonance frequencies of a rectangular cavity containing a dielectric slab are calculated using several uniform meshes. This example is chosen because the permittivity ϵ , and hence, electric field $\mathbf{E}$, are discontinuous and because the eigenvalue is given by a transcendental equation, so it can be used to test the accuracy of the new basis functions. (The transcendental equations are given in equations (2.69)–(2.73).) This subsection contains results for the same cavity using mesh refinement.

The relative error for the lowest ten eigenvalues is plotted in figure 3.6, including results from the previous chapter for comparison. The surface of the dielectric (see figure 2.8) must be a brick boundary. Thus, for some of the uniform meshes, all of the bricks are the same size, while for others, the bricks inside the dielectric are different in size than the bricks outside of the dielectric (so that the brick boundaries occur on the dielectric boundaries). To test the mesh refinement method, some of the uniform meshes are refined once for the bricks inside the dielectric. (Not all of the uniform meshes are refined because the calculation will not fit into 16 Gb of available RAM, and the calculation takes much more time once the data is transferred back and forth between RAM and the hard disk.) Some of the meshes that are refined once are refined further: there are two levels of mesh refinement inside of the dielectric and one in the layer of bricks adjacent to the dielectric. Again, not all of the meshes are refined twice because the calculation does not fit into 16 Gb of available RAM.

The results using refined meshes do not reduce the error for a given number of unknowns. Recall that for the lowest frequency modes, the field oscillates inside of the

Figure 3.6: Relative error of ten lowest resonance frequencies of cavity with dielectric slab, including calculations incorporating refined meshes.

dielectric and is exponential outside of it. The wavelength of the field inside of the dielectric is comparable to the size of the dielectric and the characteristic length of the field variation outside of the dielectric (the wavelength for the hyperbolic functions) is comparable to the size of the empty block outside of the dielectric. Since the dielectric and the empty region of the cavity are approximately the same size, then the field changes over comparable distances inside and outside of the dielectric. Thus, a uniform mesh is suitable for solving this problem. However, the eigenvalues obtained with one and two levels of mesh refinement converge to the correct values, which verifies that the mesh refinement method is correct.

3.4.2 Cavity with dielectric post

The lowest resonance frequencies of an empty rectangular box containing a dielectric post were obtained in section 2.5.2. This problem cannot be solved exactly, but the lowest eigenvalue has been measured experimentally [49], and so it can be used to test the accuracy of the new basis functions. This subsection contains results obtained using refined meshes. Figure 3.7(a) shows the lowest eigenvalue, k^2 , as a function of the number of unknowns when $\epsilon_r = 2.05$. Figure 3.7(b) shows the corresponding results when $\epsilon_r = 10$. In each case, the results are divided into three categories depending on the amount of mesh refinement. In one category, the mesh is uniform. In a second category, the mesh is refined once inside of the dielectric post. In a third category, the mesh is refined twice inside of the dielectric post and once in the layer of bricks adjacent to the post. The results with refined meshes do not show significant improvement over the results with uniform meshes for a given number of unknowns. This observation is the same as for the previous example of the dielectric slab, and indicates that the field variation is comparable inside and outside of the post. A uniform mesh is suitable for solving both problems. However, the results obtained using refined meshes are correct, which verifies that the mesh refinement method is correct.

(a) Lowest eigenvalue for cavity with dielectric post with $\epsilon_r = 2.05$.

(b) Lowest eigenvalue for cavity with dielectric post with $\epsilon_r = 10$.

Figure 3.7: Lowest eigenvalue of cavity loaded with rectangular dielectric post, including results using refined meshes. The dimensions are given in figure 2.5.

Table 3.1: Lowest eigenvalue for dielectric resonator filter.

Mesh	Uniform		Refined	
	Unknowns	Eigenvalue	Unknowns	Eigenvalue
$9 \times 8 \times 15$	18707	3.6083	38231	3.6078
$9 \times 16 \times 15$	36875	3.5865	77199	3.5861

3.4.3 Dielectric resonator filter

The lowest resonant frequencies of the dielectric resonator filter of subsection 2.5.3 are calculated with refined meshes inside of the high-K dielectric. The relative permittivity is $\epsilon_r = 38.6$, so the field varies much more rapidly inside of this dielectric than in other regions of the domain. The lowest eigenvalue is shown in table 3.1 for two meshes with and without refinement inside of the dielectric. The results using the refined meshes are less than 0.02% different than the results using the uniform meshes, in spite of the fact that there are more unknowns. The accuracy of the lowest eigenvalue is not improved significantly using mesh refinement. However, the mesh refinement algorithm has been verified on an example that is more complicated than the dielectric slab and post.

3.5 Conclusions

A method for refining the mesh by cutting selected bricks into $2 \times 2 \times 2$ bricks of equal size has been described in this chapter. The change in the node pattern at an interface where mesh refinement occurs requires that additional constraints be imposed to maintain continuity of the components E_x , E_y and E_z and the partial derivatives $\partial E_x/\partial x$, $\partial E_y/\partial y$ and $\partial E_z/\partial x$. This is accomplished by fixing the value of the field at the hanging nodes. The divergence constraints require modification at an interface where the mesh refinement changes. The constraints for the hanging nodes and the modified implementation of the divergence constraints have been given in detail.

Resonant frequencies of cavities loaded with dielectrics have been determined using

the mesh refinement algorithm described in this chapter. The mesh is refined inside of the dielectrics since the spatial variation of the field is more rapid therein. The accuracy of the eigenvalues for a given number of unknowns does not improve significantly for the refined meshes in comparison with the uniform meshes. However, the eigenvalues obtained using mesh refinement are in agreement with the exact solutions, where they exist, or with experimental data. This indicates that the mesh refinement algorithm works correctly. The mesh refinement algorithm is used in the next chapter to solve problems with singular fields where the boundary of a perfect conductor forms an edge or a corner.

Chapter 4

Edges and corners

In this thesis, the intersection of two planes in the mesh to form a line is referred to as an edge and the intersection of three planes in the mesh at a point is referred to as a corner, as shown in figure 4.1. Methods for obtaining approximate solutions to problems with singular fields caused by edges and corners are the topic of this chapter.

Background information pertaining to the behaviour of the fields at an edge is discussed in section 4.1. The singularity is described by results from an asymptotic expansion [57]. The idealization of sharp edges and corners is also discussed. Section 4.2 contains a derivation of the method that is used for treating perfectly conducting edges and corners. Example calculations of resonant cavities with sharp metal edges and

Figure 4.1: Definition of edge and corner.

corners are included. Section 4.3 describes two methods for solving problems with singularities caused by edge and corner discontinuities of the permittivity and permeability, including numerical examples.

4.1 Background information

At a plane where the permittivity, ϵ , is discontinuous, the tangential component of the electric field, $\mathbf{E}$, is continuous and the normal component of the electric field is discontinuous according to the equation

$$\epsilon_1 E_{n,1} = \epsilon_2 E_{n,2} \quad (4.1)$$

where the subscript n denotes the normal component of the field and 1 and 2 label opposite sides of the interface. In section 2.6, it was shown that the new basis functions, defined in equations (2.14)–(2.16), can exactly model the discontinuity at a planar interface.

Figure 4.2: Interface of two dielectrics forming a 90° edge.

Since the new basis functions are valid for a rectangular mesh of bricks then, in general, there are discontinuities of the material properties where the interfaces meet at 90° to form edges and corners. Figure 4.2 shows two dielectrics with permittivities ϵ_1 and

ϵ_2 and part of their boundary forming an edge parallel to the z -axis. Across the horizontal interface, E_x is continuous while it is discontinuous across the vertical interface. As the edge is approached along both interfaces, E_x must simultaneously satisfy two different equations.

$$E_{x,1} = E_{x,2} \quad \text{horizontal interface} \quad (4.2)$$

$$\epsilon_1 E_{x,1} = \epsilon_2 E_{x,2} \quad \text{vertical interface} \quad (4.3)$$

The only way for these equations to be satisfied simultaneously is for $E_{x,1} = E_{x,2} = 0$ or $E_{x,1} = E_{x,2} = \pm\infty$. The equations satisfied by E_y are similar, as are the possible solutions.

$$\epsilon_1 E_{y,1} = \epsilon_2 E_{y,2} \quad \text{horizontal interface} \quad (4.4)$$

$$E_{y,1} = E_{y,2} \quad \text{vertical interface} \quad (4.5)$$

In general, either solution (0 or ∞) may occur.

Meixner has derived an asymptotic expansion for the field near an edge for a variety of configurations in a paper published in 1972 [57]. Van Bladel [58] has plotted the field for several cases. The component of the field that is tangential to the edge is continuous and finite. The components that are perpendicular to the edge are proportional to ρ^{t-1} , where ρ is the radius in cylindrical coordinates with the z -axis on the edge. For the case where either one of the dielectrics subtends an angle of 90° ,

$$t = \frac{2}{\pi} \arccos \left(\frac{1}{2} \frac{|\epsilon_1 - \epsilon_2|}{\epsilon_1 + \epsilon_2} \right). \quad (4.6)$$

The values of t are between $2/3$ and 1 . The solution $t = 1$ occurs in the limit that $\epsilon_1 = \epsilon_2$, that is, in the limit that the permittivity is continuous, which implies that the electric field is continuous. The solution $t = 2/3$ occurs in the limit that one of the permittivities

is infinite. Thus, the radial dependence of E_x and E_y is between $\rho^{-1/3}$ and $\rho^0 = 1$. Note that in the case where a perfect electric conductor subtends 90° , the perpendicular components are proportional to $\rho^{-1/3}$, which is the same if the permittivity is infinite. Also note that the electric field for an infinitely long line charge is proportional to ρ^{-1} , so the behaviour of the field at an edge is comparable to an induced line charge density.

Note that the partial derivatives $\partial E_x/\partial x$, $\partial E_y/\partial y$ and $\partial E_z/\partial z$ must exist if the divergence is to be given by the formula [60]

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} . \quad (4.7)$$

However, at the edge the partial derivatives *do not* exist because of the singularity. In spite of this, the flux through a closed surface containing the edge of a dielectric is zero since there is no free charge inside the closed surface. This fact is used in section 4.3 to derive a method for solving problems with singularities at dielectric edges and corners.

The magnitude of the field becomes infinite and the direction varies rapidly as the edge is approached [57, 59]. The finite element method uses piecewise polynomials that cannot accurately model the singularity at an edge. There are several reasons why the finite element method can produce a reasonable approximation in this situation.

1. Matter is made up of atoms, and so when the distance scale becomes comparable to the inter-atomic spacing, the continuum assumption is invalid.
2. There are no perfectly sharp edges in the real world. Even if the edge is an arc of a circle with a very small radius, the field is finite.
3. Material properties do not remain linear as the field strength increases indefinitely. A magnetic material becomes saturated and an insulator will break down and conduct or become ionized.

While this list is not exhaustive, it does suggest that it is not necessary to model the

singularity exactly for the results to be physically accurate.

The utility of the basis functions in equations (2.14)–(2.16) stems from the fact that the divergence constraints that occur at a node that is common to more than one brick are identical for all bricks. There are two conditions that must be met for this to be true.

1. The tangential component(s) of the field are continuous across an edge or face.
2. The derivatives $\partial E_x/\partial x$, $\partial E_y/\partial y$ and $\partial E_z/\partial z$ have the same value for each of the bricks that form a common boundary.

It is possible for the perpendicular field components to be discontinuous. For example, the face constraints (A.48) and (A.49), which occur on either side of a plane $x = \text{constant}$, are identical provided E_y and E_z are continuous (which also imply that $\partial E_y/\partial y$ and $\partial E_z/\partial z$ are continuous), and also that $\partial E_x/\partial x$ has the same value on either side of the interface. There are no coefficients for E_x in these two face constraints, and so even if the values of E_x on either side of the plane are different, the constraints (A.48) and (A.49) are still identical. This is why the basis functions can exactly model the discontinuity in the normal component of the field across a planar interface, which is described by equation (4.1) and in section 2.6.

If the finite element method is used with nodal basis functions, then at an interface between sub-domains, the derivative in the perpendicular direction is, in general, discontinuous. If this derivative occurs in the functional and if it equal to the delta function, then the *square* of a delta function occurs in the functional, which leads to what Strang refers to as a “variational crime” [61, 62]. Consequently, the approximate solution may or may not converge to the exact solution. However, the functional for the curl-curl equation contains only derivatives that are tangential to the field components,

$$|\nabla \times \mathbf{E}|^2 = \left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right)^2 + \left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right)^2 + \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right)^2. \quad (4.8)$$

Specifically, the functional does not contain the derivatives

$$\frac{\partial E_x}{\partial x}, \frac{\partial E_y}{\partial y} \text{ and } \frac{\partial E_z}{\partial z}. \quad (4.9)$$

Thus, the normal component of the field can be discontinuous across an interface without producing a delta function in the functional. This fact is used to construct edge elements. It is also used for calculations with the new basis functions, equations (2.14)–(2.16), involving edges and corners.

4.2 Metal edges and corners

This section contains a description of the method used for solving problems with edges and corners at the boundary of a perfect conductor. Figure 4.3 contains two diagrams of four bricks that are adjacent to a metal edge. The perfect conductor is in brick 1, so the electric field is zero inside that brick and the tangential components are zero on the surface of the conductor. Since the metal edge is parallel to the z -axis, E_z is zero on the edge of bricks 2, 3 and 4.

$$E_{z,2} = E_{z,3} = E_{z,4} = 0 \quad (4.10)$$

Between bricks, the components of the field that are tangential to the interface are continuous.

$$E_{x,2} = E_{x,3} \quad (4.11)$$

$$E_{y,3} = E_{y,4} \quad (4.12)$$

The tangential components of $\mathbf{E}$ are zero at the surface of the perfect conductor.

$$E_{x,4} = 0 \quad (4.13)$$

$$E_{y,2} = 0 \quad (4.14)$$

(a) Four bricks with a common edge showing continuity of the tangential components of the electric field; brick 1 contains a perfect conductor.

(b) Non-zero field components at the surface of a perfect electric conductor with a 90° edge.

Figure 4.3: Diagrams of four bricks with common edge showing a continuous tangential component between bricks to satisfy divergence constraints. Brick 1 is a perfect conductor.

Figure 4.4: Eight bricks with a common corner. The perfect conductor is in brick 1.

As a result of the constraints in equations (4.10)–(4.14), the field in the bricks outside of the perfect conductor is given by

$$\mathbf{E}_2 = E_{x,2} \hat{\mathbf{x}} \quad (4.15)$$

$$\mathbf{E}_4 = E_{y,4} \hat{\mathbf{y}} \quad (4.16)$$

$$\mathbf{E}_3 = E_{x,2} \hat{\mathbf{x}} + E_{y,4} \hat{\mathbf{y}} \quad (4.17)$$

as shown in figure 4.3(b).

The constraints for the electric field at a *corner* of a perfect conductor are derived to meet the same criteria as at an *edge* of a perfect conductor: the tangential components of the field are continuous between bricks and the tangential components of the electric field are zero on the surface of the perfect conductor. Figure 4.4 shows eight bricks with a common corner, and the perfect conductor is in brick 1. The constraints at the corner

node are:

$$E_{x,1} = E_{x,4} = E_{x,5} = E_{x,8} = 0 \quad (4.18)$$

$$E_{x,2} = E_{x,3} = E_{x,6} = E_{x,7} \quad (4.19)$$

$$E_{y,1} = E_{y,2} = E_{y,5} = E_{y,6} = 0 \quad (4.20)$$

$$E_{y,3} = E_{y,4} = E_{y,7} = E_{y,8} \quad (4.21)$$

$$E_{z,1} = E_{z,2} = E_{z,3} = E_{z,4} = 0 \quad (4.22)$$

$$E_{z,5} = E_{z,6} = E_{z,7} = E_{z,8} . \quad (4.23)$$

Now consider the constraints for a time varying magnetic field, $\mathbf{H}$. (For a static magnetic field, $\nabla \times \mathbf{H} = 0$, which means that a scalar potential can be used.) The normal component of a time varying magnetic field is zero at the surface of a perfect conductor. The tangential component of $\mathbf{H}$ is discontinuous at the surface of the perfect conductor due to the surface current density. The tangential components are continuous between bricks outside of the conductor, which results in the following constraints.

$$H_{x,2} = H_{x,3} = 0 \quad (4.24)$$

$$H_{y,3} = H_{y,4} = 0 \quad (4.25)$$

The field in each brick that results from these constraints, listed below, is incorrect for brick 3.

$$\mathbf{H}_2 = H_{y,2} \hat{\mathbf{y}} \quad (4.26)$$

$$\mathbf{H}_4 = H_{x,4} \hat{\mathbf{x}} \quad (4.27)$$

$$\mathbf{H}_3 = 0 \quad (4.28)$$

The example calculation in the next subsection demonstrates that for resonant fields

(a) Four bricks with a common edge showing continuity of the tangential components of the magnetic field; brick 1 contains a perfect conductor.

(b) Non-zero field components at the surface of a perfect electric conductor with a 90° edge.

Figure 4.5: Diagrams of four bricks with common edge showing continuous tangential component between bricks to satisfy divergence constraints. Brick 1 is a perfect conductor.

where the field intensity is great near an edge, the eigenvalue is not accurate when the magnetic field formulation is used.

The constraints for a singularity in the magnetic field at a *corner* of a perfect conductor meet the same criteria as the constraints for the magnetic field at an *edge* of a perfect conductor: the tangential components of the field are continuous between bricks and the normal component of the magnetic field is zero on the surface of the perfect conductor. The brick numbers are shown in figure 4.4, and the perfect conductor is in brick 1. The constraints for the magnetic field at the node at the corner are:

$$H_{x,1} = H_{x,4} = H_{x,5} = H_{x,8} \quad (4.29)$$

$$H_{x,2} = H_{x,3} = H_{x,6} = H_{x,7} = 0 \quad (4.30)$$

$$H_{y,1} = H_{y,2} = H_{y,5} = H_{y,6} \quad (4.31)$$

$$H_{y,3} = H_{y,4} = H_{y,7} = H_{y,8} = 0 \quad (4.32)$$

$$H_{z,1} = H_{z,2} = H_{z,3} = H_{z,4} \quad (4.33)$$

$$H_{z,5} = H_{z,6} = H_{z,7} = H_{z,8} = 0 . \quad (4.34)$$

Note that this implies that $\mathbf{H}_7 = 0$ at the corner in brick 7, which is incorrect. This is a source of error, which is similar to the error in equation (4.28) for an edge.

4.2.1 Example: cavity with L-shaped cross-section

The simplest 3-dimensional problem with a 90° edge is an empty cavity with a cross-section in the shape of an “L”. The dimensions of the cavity are shown in figure 4.6. The problem is solved using the electric field formulation and the magnetic field formulation.

The lowest four resonant frequencies and fields are obtained using the electric field formulation with 12 different meshes, nine of which incorporate mesh refinement at the edge. For comparison, the problem is solved with the software package HFSS [46] using

Figure 4.6: Dimensions of L-shaped cavity.

second order edge elements and adaptive mesh refinement. The lowest four eigenvalues for each mesh are found in table 4.1 and the values from HFSS are in the last row. All of the values agree to less than 2%, so there is good agreement between the new basis functions and second order edge elements with adaptive mesh refinement.

The lowest eigenvalue is shown again in table 4.2 to illustrate the effect of mesh refinement. The bricks in the $8 \times 16 \times 16$ mesh have lengths that are one half of the lengths of the bricks in the $4 \times 8 \times 8$. If one of the bricks in the $4 \times 8 \times 8$ mesh is refined once, then the small bricks are the same size as those in the $8 \times 16 \times 16$ mesh. A brick in the $4 \times 4 \times 4$ mesh that is refined results in small bricks with lengths in two of the dimensions that are the same size as the bricks in the $4 \times 8 \times 8$ mesh. In this example, bricks that are adjacent to the edge are refined, so a brick in the uniform mesh is refined into $2 \times 2 \times 2$ smaller bricks, and then out of those, only $1 \times 1 \times 2$ that are in contact with the edge are refined further. The results in table 4.2 show that the changes in the estimate for the lowest eigenvalue arise almost entirely out of increasing the fineness of the mesh near the edge.

The resonant frequencies are obtained using the magnetic field formulation with an $8 \times 16 \times 16$ mesh and the results are in table 4.3. The field plots in figure 4.8 indicate

Figure 4.7: Magnitude of electric field, $|\mathbf{E}|$, plotted in the plane $x = 5/18$, which bisects the L-shaped cavity.

Table 4.1: Eigenvalues of cavity with L-shaped cross-section.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Refinement level	Number of unknowns
37.8868	38.9809	46.1480	61.4004	$4 \times 4 \times 4$	0	593
38.0043	38.7909	46.1455	61.1172	$4 \times 4 \times 4$	1	1465
38.1241	38.7169	46.1431	61.1044	$4 \times 4 \times 4$	2	3233
38.2804	38.6868	46.1412	61.1033	$4 \times 4 \times 4$	3	6793
38.5100	38.6747	46.1399	61.1032	$4 \times 4 \times 4$	4	13937
38.0035	38.6923	46.1395	60.8333	$4 \times 8 \times 8$	0	2625
38.1218	38.6188	46.1368	60.8208	$4 \times 8 \times 8$	1	3497
38.2782	38.5890	46.1349	60.8197	$4 \times 8 \times 8$	2	5265
38.5081	38.5770	46.1336	60.8196	$4 \times 8 \times 8$	3	8825
38.1017	38.6098	46.1208	60.7925	$8 \times 16 \times 16$	0	22785
38.2592	38.5800	46.1189	60.7915	$8 \times 16 \times 16$	1	24553
38.4895	38.5680	46.1176	60.7913	$8 \times 16 \times 16$	2	28113
37.8225	38.7006	46.1238	60.8297	HFSS	adaptive	6202

Table 4.2: The lowest eigenvalue of the cavity with L-shaped cross-section for three meshes with different levels of refinement. The level of mesh refinement near the edge is shown in parentheses.

$4 \times 4 \times 4$	$4 \times 8 \times 8$	$8 \times 16 \times 16$
37.8868 (0)		
38.0043 (1)	38.0035 (0)	
38.1241 (2)	38.1218 (1)	38.1017 (0)
38.2804 (3)	38.2782 (2)	38.2592 (1)
38.5100 (4)	38.5081 (3)	38.4895 (2)

Figure 4.8: Magnitude of magnetic field, $|\mathbf{H}|$, plotted in the plane $x = 5/18$, which bisects the L-shaped cavity. For modes 1 and 2, the magnitude of the magnetic field, $|\mathbf{H}|$, becomes increasingly large as the mesh is made finer. The inaccuracy of the eigenvalues for those modes is due to the inaccurate edge condition for $\mathbf{H}$, equations (4.26)–(4.28). The computed eigenvalues for modes 3 and 4 are accurate because, for those modes, $|\mathbf{H}|$ is not infinite at the edge.

that the field intensity is greatest near the edge for modes 1 and 2. However, in equation (4.28), the magnetic field is set to zero at the edge in the brick that is opposite to the conductor, which is not accurate for these cases. The eigenvalues for these modes are not accurate, as shown in the table. In the magnetic field formulation, the natural boundary condition will ensure that the flux of the Poynting vector through the cavity wall is zero. However, it is not exact and converges to zero as the accuracy of the approximation increases. (See subsection 2.4.2 for further discussion.) The flux of the Poynting vector through the surfaces that form the edge, P' , is high for these modes compared to the total flux P . For modes 3 and 4, the plots in figure 4.8 indicate that the field intensity is low near the edge. The eigenvalues for these modes agree with the results from HFSS to less than 0.07%. Since the results are not accurate for modes where the field intensity is great near an edge, the method of solving problems with perfectly conducting edges using the magnetic field formulation is not used any further.

Table 4.3: Eigenvalues of cavity with L-shaped cross-section using magnetic field formulation. The mesh is $8 \times 16 \times 16$, there are two levels of refinement near the edge and there are 32481 unknowns. P is proportional to the flux of the Poynting vector through the cavity walls and is defined in equation (2.66). P' is the contribution to P from the surfaces that form the edge – the two planes that form the inner part of the “L”.

HFSS	Eigenvalue	P'	P	$\langle c_{211}^x \rangle_{RMS}$
37.8225	43.9990	1.0×10^5	1.0×10^5	9.2×10^{-2}
38.7006	45.6718	1.1×10^5	1.2×10^5	2.0×10^{-1}
46.1238	46.1174	-3.0	-2.9	1.1×10^{-4}
60.8297	60.8011	-8.1	-8.3	1.2×10^{-3}

The electric and magnetic fields for the lowest resonant frequency are plotted in figure 4.9. Figure 4.9(a) shows the components of the electric field that lie in the plane that cuts the cavity in half, that is, if one boundary is at $x = 0$ and the opposite boundary is at $x = 5/9$, then $E_y \hat{\mathbf{y}} + E_z \hat{\mathbf{z}}$ is plotted in the plane $x = 5/18$. Figure 4.9(b) shows $H_y \hat{\mathbf{y}} + H_z \hat{\mathbf{z}}$ in the plane $x = 0$. The plots are given to show that for both cases, the

(a) Electric field components $E_y\hat{\mathbf{y}} + E_z\hat{\mathbf{z}}$ of the lowest resonant mode in the plane $x = 5/18$, which bisects L-shaped cavity.

(b) Magnetic field components $H_y\hat{\mathbf{y}} + H_z\hat{\mathbf{z}}$ of the lowest resonant mode in the plane $x = 0$.

Figure 4.9: Projection of $\mathbf{E}$ and $\mathbf{H}$ of the lowest resonant mode into the planes $x = 5/18$ and $x = 0$, respectively, to illustrate that the fields “turn the corner”.

Figure 4.10: Dimensions of T-shaped cavity.

direction of the field “turns” due to the presence of the corner. This does not occur for all finite element methods, as shown in Figure 2.3 of the paper by Arnold, Falk and Winther [63].

4.2.2 Example: cavity with T-shaped cross-section

This subsection contains results for the resonant frequencies of an empty cavity in the shape of a waveguide T-junction with all three ports terminated by the perfect conductor. The dimensions of the cavity are shown in figure 4.10.

The resonant frequencies are obtained using the electric field formulation. The four lowest eigenvalues for the $4 \times 8 \times 12$ and $8 \times 16 \times 24$ meshes are listed in table 4.4, including results with mesh refinement in the bricks adjacent to the edges. The eigenvalues obtained using the $4 \times 8 \times 12$ mesh with $n + 1$ levels of mesh refinement around the edges are in close agreement with the eigenvalues obtained using the $8 \times 16 \times 24$ mesh with n levels of mesh refinement. Although the accuracy is the same, there are less unknowns using the $4 \times 8 \times 12$ with one greater level of refinement and, thus, using a refined mesh is more efficient in this case.

Figure 4.11: Magnitude of electric field, $|\mathbf{E}|$, plotted in the plane $x = 1/2$, which bisects the T-shaped cavity.

Table 4.4: Eigenvalues, k^2 , of cavity with T-shaped cross-section.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Refinement level	Number of unknowns
8.2067	11.0978	11.5487	13.9562	$4 \times 8 \times 12$	0	3521
8.1832	11.1156	11.5896	13.9430	$4 \times 8 \times 12$	1	5265
8.1737	11.1393	11.6428	13.9380	$4 \times 8 \times 12$	2	8801
8.1699	11.1741	11.7209	13.9360	$4 \times 8 \times 12$	3	15921
8.1814	11.1103	11.5834	13.9384	$8 \times 16 \times 24$	0	30465
8.1719	11.1342	11.6370	13.9334	$8 \times 16 \times 24$	1	34001
8.1681	11.1690	11.7152	13.9314	$8 \times 16 \times 24$	2	41121
8.1666	11.2211	11.8333	13.9306	$8 \times 16 \times 24$	3	55409

The magnitude of the electric field, $|\mathbf{E}|$, of the four lowest resonant modes is plotted in the plane $x = 1/2$, which bisects the cavity, in figure 4.11. At the edge, the electric field is zero for modes 1 and 4, while for modes 2 and 3 it is large. Table 4.4 shows that as the mesh is refined, the eigenvalues for modes 1 and 4 are decreasing (converging), while for modes 2 and 3 the eigenvalues are increasing (diverging). This is because the infinite electric field at the edge cannot be modelled accurately using polynomials.

4.2.3 Example: cavity with square U-shaped cross-section

This subsection contains results for a cavity with a cross-section in the shape of a “U” with square corners. The dimensions of the cavity are shown in figure 4.12.

Table 4.5 contains the four lowest eigenvalues, k^2 , calculated with meshes that are $4 \times 8 \times 12$ and $8 \times 16 \times 24$. The meshes are refined in bricks that are adjacent to the edges. The magnitude of the electric field, $|\mathbf{E}|$, is plotted in the plane $x = 1/2$, which bisects the cavity, for the four lowest modes in figure 4.13. The electric field is zero at the edges for modes 1 and 2, while it is non-zero for modes 3 and 4. The eigenvalues of modes 1 and 2 are converging as the mesh is refined while for modes 3 and 4 the eigenvalues

Figure 4.12: Dimensions of the square U-shaped cavity.

are diverging as the mesh is refined. This behaviour is also observed with the T-shaped cavity of the preceding example. It occurs because the infinite field at the edge cannot be modelled accurately with piecewise continuous polynomials.

Mesh refinement in the bricks adjacent to the edges for the square U-shaped cavity produces the same effect as for the T-shaped cavity: refinement of n levels for the $8 \times 16 \times 24$ mesh results in the same eigenvalues as $n + 1$ levels of refinement for the $4 \times 8 \times 12$ mesh. However, the number of unknowns in the latter mesh are less than former mesh, as seen in table 4.5. In comparison with a uniformly finer mesh, mesh refinement at perfect conductor edges achieves the same accuracy with fewer unknowns and thus is more efficient.

4.2.4 Example: cavity with perfectly conducting post

The subsection contains results for the resonant frequencies of a cavity containing a rectangular post. This problem contains singularities at the edges and the corners. The dimensions are the same as for the cavity with the dielectric post, shown in figure 2.5, except that the dielectric post is replaced by a perfect electric conductor.

The magnitude of the electric field is plotted above the post in figure 4.14 and the tangential components of the field are plotted below the post height in figure 4.15. The

Figure 4.13: Magnitude of electric field, $|\mathbf{E}|$, plotted in the plane $x = 1/2$, which bisects the square U-shaped cavity.

Table 4.5: Eigenvalues, k^2 , of a cavity with square U-shaped cross-section.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Refinement level	Number of unknowns
9.0748	10.1945	10.4016	11.9758	$4 \times 8 \times 12$	0	4417
9.0571	10.1760	10.4256	12.0026	$4 \times 8 \times 12$	1	6161
9.0499	10.1685	10.4590	12.0365	$4 \times 8 \times 12$	2	9697
9.0470	10.1655	10.5086	12.0850	$4 \times 8 \times 12$	3	16817
9.0546	10.1738	10.4202	11.9969	$8 \times 16 \times 24$	0	38145
9.0475	10.1663	10.4538	12.0310	$8 \times 16 \times 24$	1	41681
9.0446	10.1633	10.5034	12.0796	$8 \times 16 \times 24$	2	48801

electric field of the four lowest modes is plotted on the surface of the post in figure 4.16.

The eigenvalues for the four lowest modes using three meshes with refinement are given in table 4.6. Results from HFSS [46], using second order edge elements with adaptive mesh refinement, are also included in the table. The eigenvalues diverge as the mesh is refined with edge elements and with the new basis functions defined in equations (2.14)–(2.16). This occurs with the new basis functions and with edge elements because piecewise continuous polynomials cannot accurately model the infinite field at the edges and corners.

4.3 Dielectric edges and corners

This section describes two methods for solving problems where the electric field is singular at an edge or corner of a dielectric. The same methods apply in cases where the magnetic field is singular at an edge or corner of a magnetic material. In the first method, permittivity, ϵ , is approximated as continuous at the edge or corner. The second method uses constraints to ensure that the flux is zero through a closed surface surrounding the edge or corner. There are three examples of resonant cavities loaded with dielectrics to

Figure 4.14: Magnitude of electric field, $|\mathbf{E}|$, plotted in the plane $x = \frac{1}{3}$ for the $8 \times 16 \times 12$ mesh, or one layer of bricks above the post height. (The dimensions of the cavity are given in figure 2.5.)

Figure 4.15: Electric field components $E_y\hat{\mathbf{y}} + E_z\hat{\mathbf{z}}$ plotted in the plane $x = \frac{2}{9}$ for the $8 \times 16 \times 12$ mesh, or one layer of bricks below the post height. (The dimensions of the cavity are given in figure 2.5.)

Figure 4.16: The electric field, $\mathbf{E}$, on the surface of the post for the $8 \times 16 \times 12$ mesh.

Table 4.6: Eigenvalues, k^2 , of a cavity with perfectly conducting post. The mesh is refined in two different ways using the basis functions in equations (2.14)–(2.16): (a) around the edges and corners, and (b) above the post. Results from the software package HFSS [46] are given at the bottom of the table, labelled as (c). The results from HFSS were obtained using second order edge elements with adaptive mesh refinement. The parameter to determine the amount of mesh refinement, λ_{target} , is given in the table.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Refinement level	Number of unknowns
13.7673	35.5501	41.9713	70.2255	$8 \times 16 \times 12$	0	18793
14.7677	36.9472	43.0083	70.5985	$8 \times 16 \times 12$	1 (a)	29033
16.2694	38.9453	44.4724	71.1028	$8 \times 16 \times 12$	2 (a)	50025
13.6635	35.4077	41.8743	70.2023	$8 \times 16 \times 12$	1 (b)	32913
13.9011	35.9820	41.9947	70.3489	$8 \times 8 \times 8$	0	5985
13.6128	35.5665	41.7324	70.2753	$8 \times 8 \times 8$	1 (b)	10361
13.6128	35.5664	41.7324	70.2753	$8 \times 8 \times 8$	2 (b)	19273
13.5940	35.3420	41.9028	70.0946	$8 \times 12 \times 8$	0	9145
13.3613	35.0608	41.6511	70.0464	$8 \times 12 \times 8$	1 (b)	15905
13.3612	35.0608	41.6510	70.0464	$8 \times 12 \times 8$	2 (b)	34529
11.9471	32.3882	39.3926	65.9806	tetrahedra	$\lambda_{target} = 0.40$ (c)	957
11.9904	32.4101	39.6445	66.2660	tetrahedra	$\lambda_{target} = 0.20$ (c)	1122
11.9471	32.3882	39.3926	65.9806	tetrahedra	$\lambda_{target} = 0.10$ (c)	957
11.9892	32.5549	39.6117	66.3372	tetrahedra	$\lambda_{target} = 0.04$ (c)	1173
12.1092	32.9652	40.0182	67.4443	tetrahedra	$\lambda_{target} = 0.02$ (c)	2538
12.2847	33.6215	40.6218	68.9129	tetrahedra	$\lambda_{target} = 0.01$ (c)	23430

demonstrate both methods.

4.3.1 Preliminary remarks

If there are no constraints used at an edge or corner, that is, the normal components are discontinuous and free to vary, then there are spurious modes. The eigenvalue, k^2 , of the spurious modes increases as the mesh is made finer around the edges and corners. Constraints are applied at the singularity to remove the spurious modes.

Mesh refinement around the edges and corners does *not* improve convergence when the constraints are applied (in most cases, it worsens) and so it is not used. Instead, the mesh is refined according to two criteria which were determined heuristically. The first is that the fraction of bricks that are inside the dielectric materials increases as more bricks are added to the mesh. The second criterion is that the size of each brick is as close to cubic as possible.

4.3.2 Method 1: Continuous permittivity approximation

The first method for treating the singularity of the field at edges and corners is to make the field continuous at the edges and corners. Since the field is continuous, the normal component of the field is continuous which implies that the permittivity is continuous at the edge or corner. This has the effect of “rounding-off” the corner. The field has the correct discontinuity at the other nodes – those not on the edge or corner – but is continuous on the edge or corner.

Between the nodes, the discontinuity of the normal component is not constant, and thus, the approximation also introduces a non-constant permittivity. In fact, the discontinuity of the field depends on the field itself, which implies that the permittivity depends on the field, that is, the permittivity is nonlinear. However, the permittivity is treated as piecewise constant for the implementation of the divergence constraints, which is a source of error. The method is still used since the infinite field occurring at edges and

Figure 4.17: Diagram for flux constraints.

corners does not physically exist, as the discussed in section 4.1.

Other methods where the permittivity is approximated at discontinuities include the finite difference time domain method [66] and the plane wave method discussed in section 1.3.6 [38].

4.3.3 Method 2: Flux constraints

In section 4.1, it was noted that the continuity of the tangential components of the field ensures that delta functions do not appear in the functional due to the terms containing the curl. (See equation (4.8).) In fact, since the tangential components of the field are continuous between bricks, then the derivatives that occur in the curl are also continuous between those bricks. This implies that the line integral of the field around a square with sides of length $2L$ that encloses an edge (see figure 4.17) is also zero in the limit that $L \rightarrow 0$. This suggests an analogous method for treating the singularities at corners and edges: derive a constraint such that the flux through a closed surface surrounding the edge or corner is zero. This follows from the integral form of Gauss' law, since there is no free charge on the edge or corner.

Consider an edge parallel to the z -axis, as shown in figure 4.17. The flux through a square of dimensions $2L \times 2L$ is evaluated in the limit that $L \rightarrow 0$, which means that the components of the field can be considered constant over the surface. Let ϵ_{in} be the permittivity in brick 1 and ϵ_{out} be the permittivity in bricks 2, 3 and 4. Note that the tangential components of the field are continuous, as discussed in section 4.1, that is, $E_{x,1} = E_{x,4}$, $E_{x,2} = E_{x,3}$, $E_{y,1} = E_{y,2}$ and $E_{y,3} = E_{y,4}$. The total electric flux through the square is zero, which is used to derive the constraint.

$$\begin{aligned} & -L \epsilon_{in} E_{x,1} - L \epsilon_{in} E_{y,1} + L \epsilon_{out} E_{x,2} - L \epsilon_{out} E_{y,2} \\ & + L \epsilon_{out} E_{x,3} + L \epsilon_{out} E_{y,3} - L \epsilon_{out} E_{x,4} + L \epsilon_{out} E_{y,4} = 0 \end{aligned} \quad (4.35)$$

$$\begin{aligned} \Rightarrow & -\epsilon_{in} E_{x,1} - \epsilon_{in} E_{y,1} + \epsilon_{out} E_{x,2} - \epsilon_{out} E_{y,2} \\ & + \epsilon_{out} E_{x,3} + \epsilon_{out} E_{y,3} - \epsilon_{out} E_{x,4} + \epsilon_{out} E_{y,4} = 0 \end{aligned} \quad (4.36)$$

$$\Rightarrow -(\epsilon_{in} + \epsilon_{out}) E_{x,1} - (\epsilon_{in} + \epsilon_{out}) E_{y,1} + 2\epsilon_{out} E_{x,3} + 2\epsilon_{out} E_{y,3} = 0 \quad (4.37)$$

$$\begin{aligned} \Rightarrow & E_{x,1} = -E_{y,1} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} E_{x,3} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} E_{y,3} \end{aligned} \quad (4.38)$$

$$(4.39)$$

If $\epsilon_{in} = \epsilon_{out}$, then equation (4.38) becomes $E_{x,1} = -E_{y,1} + E_{x,3} + E_{y,3}$, which is true for a continuous field. Since brick 1 is inside of the dielectric and brick 3 is outside of the dielectric, then equation (4.38) can be rewritten as

$$E_{x,in} = -E_{y,in} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} (E_{x,out} + E_{y,out}) . \quad (4.40)$$

Similarly, the constraint for an edge that is parallel to the x -axis is

$$E_{y,in} = -E_{z,in} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} (E_{y,out} + E_{z,out}) \quad (4.41)$$

and the constraint for an edge parallel to the y -axis is

$$E_{z,in} = -E_{x,in} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} (E_{z,out} + E_{x,out}) . \quad (4.42)$$

The constraint for a corner can be derived in a way similar to equation (4.41). The corner constraint is

$$E_{x,in} = -E_{y,in} - E_{z,in} + \frac{4\epsilon_{out}}{\epsilon_{in} + 3\epsilon_{out}} (E_{x,out} + E_{y,out} + E_{z,out}) . \quad (4.43)$$

The constraint for an edge that is parallel to the z -axis, equation (4.41), is derived for the case where the dielectric is in brick 1. If the dielectric is in brick 2, then the constraint can be derived from equation (4.41) by letting $E_{x,in} \rightarrow -E_{x,in}$ and $E_{x,out} \rightarrow -E_{x,out}$.

$$E_{x,in} = E_{y,in} + \frac{2\epsilon_{out}}{\epsilon_{in} + \epsilon_{out}} (E_{x,out} - E_{y,out}) \quad (4.44)$$

If the dielectric is in brick 4, then the constraint can be derived from equation (4.41) by letting $E_{y,in} \rightarrow -E_{y,in}$ and $E_{y,out} \rightarrow -E_{y,out}$, which results in equation (4.44) as well. If the dielectric is in brick 3, then the constraint can be derived from equation (4.41) by letting $E_{x,in} \rightarrow -E_{x,in}$, $E_{x,out} \rightarrow -E_{x,out}$, $E_{y,in} \rightarrow -E_{y,in}$ and $E_{y,out} \rightarrow -E_{y,out}$, which results in the same constraint as equation (4.41). Similar transformations apply for the constraints for the edges parallel to the x - and y -axes, equations (4.41) and (4.42), respectively, as well as for the constraint at a corner, equation (4.43).

4.3.4 Example: Cavity with dielectric bar

This subsection contains the results of a cavity containing a dielectric with perfectly conducting walls in the shape of a rectangular box. The dimensions of the cavity are shown in figure 4.18. This example is chosen to test the constraints for singularities on the edges. There are no singularities at the corners because $E_y = 0$ and $E_z = 0$ since

Figure 4.18: Dimensions of cavity with dielectric bar.

they are located on the surface of the perfectly conducting box.

The problem is solved for two different permittivities. In the first example, the relative permittivity, ϵ_r , is 2.05, while in the second example $\epsilon_r = 10$. The discontinuity in the normal component of the field is relatively small in the first case and larger in the second, and thus the edge constraints are tested under different circumstances.

The eigenvalues, k^2 , for the dielectric bar with $\epsilon_r = 2.05$ obtained with the continuous permittivity approximation, the flux constraints and the software package HFSS [46] are found in tables 4.7, 4.8 and 4.9, respectively. The values obtained with HFSS use second order edge elements with adaptive mesh refinement. For the different meshes in the tables, the lowest eigenvalue, k_1^2 , differs by 0.25%, 0.02% and 1%, respectively, for the three different methods. For the second lowest resonant frequency, k_2^2 , the eigenvalues differ by 0.002%, 0.002% and 0.13% for the three different methods, respectively. For the third lowest resonant frequency, k_3^2 , the eigenvalues differ by 0.2%, 0.014% and 2% for the three different methods, respectively. For the fourth lowest resonant frequency, k_4^2 , the eigenvalues differ by 0.26%, 0.03% and 1% for the three different methods, respectively. Although the values obtained with different meshes using HFSS differ by the

Table 4.7: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 2.05$ obtained with the continuous permittivity approximation at the edges.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
27.7766	35.5278	51.2953	56.8074	$8 \times 8 \times 12$	$8 \times 5 \times 6$	11265
27.7859	35.5277	51.3049	56.7884	$10 \times 8 \times 16$	$10 \times 5 \times 8$	19009
27.7987	35.5277	51.3237	56.7918	$10 \times 8 \times 18$	$10 \times 5 \times 10$	21425
27.8103	35.5275	51.3526	56.8633	$10 \times 10 \times 18$	$10 \times 8 \times 10$	26961
27.7920	35.5271	51.3151	56.8300	$10 \times 10 \times 18$	$10 \times 7 \times 10$	26961
27.7918	35.5271	51.3150	56.8299	$12 \times 10 \times 18$	$12 \times 7 \times 10$	32497
27.7913	35.5270	51.3125	56.8792	$12 \times 12 \times 18$	$12 \times 9 \times 10$	39169
27.8091	35.5270	51.3409	56.8487	$12 \times 12 \times 24$	$12 \times 9 \times 14$	52417
27.8248	35.5270	51.3685	56.8772	$12 \times 12 \times 24$	$12 \times 9 \times 16$	52417
27.8474	35.5271	51.4117	56.9349	$12 \times 12 \times 24$	$12 \times 9 \times 18$	52417
27.8239	35.5270	51.3672	56.8990	$12 \times 13 \times 24$	$12 \times 10 \times 16$	56881
27.8268	35.5270	51.3705	56.8583	$12 \times 11 \times 24$	$12 \times 8 \times 16$	47953
27.8268	35.5270	51.3705	56.8582	$13 \times 11 \times 24$	$13 \times 8 \times 16$	52037
27.8267	35.5270	51.3705	56.8582	$14 \times 11 \times 24$	$14 \times 8 \times 16$	56121
27.8416	35.5270	51.3916	56.8674	$14 \times 11 \times 26$	$14 \times 8 \times 18$	60849

Table 4.8: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 2.05$ obtained with the flux constraints at the edges.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
27.7771	35.5278	51.2588	56.8266	$8 \times 8 \times 12$	$8 \times 5 \times 6$	11295
27.7781	35.5277	51.2592	56.8161	$10 \times 8 \times 16$	$10 \times 5 \times 8$	19047
27.7788	35.5277	51.2598	56.8147	$10 \times 8 \times 18$	$10 \times 5 \times 10$	21463
27.7827	35.5275	51.2648	56.8157	$10 \times 10 \times 18$	$10 \times 8 \times 10$	26999
27.7781	35.5271	51.2581	56.8168	$10 \times 10 \times 18$	$10 \times 7 \times 10$	26999
27.7779	35.5271	51.2580	56.8166	$12 \times 10 \times 18$	$12 \times 7 \times 10$	32543
27.7782	35.5270	51.2575	56.8205	$12 \times 12 \times 18$	$12 \times 9 \times 10$	39215
27.7808	35.5270	51.2613	56.8165	$12 \times 12 \times 24$	$12 \times 9 \times 14$	52463
27.7804	35.5270	51.2599	56.8209	$12 \times 12 \times 24$	$12 \times 9 \times 16$	52463
27.7810	35.5271	51.2583	56.8342	$12 \times 12 \times 24$	$12 \times 9 \times 18$	52463
27.7807	35.5270	51.2597	56.8230	$12 \times 13 \times 24$	$12 \times 10 \times 16$	56927
27.7803	35.5270	51.2601	56.8191	$12 \times 11 \times 24$	$12 \times 8 \times 16$	47999
27.7802	35.5270	51.2601	56.8190	$13 \times 11 \times 24$	$13 \times 8 \times 16$	52087
27.7802	35.5270	51.2601	56.8190	$14 \times 11 \times 24$	$14 \times 8 \times 16$	56175
27.7812	35.5270	51.2611	56.8202	$14 \times 11 \times 26$	$14 \times 8 \times 18$	60903

Table 4.9: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 2.05$ obtained with the software package HFSS [46]. The calculations were performed using second order edge elements with adaptive mesh refinement. The convergence parameter for the adaptive mesh refinement is λ_{target} .

k_1^2	k_2^2	k_3^2	k_4^2	λ_{target}	Number of unknowns
28.0575	35.5718	52.2959	57.4497	0.40	618
28.0575	35.5718	52.2959	57.4497	0.20	618
28.0575	35.5718	52.2959	57.4497	0.10	618
27.7714	35.5260	51.3091	56.7945	0.04	1383
27.7705	35.5275	51.2484	56.7858	0.02	7590
27.7719	35.5268	51.2518	56.7959	0.01	44928

most out of the three methods, the number of unknowns varies by approximately 2 orders of magnitude and the eigenvalues are converging. Using the continuous permittivity approximation, there is a trend that k_1^2 , k_3^2 and k_4^2 are increasing. Using the flux constraints, the four lowest eigenvalues vary by at most 0.03%. The reason that the values for different meshes are close together is that the change in the permittivity is 2.05 at the interface and the edges, and so the discontinuity in the normal component of the field is only 2.05. The flux constraints will be tested more severely if the permittivity is increased, which is why the problem is solved again with $\epsilon_r = 10$.

The eigenvalues, k^2 , for the resonant frequencies of a cavity containing a dielectric bar with $\epsilon_r = 10$ are obtained using the new basis functions and the software package HFSS [46]. The new basis functions utilize the continuous permittivity approximation and the flux constraints, and the results are contained in tables 4.10 and 4.11, respectively. The results obtained with HFSS using second order edge elements with adaptive mesh refinement are contained in table 4.12. The magnitude of the electric field is plotted in the plane $x = 5/18$, which bisects the cavity, in figure 4.19. Modes 1 and 3 show discontinuities in the magnitude of the field, and hence the normal components of the

Table 4.10: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 10$ obtained with the continuous permittivity approximation at the edges.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
7.9557	8.2778	12.8663	15.3235	$8 \times 8 \times 12$	$8 \times 5 \times 6$	11265
7.9618	8.2777	12.8601	15.3217	$10 \times 8 \times 16$	$10 \times 5 \times 8$	19009
7.9734	8.2777	12.8607	15.3213	$10 \times 8 \times 18$	$10 \times 5 \times 10$	21425
7.9992	8.2776	12.8719	15.3214	$10 \times 10 \times 18$	$10 \times 8 \times 10$	26961
7.9784	8.2776	12.8614	15.3210	$10 \times 10 \times 18$	$10 \times 7 \times 10$	26961
7.9783	8.2776	12.8614	15.3210	$12 \times 10 \times 18$	$12 \times 7 \times 10$	32497
7.9924	8.2775	12.8631	15.3210	$12 \times 12 \times 18$	$12 \times 9 \times 10$	39169
8.0005	8.2775	12.8616	15.3207	$12 \times 12 \times 24$	$12 \times 9 \times 14$	52417
8.0220	8.2775	12.8671	15.3207	$12 \times 12 \times 24$	$12 \times 9 \times 16$	52417
8.0559	8.2776	12.8782	15.3210	$12 \times 12 \times 24$	$12 \times 9 \times 18$	52417
8.0292	8.2775	12.8679	15.3207	$12 \times 13 \times 24$	$12 \times 10 \times 16$	56881
8.0169	8.2775	12.8663	15.3207	$12 \times 11 \times 24$	$12 \times 8 \times 16$	47953
8.0169	8.2775	12.8662	15.3207	$13 \times 11 \times 24$	$13 \times 8 \times 16$	52037
8.0169	8.2775	12.8662	15.3207	$14 \times 11 \times 24$	$14 \times 8 \times 16$	56121
8.0319	8.2775	12.8678	15.3207	$14 \times 11 \times 26$	$14 \times 8 \times 18$	60849

Table 4.11: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 10$ obtained with the flux constraints at the edges.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
7.9822	8.2778	12.8394	15.3235	$8 \times 8 \times 12$	$8 \times 5 \times 6$	11295
7.9816	8.2777	12.8378	15.3217	$10 \times 8 \times 16$	$10 \times 5 \times 8$	19047
7.9806	8.2777	12.8374	15.3213	$10 \times 8 \times 18$	$10 \times 5 \times 10$	21463
7.9813	8.2776	12.8379	15.3214	$10 \times 10 \times 18$	$10 \times 8 \times 10$	26999
7.9796	8.2776	12.8372	15.3210	$10 \times 10 \times 18$	$10 \times 7 \times 10$	26999
7.9796	8.2776	12.8371	15.3210	$12 \times 10 \times 18$	$12 \times 7 \times 10$	32543
7.9797	8.2775	12.8371	15.3210	$12 \times 12 \times 18$	$12 \times 9 \times 10$	39215
7.9808	8.2775	12.8369	15.3207	$12 \times 12 \times 24$	$12 \times 9 \times 14$	52463
7.9792	8.2775	12.8369	15.3207	$12 \times 12 \times 24$	$12 \times 9 \times 16$	52463
7.9805	8.2776	12.8375	15.3210	$12 \times 12 \times 24$	$12 \times 9 \times 18$	52463
7.9794	8.2775	12.8369	15.3207	$12 \times 13 \times 24$	$12 \times 10 \times 16$	56927
7.9791	8.2775	12.8369	15.3207	$12 \times 11 \times 24$	$12 \times 8 \times 16$	47999
7.9791	8.2775	12.8369	15.3207	$13 \times 11 \times 24$	$13 \times 8 \times 16$	52087
7.9791	8.2775	12.8369	15.3207	$14 \times 11 \times 24$	$14 \times 8 \times 16$	56175
7.9792	8.2775	12.8369	15.3207	$14 \times 11 \times 26$	$14 \times 8 \times 18$	60903

(a) Singularities at edges treated using the continuous permittivity approximation.

(b) Singularities at edges treated using the flux constraints.

Figure 4.19: The magnitude of the electric field, $|\mathbf{E}|$, plotted in the plane $x = 5/18$, which bisects the cavity containing the dielectric bar with $\epsilon_r = 10$. The field is parallel to the edges for modes 2 and 4, and so it is continuous there (which implies that the magnitude of the field is also continuous).

Table 4.12: Eigenvalues of the cavity containing the dielectric bar with relative permittivity $\epsilon_r = 10$ obtained with the software package HFSS [46]. The calculations were performed using second order edge elements with adaptive mesh refinement. The convergence parameter for the adaptive mesh refinement is λ_{target} .

k_1^2	k_2^2	k_3^2	k_4^2	λ_{target}	Number of unknowns
7.9395	8.2868	12.8347	15.4599	0.40	867
7.9395	8.2868	12.8347	15.4599	0.20	867
7.9395	8.2868	12.8347	15.4599	0.10	867
7.9698	8.2795	12.8570	15.3717	0.04	1650
7.9665	8.2777	12.8355	15.3221	0.02	10131
7.9674	8.2775	12.8356	15.3205	0.01	58821

field, at the boundary of the dielectric. The magnitudes of modes 2 and 4 are continuous across the boundary of the dielectric because the field is parallel to the edges. Thus, k_1^2 and k_3^2 are more sensitive to the edge conditions than k_2^2 and k_4^2 , which is verified in the tables. The values of k_1^2 differ by 1.3% and have an increasing (diverging) trend as the mesh is made finer assuming the continuous permittivity approximation. The values of k_3^2 differ by 0.14%, but there is no trend. With the flux constraints, the values of k_1^2 differ by 0.04%, while the values of k_3^2 differ by 0.02%. Both have a decreasing (converging) trend. The values of k_1^2 obtained with HFSS differ by 0.4% with an increasing (diverging) trend, while the values of k_3^2 differ by 0.2% with no trend.

To begin the comparison between the three methods, note that k_2^2 converges to 8.2775 for all three methods, and that k_4^2 converges to 15.3207 for the continuous permittivity approximation and the flux constraints, while it converges to 15.3205 with HFSS, a difference of only 0.0013%. This is because the field is parallel to the edges for modes 2 and 4, which is illustrated in figure 4.19 because the magnitude of $\mathbf{E}$ is continuous. The values of k_1^2 obtained with the flux constraints and HFSS differ by 0.15% for the solutions with the greatest number of unknowns (the bottom of tables 4.11 and 4.12).

The corresponding value obtained with the continuous permittivity approximation is greater than the value obtained with the flux constraints by 0.66% and greater than the value obtained with HFSS by 0.8%. The value of k_3^2 with the greatest number of unknowns differs by 0.01% using the flux constraints and HFSS. The value obtained with the continuous permittivity approximation differs by 0.24% from the value obtained with the flux constraints and 0.25% from the value obtained with HFSS. Thus, the eigenvalues obtained with the flux constraints are in closer agreement to the eigenvalues obtained using edge elements (HFSS) compared to the eigenvalues obtained using the continuous permittivity approximation.

4.3.5 Example: Cavity with dielectric post

The cavity containing a dielectric post, which was solved in section 2.5.2 using the magnetic field, is solved in this subsection using the electric field formulation with the edge and corner constraints described in this chapter. The dimensions of the cavity are given in figure 2.5. The relative permittivity of the dielectric post is $\epsilon_r = 2.05$. The problem is also solved with $\epsilon_r = 10$ to provide a more demanding test of the edge and corner constraints, as the discontinuity in the field is greater at the surface of the dielectric. Note that the dielectric bar of the preceding subsection has edges where the field is singular, whereas the dielectric post has both edges and corners where the field is singular.

The lowest four eigenvalues for the cavity containing the dielectric post with $\epsilon_r = 2.05$ are listed in tables 4.13, 4.14 and 4.15 for the continuous permittivity approximation, the flux constraints and the software package HFSS [46], respectively. The tables are given so that the effect of the mesh on the eigenvalues can be observed. The lowest eigenvalue, k_1^2 , is plotted in figure 4.20, which includes the results obtained using the magnetic field formulation in section 2.5.2. The figure illustrates that the flux constraints result in a closer approximation to eigenvalues obtained with the magnetic field results and with edge elements (HFSS) than the continuous permittivity approximation. The eigenvalues

Table 4.13: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 2.05$ obtained with the continuous permittivity approximation at the edges and corners. ‘Post mesh’ refers to the number of bricks in the mesh that are inside the dielectric post.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
30.9752	49.7311	56.3728	62.7384	$8 \times 12 \times 10$	$5 \times 6 \times 4$	14177
30.9853	49.7511	56.3863	62.6789	$8 \times 16 \times 10$	$5 \times 8 \times 4$	19009
30.9976	49.7742	56.4064	62.6725	$8 \times 18 \times 10$	$5 \times 10 \times 4$	21425
30.9966	49.7722	56.4028	62.6570	$8 \times 20 \times 10$	$5 \times 10 \times 4$	23841
31.0111	49.7990	56.4280	62.6745	$8 \times 20 \times 10$	$5 \times 12 \times 4$	23841
31.1014	49.7580	56.4769	62.7550	$8 \times 20 \times 12$	$5 \times 12 \times 6$	28737
31.2031	49.7193	56.5276	62.8434	$8 \times 20 \times 16$	$5 \times 12 \times 8$	38529
31.0233	49.8279	56.4186	62.7796	$11 \times 20 \times 12$	$7 \times 12 \times 6$	39873
31.0516	49.8783	56.4418	62.8081	$11 \times 20 \times 12$	$8 \times 12 \times 6$	39873
31.0630	49.9000	56.4615	62.8032	$11 \times 22 \times 12$	$8 \times 14 \times 6$	43913
31.1479	49.8762	56.5064	62.8900	$11 \times 22 \times 14$	$8 \times 14 \times 8$	51393
31.0604	49.8959	56.4548	62.7609	$11 \times 24 \times 12$	$8 \times 14 \times 6$	47953
31.0756	49.9235	56.4823	62.8041	$11 \times 24 \times 12$	$8 \times 16 \times 6$	47953
31.0566	50.0505	56.4521	62.8738	$14 \times 22 \times 12$	$11 \times 14 \times 6$	56177

Table 4.14: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 2.05$ obtained with the flux constraints at the edges and corners. ‘Post mesh’ refers to the number of bricks in the mesh that are inside the dielectric post.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
30.9552	49.6902	56.3369	62.7369	$8 \times 12 \times 10$	$5 \times 6 \times 4$	14257
30.9564	49.6936	56.3377	62.7129	$8 \times 16 \times 10$	$5 \times 8 \times 4$	19097
30.9572	49.6950	56.3385	62.7089	$8 \times 18 \times 10$	$5 \times 10 \times 4$	21521
30.9591	49.6987	56.3413	62.7056	$8 \times 20 \times 10$	$5 \times 10 \times 4$	23937
30.9581	49.6965	56.3397	62.7081	$8 \times 20 \times 10$	$5 \times 12 \times 4$	23945
30.9645	49.6898	56.3431	62.7136	$8 \times 20 \times 12$	$5 \times 12 \times 6$	28849
30.9871	49.6848	56.3544	62.7336	$8 \times 20 \times 16$	$5 \times 12 \times 8$	38649
30.9532	49.7050	56.3334	62.7201	$11 \times 20 \times 12$	$7 \times 12 \times 6$	40001
30.9585	49.6969	56.3377	62.7162	$11 \times 20 \times 12$	$8 \times 12 \times 6$	40009
30.9592	49.6982	56.3387	62.7158	$11 \times 22 \times 12$	$8 \times 14 \times 6$	44057
30.9654	49.6978	56.3416	62.7222	$11 \times 22 \times 14$	$8 \times 14 \times 8$	51545
30.9606	49.7013	56.3412	62.7083	$11 \times 24 \times 12$	$8 \times 14 \times 6$	48097
30.9601	49.6996	56.3398	62.7164	$11 \times 24 \times 12$	$8 \times 16 \times 6$	48105
30.9608	49.7080	56.3383	62.7220	$14 \times 22 \times 12$	$11 \times 14 \times 6$	56345

Table 4.15: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 2.05$ obtained with the software package HFSS [46]. The calculations were performed using second order edge elements with adaptive mesh refinement. The convergence parameter for the adaptive mesh refinement is λ_{target} .

k_1^2	k_2^2	k_3^2	k_4^2	λ_{target}	Number of unknowns
30.9139	49.6149	56.3434	62.6236	0.40	1329
30.9139	49.6149	56.3434	62.6236	0.20	1329
30.9113	49.6209	56.3207	62.5655	0.10	1143
30.9245	49.6468	56.3126	62.6519	0.04	5619
30.9307	49.6585	56.3198	62.6717	0.02	38052
30.9314	49.6597	56.3207	62.6733	0.01	58398

obtained with the flux constraints do not increase or decrease monotonically due the eigenvalues from the $8 \times 20 \times 12$ and $8 \times 20 \times 16$ meshes. However, the values of k_1^2 obtained with different meshes using the flux constraints differ by only 0.1%.

Tables 4.16, 4.17 and 4.18 contain results for the lowest four eigenvalues, k^2 , with different meshes in the case where $\epsilon_r = 10$ for the post. The tables are included so that the effect of the choice of mesh on the eigenvalues can be observed. The lowest eigenvalue, k_1^2 , is plotted in figure 4.21, including results obtained using the magnetic field formulation and the software package HFSS [46]. The eigenvalues obtained using the continuous permittivity approximation show an increasing trend and they do not approach a horizontal asymptote. The eigenvalues obtained with the flux constraints show a converging trend apart from those obtained with the $8 \times 20 \times 16$ and $11 \times 20 \times 12$ (with a $7 \times 12 \times 6$ post) meshes in the middle column of table 4.17. The eigenvalues, k_1^2 , obtained with the flux constraints vary by 1.1% among all of the meshes that were used. The values obtained with HFSS using second order edge elements and adaptive mesh refinement vary by 1.3%, although they are monotone increasing. The values obtained using the new basis functions with the magnetic field formulation vary by 0.2% and they

Figure 4.20: The eigenvalue for the lowest frequency resonant mode for the cavity containing a dielectric post with relative permittivity $\epsilon_r = 2.05$. The results obtained with the new basis functions use the magnetic field formulation and the electric field formulation with two methods to treat the singularities at the edges and corners. The results obtained with HFSS second order edge elements with adaptive mesh refinement. The scale for k^2 varies by only 1.6%.

Table 4.16: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 10$ obtained with the continuous permittivity approximation at the edges and corners. ‘Post mesh’ refers to the number of bricks in the mesh that are inside the dielectric post.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
13.7590	16.1239	25.1960	28.7791	$8 \times 12 \times 10$	$5 \times 6 \times 4$	14177
13.8277	16.1100	25.2404	29.0423	$8 \times 16 \times 10$	$5 \times 8 \times 4$	19009
13.9137	16.1094	25.2876	29.3144	$8 \times 18 \times 10$	$5 \times 10 \times 4$	21425
13.9013	16.1049	25.2826	29.2748	$8 \times 20 \times 10$	$5 \times 10 \times 4$	23841
14.0004	16.1108	25.3331	29.5597	$8 \times 20 \times 10$	$5 \times 12 \times 4$	23841
14.4752	16.1356	25.3702	30.1060	$8 \times 20 \times 12$	$5 \times 12 \times 6$	28737
14.9997	16.1625	25.4217	30.1703	$8 \times 20 \times 16$	$5 \times 12 \times 8$	38529
14.4614	16.1251	25.5099	30.0816	$11 \times 20 \times 12$	$7 \times 12 \times 6$	39873
14.7082	16.1325	25.6051	30.1138	$11 \times 20 \times 12$	$8 \times 12 \times 6$	39873
14.7899	16.1337	25.6415	30.1288	$11 \times 22 \times 12$	$8 \times 14 \times 6$	43913
15.2908	16.1600	25.7034	30.1911	$11 \times 22 \times 14$	$8 \times 14 \times 8$	51393
14.7333	16.1249	25.6254	30.1205	$11 \times 24 \times 12$	$8 \times 14 \times 6$	47953
14.8815	16.1358	25.6804	30.1447	$11 \times 24 \times 12$	$8 \times 16 \times 6$	47953
15.2550	16.1372	25.8970	30.1594	$14 \times 22 \times 12$	$11 \times 14 \times 6$	56177

Table 4.17: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 10$ obtained with the flux constraints at the edges and corners. ‘Post mesh’ refers to the number of bricks in the mesh that are inside the dielectric post.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Post mesh	Number of unknowns
15.1099	16.0948	25.6041	30.1485	$8 \times 12 \times 10$	$5 \times 6 \times 4$	14257
15.0895	16.0901	25.6024	30.1287	$8 \times 16 \times 10$	$5 \times 8 \times 4$	19097
15.0799	16.0891	25.5998	30.1227	$8 \times 18 \times 10$	$5 \times 10 \times 4$	21521
15.1040	16.0889	25.6087	30.1265	$8 \times 20 \times 10$	$5 \times 10 \times 4$	23937
15.0770	16.0887	25.5990	30.1207	$8 \times 20 \times 10$	$5 \times 12 \times 4$	23945
15.0638	16.0885	25.5829	30.1193	$8 \times 20 \times 12$	$5 \times 12 \times 6$	28849
15.1990	16.0938	25.5948	30.1332	$8 \times 20 \times 16$	$5 \times 12 \times 8$	38649
15.0964	16.0874	25.6103	30.1165	$11 \times 20 \times 12$	$7 \times 12 \times 6$	40001
15.0353	16.0874	25.5813	30.1142	$11 \times 20 \times 12$	$8 \times 12 \times 6$	40009
15.0340	16.0872	25.5808	30.1133	$11 \times 22 \times 12$	$8 \times 14 \times 6$	44057
15.0384	16.0874	25.5797	30.1135	$11 \times 22 \times 14$	$8 \times 14 \times 8$	51545
15.0459	16.0867	25.5860	30.1160	$11 \times 24 \times 12$	$8 \times 14 \times 6$	48097
15.0343	16.0872	25.5808	30.1130	$11 \times 24 \times 12$	$8 \times 16 \times 6$	48105
15.0416	16.0872	25.5833	30.1132	$14 \times 22 \times 12$	$11 \times 14 \times 6$	56345

Table 4.18: Eigenvalues of the cavity containing the dielectric post with relative permittivity $\epsilon_r = 10$ obtained with the software package HFSS [46]. The calculations were performed using second order edge elements with adaptive mesh refinement. The convergence parameter for the adaptive mesh refinement is λ_{target} .

k_1^2	k_2^2	k_3^2	k_4^2	λ_{target}	Number of unknowns
14.5226	16.1306	25.4529	30.1676	0.40	1341
14.5226	16.1306	25.4529	30.1676	0.20	1341
14.5959	16.1026	25.4837	30.2778	0.10	2181
14.6530	16.0790	25.4653	30.0831	0.04	9852
14.7232	16.0784	25.4952	30.0821	0.02	53436

Figure 4.21: The eigenvalue for the lowest frequency resonant mode for the cavity containing a dielectric post with relative permittivity $\epsilon_r = 10$. The results obtained with the new basis functions use the magnetic field formulation and the electric field formulation with two methods to treat the singularities at the edges and corners. The results obtained with HFSS second order edge elements with adaptive mesh refinement. The scale for k^2 varies by approximately 7%.

are converging. (Note that if the magnetic field formulation were used with edge elements, then the boundary condition $\mathbf{H} \cdot \mathbf{n} = 0$ could not be imposed since the normal component of the field on the face of a tetrahedron is not one of the degrees of freedom.) The range of all of the eigenvalues, k_1^2 , is 4.6% among those obtained with the flux constraints, the magnetic field formulation and HFSS. In spite of the fact that the piecewise polynomials cannot accurately model the infinite electric field on the edges and corners, the values obtained using the different methods agree reasonably well.

4.3.6 Example: Dielectric resonator filter

This subsection contains results for the dielectric resonator developed by Zhang and Mansour [51–53]. The problem was solved in section 2.5.3 using the magnetic field formulation. The dimensions of the filter are given in figure 2.7. The new results in this subsection are obtained using the electric field formulation with both of the methods for treating the singularities at edges and corners described in this chapter.

Table 4.19 contains the four lowest eigenvalues for different meshes, as well as the results of section 2.5.3 obtained with the magnetic field formulation. Results from the software package HFSS [46] with second order edge elements and adaptive mesh refinement are included at the bottom of the table. The lowest eigenvalue, k_1^2 , is plotted in figure 4.22. The values obtained using all four methods are converging. The values obtained from each method with the greatest number of unknowns differ by 0.5%.

The second and fourth lowest eigenvalues obtained using the continuous field approximation are not in agreement with the other methods. The projection of the electric field in the plane $x = 5/18$ is plotted for the lowest four resonant modes in figure 4.23 using both methods for treating the singularities. The field patterns for modes 2, 3 and 4 are noticeably different between the two different methods. The eigenvalues obtained using the flux constraints are in better agreement with the other methods, and the field pattern is much different from the continuous field approximation.

Table 4.19: Eigenvalues of the dielectric resonator developed by Zhang and Mansour. The dimensions are given in figure 2.7.

k_1^2	k_2^2	k_3^2	k_4^2	Mesh	Unknowns	Method
3.5756	3.6123	3.8727	4.2503	$9 \times 8 \times 15$	15973	continuous ϵ
3.5340	3.6513	3.8703	4.2393	$9 \times 16 \times 15$	32485	continuous ϵ
3.5287	3.5435	3.8188	4.1657	$9 \times 16 \times 30$	65545	continuous ϵ
3.5427	3.7457	4.1651	4.9983	$9 \times 8 \times 15$	16379	flux constraints
3.5316	3.7456	4.1516	4.9471	$9 \times 16 \times 15$	33019	flux constraints
3.5302	3.7178	4.0392	4.9218	$9 \times 16 \times 30$	66279	flux constraints
3.6083	3.7560	4.0288	4.8539	$9 \times 8 \times 15$	18707	magnetic field
3.5865	3.7164	3.9763	4.8218	$9 \times 16 \times 15$	36875	magnetic field
3.5412	3.7019	3.9581	4.7910	$9 \times 16 \times 30$	73175	magnetic field
3.5385	3.6971	3.9523	4.7869	$9 \times 24 \times 30$	109223	magnetic field
3.5250	3.6668	3.9122	4.7257	$\lambda_{target} = 0.40$	8670	HFSS
3.5259	3.6708	3.9142	4.7362	$\lambda_{target} = 0.20$	9426	HFSS
3.5200	3.6712	3.9163	4.7414	$\lambda_{target} = 0.10$	20961	HFSS
3.5193	3.6738	3.9203	4.7452	$\lambda_{target} = 0.04$	63369	HFSS
3.5193	3.6759	3.9242	4.7509	$\lambda_{target} = 0.02$	199884	HFSS

Figure 4.22: The eigenvalue for the lowest frequency resonant mode for the dielectric resonator filter. The results obtained with the new basis functions use the magnetic field formulation and the electric field formulation with two methods to treat the singularities at the edges and corners. The results from HFSS were obtained using second order edge elements with adaptive mesh refinement.

(a) Singularities at edges treated using method 1, the continuous field approximation.

(b) Singularities at edges treated using method 2, ensuring that the flux is zero through a surface containing each edge.

Figure 4.23: Electric field components $E_y\hat{\mathbf{y}} + E_z\hat{\mathbf{z}}$ plotted in the plane $x = 5/18$ for the $9 \times 16 \times 30$ mesh. The dimensions are given in figure 2.7. (The plane $x = 0$ corresponds to the bottom of the metal case.)

4.4 Conclusions

This chapter described methods for solving problems where the field possesses singularities at edges and corners of material boundaries. The results for perfect conductors using the electric field formulation are summarized in the following list.

1. There are no spurious modes and the eigenvalues are reasonably accurate (on the order of 1%).
2. As the mesh is refined, the eigenvalues converge if the field is zero on the edge and they diverge if the magnitude of the field is infinite.
3. Refining the bricks adjacent to an edge of a perfect conductor is effective.
4. The eigenvalues for problems containing corners of perfect conductors depend sensitively on the mesh.

In contrast, the method developed for edges and corners of perfect conductors using the magnetic field formulation is not accurate. The constraints result in $\mathbf{H} = 0$ in one of the bricks opposite to the edge or corner. The eigenvalues are accurate if the field *is* zero at the edge or corner, but in cases where the magnitude of the field is infinite, the approximation is poor.

The methods for solving problems using the electric field formulation that possess singularities at edges and corners of dielectric boundaries are equally applicable to solving problems using the magnetic field formulation that possess the corresponding singularities at magnetic material boundaries. The results are summarized in the following list.

1. If there are no constraints used at an edge or corner, that is, if the normal components of the field are discontinuous and free to vary, then there are spurious modes. The eigenvalues of the spurious modes increase as the mesh is refined around the edges and corners.

2. The constraints are used to eliminate the spurious modes. There are two sets of constraints that can be applied: the continuous permittivity approximation and the flux constraints.
3. Mesh refinement around the edges and corners is not used with the constraints because in most cases the accuracy of the eigenvalues is worse.
4. The flux constraints result in better agreement with the magnetic field formulation, where the field is continuous across dielectric boundaries, and edge elements compared to the continuous permittivity approximation.
5. The continuous permittivity approximation contains an inconsistency: the resulting permittivity depends on the electric field, that is, the permittivity is non-linear and inhomogeneous within the brick at the edge or corner, and yet it is assumed to be constant when implementing the divergence constraints.
6. The eigenvalues of modes possessing singularities depend sensitively on the mesh. There were two heuristically determined criteria used for refining the mesh: the relative number of bricks inside the dielectric should increase while keeping the bricks as close to cubic as possible. This is not an algorithm with unique output, but rather a guide for “trial and error”. The eigenvalues for modes that did not possess singularities did not depend sensitively on the mesh.

The eigenvalues obtained with the software package HFSS [46] used second order edge elements with adaptive mesh refinement. Those eigenvalues were insensitive to the mesh in cases where the field was continuous across the edges and they diverged as the mesh was refined if the magnitude of the field was infinite. However, the range of the eigenvalues obtained with different meshes was smaller using HFSS than with the new basis functions in cases where the fields are singular.

A suggestion for future work is to develop basis functions that contain the singular behaviour of the field at edges and corners. A major challenge is to simultaneously solve

the curl and divergence equations, as well to maintain continuity of the field between neighbouring subdomains that do not contain the singularity. However, it is also noteworthy that the polarizability of the dielectric does not remain linear as the electric field increases indefinitely, and thus ϵ is not constant. For physical devices, the edges and corners are not perfectly sharp. Furthermore, as the distance scale near the interface decreases, the continuum hypothesis breaks down and the atomic nature of matter becomes significant.

Chapter 5

Conclusions

5.1 Summary of thesis

This thesis describes new basis functions for solving partial differential equations of vector fields using the finite element method. The basis functions are a combination of cubic Hermite splines and second order Lagrange interpolation polynomials, defined in equations (2.14)–(2.16). They are used to solve the curl equation while the divergence of the field is set as a constraint for problems where the geometry conforms to a Cartesian coordinate system. The domain is divided into a mesh of bricks and the divergence is modelled to second order in x , y and z within each brick.

The method is modified to incorporate mesh refinement. The mesh is refined by cutting selected bricks into $2 \times 2 \times 2$ bricks of equal size. There is a change in the node pattern at an interface where mesh refinement occurs, which necessitates additional constraints for the hanging nodes and a modified implementation of the divergence constraints.

There are methods for solving problems containing singularities at material interfaces that form edges and corners. This includes perfect conductors, dielectrics causing singularities in the electric field and magnetic materials causing singularities in the magnetic field.

The primary test problem is the calculation of resonant frequencies of 3-dimensional cavities. The variational formulation for this problem is described using both the electric field and the magnetic field. This formulation does not determine the divergence of the field which is why the divergence needs to be set as a constraint. This is an eigenvalue problem: if the divergence is not set as a constraint then there are additional non-physical eigenvalues and eigenfunctions, referred to as spurious modes. This is the reason why the resonant cavity is the test problem. When the electric field formulation is used, there are no spurious modes. When the magnetic field formulation is used, there are some spurious modes that arise because not all of the boundary conditions and divergence constraints can be imposed simultaneously. However, these modes can easily be identified by examining the magnetic field on the cavity boundary.

The resonant frequencies of several different cavities are calculated using the new basis functions. There is good agreement with exact values in cases where they exist. In other cases, the agreement with experimental measurements and other numerical methods, notably with second order edge elements with adaptive mesh refinement via the commercial software package HFSS, is good.

The method has been modified for cylindrical coordinates provided the domain does not contain the origin, as discussed in Appendix C.

5.2 Key contributions

The key contributions of this thesis are:

1. The basis functions defined in equations (2.14)–(2.16) are used to solve the curl equation while allowing for the divergence to be implemented as a constraint.
2. A mesh refinement procedure has been developed to increase the number of degrees of freedom in a given region.

3. The method is modified to solve problems with singularities where material boundaries form edges and corners.
4. The method is extended to cylindrical coordinates provided the domain does not contain the coordinate axis. (The new basis functions result in infinite divergence and curl on the coordinate axis.)

5.3 Future work

There are six suggestions for future work.

1. The example calculations have been resonant cavities with perfectly conducting walls. The tangential components of the electric field or the normal component of the magnetic field are set to zero on the boundary. For unbounded problems, such as scattering, a method for truncating the domain needs to be implemented. Based on a preliminary investigation, the perfectly matched layer method [64, 65] is appropriate for the basis functions and will require the least amount of time to implement in the code.
2. The example calculations have been done in the frequency domain. The work can be extended for use in the time domain, including a dispersion analysis.
3. The example calculations have been resonant cavities with rectangular or cylindrical geometries. However, the method is applicable to other problems with rectangular or cylindrical geometries involving partial differential equations of vector fields, such as microstrip circuits [66] and ultrasonic motors [67].
4. Basis functions that contain the singular behaviour of the field at edges and corners would increase the accuracy of the calculations for a given number of unknowns. However, it is not easy to find basis functions that can simultaneously solve the

curl and divergence equations, as well to maintain continuity of the field between neighbouring subdomains that do not contain the singularity.

5. The mesh refinement procedure can be modified so that it is done adaptively. Presently, a list of bricks to be refined is given as input. However, the list could be generated automatically in an iterative way: compute the solution with a uniform mesh, refine bricks where the changes in the field are greatest, compute the solution for the modified mesh, and repeat until a convergence criterion is met.
6. Attempts to generalize the method for arbitrary, hexahedral bricks were not successful. For a hexahedral brick, the local coordinate system is not orthogonal. Additional terms in the divergence equation do not yield simple, non-trivial constraints if a product of cubic Hermite splines and second order Lagrange interpolation polynomials are used. However, the method is successfully applied in cylindrical coordinates provided that the singularity in the coordinate transformation at the axis is excluded, as discussed in Appendix C. This suggests that the method can be extended for a mesh consisting of orthogonal, curvilinear bricks provided there are no singularities in the coordinate transformation.

Appendix A

List of divergence constraints

The vector field is expanded in terms of a linear combination of cubic Hermite splines and second order Lagrange interpolation polynomials, which is given in equations (2.14) – (2.16). The definition of the basis functions is repeated here for convenience.

$$E_x(x, y, z) = \sum_{i=0}^3 \sum_{j=0}^2 \sum_{k=0}^2 c_{ijk}^x \Delta_{xi} H_i(x) L_j(y) L_k(z) \quad (\text{A.1})$$

$$E_y(x, y, z) = \sum_{i=0}^2 \sum_{j=0}^3 \sum_{k=0}^2 c_{ijk}^y \Delta_{yj} L_i(x) H_j(y) L_k(z) \quad (\text{A.2})$$

$$E_z(x, y, z) = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^3 c_{ijk}^z \Delta_{zk} L_i(x) L_j(y) H_k(z) \quad (\text{A.3})$$

The mixture of cubic and quadratic polynomials is chosen such that the divergence can be expressed as a product of second order Lagrange interpolation polynomials in each Cartesian coordinate. There are three degrees of freedom for each quadratic polynomial and so a product of three polynomials means there are 27 degrees of freedom for the divergence in each brick. The divergence constraints are obtained by evaluating the divergence at each corner of the brick, the midpoint of each edge, the centre of each face and the centre of the brick. The constraints that arise from each corner are similar to each other. Likewise, the constraints at the midpoint of each edge are similar and the constraints at the centre of each face are similar to each other. All of the constraints are

listed below for completeness.

Each coefficient in the basis functions corresponds to the value of one of the field components E_x , E_y or E_z or the one of the partial derivatives $\partial E_x/\partial x$, $\partial E_y/\partial y$ or $\partial E_z/\partial z$. The positions of all of the nodes are plotted in figures A.1 – A.3. Each node is labeled by its appropriate coefficient for reference.

A.1 Corner constraints

The corner constraints are listed beside the node for the divergence in the local coordinate system.

$$(0, 0, 0) \quad d_{000} = c_{100}^x + c_{010}^y + c_{001}^z \quad (\text{A.4})$$

$$(0, 0, 1) \quad d_{002} = c_{102}^x + c_{012}^y + c_{003}^z \quad (\text{A.5})$$

$$(0, 1, 0) \quad d_{020} = c_{120}^x + c_{030}^y + c_{021}^z \quad (\text{A.6})$$

$$(0, 1, 1) \quad d_{022} = c_{122}^x + c_{032}^y + c_{023}^z \quad (\text{A.7})$$

$$(1, 0, 0) \quad d_{200} = c_{300}^x + c_{210}^y + c_{201}^z \quad (\text{A.8})$$

$$(1, 0, 1) \quad d_{202} = c_{302}^x + c_{212}^y + c_{203}^z \quad (\text{A.9})$$

$$(1, 1, 0) \quad d_{220} = c_{320}^x + c_{230}^y + c_{221}^z \quad (\text{A.10})$$

$$(1, 1, 1) \quad d_{222} = c_{322}^x + c_{232}^y + c_{223}^z \quad (\text{A.11})$$

Let the subscripts be appended by three integers, (l, m, n) , representing the position of a given brick in the mesh. Using local coordinates for each brick, $x = 1$ for the l^{th} coincides with $x = 0$ for the $(l + 1)^{\text{th}}$ brick. The constraint at the corner $(1, 1, 1)$ for the brick labeled by (l, m, n) needs to be compared to the constraints from the seven other bricks that share that corner, for example, at the corner $(0, 0, 0)$ for the brick labeled by

(a) Coefficients for E_x . (b) Coefficients for $\partial E_x / \partial x$.Figure A.1: Node locations for E_x and $\partial E_x / \partial x$.

(a) Coefficients for E_y . (b) Coefficients for $\partial E_y / \partial y$.Figure A.2: Node locations for E_y and $\partial E_y / \partial y$.

(a) Coefficients for E_z . (b) Coefficients for $\partial E_z / \partial z$.Figure A.3: Node locations for E_z and $\partial E_z / \partial z$.

$(l+1, m+1, n+1)$. The constraints are listed equations (A.12)–(A.19) below.

$$d_{0,0,0,l+1,m+1,n+1} = c_{1,0,0,l+1,m+1,n+1}^x + c_{0,1,0,l+1,m+1,n+1}^y + c_{0,0,1,l+1,m+1,n+1}^z \quad (\text{A.12})$$

$$d_{0,0,2,l+1,m+1,n} = c_{1,0,2,l+1,m+1,n}^x + c_{0,1,2,l+1,m+1,n}^y + c_{0,0,3,l+1,m+1,n}^z \quad (\text{A.13})$$

$$d_{0,2,0,l+1,m,n+1} = c_{1,2,0,l+1,m,n+1}^x + c_{0,3,0,l+1,m,n+1}^y + c_{0,2,1,l+1,m,n+1}^z \quad (\text{A.14})$$

$$d_{0,2,2,l+1,m,n} = c_{1,2,2,l+1,m,n}^x + c_{0,3,2,l+1,m,n}^y + c_{0,2,3,l+1,m,n}^z \quad (\text{A.15})$$

$$d_{2,0,0,l,m+1,n+1} = c_{3,0,0,l,m+1,n+1}^x + c_{2,1,0,l,m+1,n+1}^y + c_{2,0,1,l,m+1,n+1}^z \quad (\text{A.16})$$

$$d_{2,0,2,l,m+1,n} = c_{3,0,2,l,m+1,n}^x + c_{2,1,2,l,m+1,n}^y + c_{2,0,3,l,m+1,n}^z \quad (\text{A.17})$$

$$d_{2,2,0,l,m,n+1} = c_{3,2,0,l,m,n+1}^x + c_{2,3,0,l,m,n+1}^y + c_{2,2,1,l,m,n+1}^z \quad (\text{A.18})$$

$$d_{2,2,2,l,m,n} = c_{3,2,2,l,m,n}^x + c_{2,3,2,l,m,n}^y + c_{2,2,3,l,m,n}^z \quad (\text{A.19})$$

If the partial derivatives and the divergence are continuous, then

$$\begin{aligned} c_{1,0,0,l+1,m+1,n+1}^x &= c_{1,0,2,l+1,m+1,n}^x = c_{1,2,0,l+1,m,n+1}^x = c_{1,2,2,l+1,m,n}^x \\ &= c_{3,0,0,l,m+1,n+1}^x = c_{3,0,2,l,m+1,n}^x = c_{3,2,0,l,m,n+1}^x = c_{3,2,2,l,m,n}^x \end{aligned} \quad (\text{A.20})$$

$$\begin{aligned} c_{0,1,0,l+1,m+1,n+1}^y &= c_{0,1,2,l+1,m+1,n}^y = c_{0,3,0,l+1,m,n+1}^y = c_{0,3,2,l+1,m,n}^y \\ &= c_{2,1,0,l,m+1,n+1}^y = c_{2,1,2,l,m+1,n}^y = c_{2,3,0,l,m,n+1}^y = c_{2,3,2,l,m,n}^y \end{aligned} \quad (\text{A.21})$$

$$\begin{aligned} c_{0,0,1,l+1,m+1,n+1}^z &= c_{0,0,3,l+1,m+1,n}^z = c_{0,2,1,l+1,m,n+1}^z = c_{0,2,3,l+1,m,n}^z \\ &= c_{2,0,1,l,m+1,n+1}^z = c_{2,0,3,l,m+1,n}^z = c_{2,2,1,l,m,n+1}^z = c_{2,2,3,l,m,n}^z \end{aligned} \quad (\text{A.22})$$

$$\begin{aligned}
d_{0,0,0,l+1,m+1,n+1} &= d_{0,0,2,l+1,m+1,n} = d_{0,2,0,l+1,m,n+1} = d_{0,2,2,l+1,m,n} \\
&= d_{2,0,0,l,m+1,n+1} = d_{2,0,2,l,m+1,n} = d_{2,2,0,l,m,n+1} = d_{2,2,2,l,m,n}
\end{aligned} \tag{A.23}$$

which means that the divergence constraints are identical for the corner that is common to all eight bricks. Thus, there is only one independent constraint for each corner in the mesh.

A.2 Edge constraints

There is a divergence constraint at the midpoint of each of the 12 edges of each brick. All of these divergence constraints are listed below beside the position where they occur.

$$(0, 0, \frac{1}{2}) \quad d_{001} = c_{101}^x + c_{011}^y - \frac{3}{2\delta_z} c_{000}^z - \frac{1}{4} c_{001}^z + \frac{3}{2\delta_z} c_{002}^z - \frac{1}{4} c_{003}^z \tag{A.24}$$

$$(0, 1, \frac{1}{2}) \quad d_{021} = c_{121}^x + c_{031}^y - \frac{3}{2\delta_z} c_{020}^z - \frac{1}{4} c_{021}^z + \frac{3}{2\delta_z} c_{022}^z - \frac{1}{4} c_{023}^z \tag{A.25}$$

$$(1, 0, \frac{1}{2}) \quad d_{201} = c_{301}^x + c_{211}^y - \frac{3}{2\delta_z} c_{200}^z - \frac{1}{4} c_{201}^z + \frac{3}{2\delta_z} c_{202}^z - \frac{1}{4} c_{203}^z \tag{A.26}$$

$$(1, 1, \frac{1}{2}) \quad d_{221} = c_{321}^x + c_{231}^y - \frac{3}{2\delta_z} c_{220}^z - \frac{1}{4} c_{221}^z + \frac{3}{2\delta_z} c_{222}^z - \frac{1}{4} c_{223}^z \tag{A.27}$$

$$(\frac{1}{2}, 0, 0) \quad d_{100} = c_{110}^y + c_{101}^z - \frac{3}{2\delta_x} c_{000}^x - \frac{1}{4} c_{100}^x + \frac{3}{2\delta_x} c_{200}^x - \frac{1}{4} c_{300}^x \tag{A.28}$$

$$(\frac{1}{2}, 0, 1) \quad d_{102} = c_{112}^y + c_{103}^z - \frac{3}{2\delta_x} c_{002}^x - \frac{1}{4} c_{102}^x + \frac{3}{2\delta_x} c_{202}^x - \frac{1}{4} c_{302}^x \tag{A.29}$$

$$(\frac{1}{2}, 1, 0) \quad d_{120} = c_{130}^y + c_{121}^z - \frac{3}{2\delta_x} c_{020}^x - \frac{1}{4} c_{120}^x + \frac{3}{2\delta_x} c_{220}^x - \frac{1}{4} c_{320}^x \tag{A.30}$$

$$(\frac{1}{2}, 1, 1) \quad d_{122} = c_{132}^y + c_{123}^z - \frac{3}{2\delta_x} c_{022}^x - \frac{1}{4} c_{122}^x + \frac{3}{2\delta_x} c_{222}^x - \frac{1}{4} c_{322}^x \tag{A.31}$$

$$(0, \frac{1}{2}, 0) \quad d_{010} = c_{011}^z + c_{110}^x - \frac{3}{2\delta_y} c_{000}^y - \frac{1}{4} c_{010}^y + \frac{3}{2\delta_y} c_{020}^y - \frac{1}{4} c_{030}^y \tag{A.32}$$

$$(0, \frac{1}{2}, 1) \quad d_{012} = c_{013}^z + c_{112}^x - \frac{3}{2\delta_y} c_{002}^y - \frac{1}{4} c_{012}^y + \frac{3}{2\delta_y} c_{022}^y - \frac{1}{4} c_{032}^y \tag{A.33}$$

$$(1, \frac{1}{2}, 0) \quad d_{210} = c_{211}^z + c_{310}^x - \frac{3}{2\delta_y} c_{200}^y - \frac{1}{4} c_{210}^y + \frac{3}{2\delta_y} c_{220}^y - \frac{1}{4} c_{230}^y \quad (\text{A.34})$$

$$(1, \frac{1}{2}, 1) \quad d_{212} = c_{213}^z + c_{312}^x - \frac{3}{2\delta_y} c_{202}^y - \frac{1}{4} c_{212}^y + \frac{3}{2\delta_y} c_{222}^y - \frac{1}{4} c_{232}^y \quad (\text{A.35})$$

Each edge is common to four bricks, except at the boundary. The first four constraints listed above are for edges that are parallel to the z -axis. Consider the constraint that is common to the edge whose midpoint is at $(1, 1, \frac{1}{2})$ of the brick labeled by the integers (l, m, n) .

$$\begin{aligned} d_{0,0,1,l+1,m+1,n} &= c_{1,0,1,l+1,m+1,n}^x + c_{0,1,1,l+1,m+1,n}^y \\ &\quad - \frac{3}{2\delta_{z,l+1,m+1,n}} c_{0,0,0,l+1,m+1,n}^z - \frac{1}{4} c_{0,0,1,l+1,m+1,n}^z \\ &\quad + \frac{3}{2\delta_{z,l+1,m+1,n}} c_{0,0,2,l+1,m+1,n}^z - \frac{1}{4} c_{0,0,3,l+1,m+1,n}^z \end{aligned} \quad (\text{A.36})$$

$$\begin{aligned} d_{0,2,1,l+1,m,n} &= c_{1,2,1,l+1,m,n}^x + c_{0,3,1,l+1,m,n}^y \\ &\quad - \frac{3}{2\delta_{z,l+1,m,n}} c_{0,2,0,l+1,m,n}^z - \frac{1}{4} c_{0,2,1,l+1,m,n}^z \\ &\quad + \frac{3}{2\delta_{z,l+1,m,n}} c_{0,2,2,l+1,m,n}^z - \frac{1}{4} c_{0,2,3,l+1,m,n}^z \end{aligned} \quad (\text{A.37})$$

$$\begin{aligned} d_{2,0,1,l,m+1,n} &= c_{3,0,1,l,m+1,n}^x + c_{2,1,1,l,m+1,n}^y \\ &\quad - \frac{3}{2\delta_{z,l,m+1,n}} c_{2,0,0,l,m+1,n}^z - \frac{1}{4} c_{2,0,1,l,m+1,n}^z \\ &\quad + \frac{3}{2\delta_{z,l,m+1,n}} c_{2,0,2,l,m+1,n}^z - \frac{1}{4} c_{2,0,3,l,m+1,n}^z \end{aligned} \quad (\text{A.38})$$

$$\begin{aligned} d_{2,2,1,l,m,n} &= c_{3,2,1,l,m,n}^x + c_{2,3,1,l,m,n}^y \\ &\quad - \frac{3}{2\delta_{z,l,m,n}} c_{2,2,0,l,m,n}^z - \frac{1}{4} c_{2,2,1,l,m,n}^z \\ &\quad + \frac{3}{2\delta_{z,l,m,n}} c_{2,2,2,l,m,n}^z - \frac{1}{4} c_{2,2,3,l,m,n}^z \end{aligned} \quad (\text{A.39})$$

The bricks are common to an edge that is parallel to the z -axis and so all four bricks have the same height, that is,

$$\delta_{z,l+1,m+1,n} = \delta_{z,l+1,m,n} = \delta_{z,l,m+1,n} = \delta_{z,l,m,n} . \quad (\text{A.40})$$

If the component of the field parallel to the z -axis is continuous, then

$$c_{0,0,0,l+1,m+1,n}^z = c_{0,2,0,l+1,m,n}^z = c_{2,0,0,l,m+1,n}^z = c_{2,2,0,l,m,n}^z \quad (\text{A.41})$$

$$c_{0,0,1,l+1,m+1,n}^z = c_{0,2,1,l+1,m,n}^z = c_{2,0,1,l,m+1,n}^z = c_{2,2,1,l,m,n}^z \quad (\text{A.42})$$

$$c_{0,0,2,l+1,m+1,n}^z = c_{0,2,2,l+1,m,n}^z = c_{2,0,2,l,m+1,n}^z = c_{2,2,2,l,m,n}^z \quad (\text{A.43})$$

$$c_{0,0,3,l+1,m+1,n}^z = c_{0,2,3,l+1,m,n}^z = c_{2,0,3,l,m+1,n}^z = c_{2,2,3,l,m,n}^z . \quad (\text{A.44})$$

If the partial derivatives of the field components perpendicular to the edge are continuous, then

$$c_{1,0,1,l+1,m+1,n}^x = c_{1,2,1,l+1,m,n}^x = c_{3,0,1,l,m+1,n}^x = c_{3,2,1,l,m,n}^x \quad (\text{A.45})$$

$$c_{0,1,1,l+1,m+1,n}^y = c_{0,3,1,l+1,m,n}^y = c_{2,1,1,l,m+1,n}^y = c_{2,3,1,l,m,n}^y \quad (\text{A.46})$$

and also

$$d_{0,0,1,l+1,m+1,n} = d_{0,2,1,l+1,m,n} = d_{2,0,1,l,m+1,n} = d_{2,2,1,l,m,n} . \quad (\text{A.47})$$

This means that the constraints at the midpoint of an edge parallel to the z -axis are the same for all four bricks that share that edge. Similar results are obtained for edges that are parallel to the x -axis and the y -axis. Thus, there is only one independent constraint at the midpoint of each edge in the mesh.

A.3 Face constraints

There is a node for the divergence equation at the centre of each of the six faces of each brick. For the face that is in the plane $x = 0$ the node is located at $(0, \frac{1}{2}, \frac{1}{2})$ and the divergence constraint is

$$\begin{aligned} d_{011} = c_{111}^x & - \frac{3}{2\delta_y} c_{001}^y - \frac{1}{4} c_{011}^y + \frac{3}{2\delta_y} c_{021}^y - \frac{1}{4} c_{031}^y \\ & - \frac{3}{2\delta_z} c_{010}^z - \frac{1}{4} c_{011}^z + \frac{3}{2\delta_z} c_{012}^z - \frac{1}{4} c_{013}^z \end{aligned} \quad (\text{A.48})$$

while for the face that is in the plane $x = 1$ the node is located at $(1, \frac{1}{2}, \frac{1}{2})$ and the divergence constraint is

$$\begin{aligned} d_{211} = c_{311}^x & - \frac{3}{2\delta_y} c_{201}^y - \frac{1}{4} c_{211}^y + \frac{3}{2\delta_y} c_{221}^y - \frac{1}{4} c_{231}^y \\ & - \frac{3}{2\delta_z} c_{210}^z - \frac{1}{4} c_{211}^z + \frac{3}{2\delta_z} c_{212}^z - \frac{1}{4} c_{213}^z . \end{aligned} \quad (\text{A.49})$$

For the face that is in the plane $y = 0$ the node for the divergence equation is located at $(\frac{1}{2}, 0, \frac{1}{2})$ and the divergence constraint is

$$\begin{aligned} d_{101} = c_{111}^y & - \frac{3}{2\delta_z} c_{100}^z - \frac{1}{4} c_{101}^z + \frac{3}{2\delta_z} c_{102}^z - \frac{1}{4} c_{103}^z \\ & - \frac{3}{2\delta_x} c_{001}^x - \frac{1}{4} c_{101}^x + \frac{3}{2\delta_x} c_{201}^x - \frac{1}{4} c_{301}^x \end{aligned} \quad (\text{A.50})$$

while for the face that is in the plane $y = 1$ the node for the divergence equation is at $(\frac{1}{2}, 1, \frac{1}{2})$ and the divergence constraint is

$$\begin{aligned} d_{121} = c_{131}^y & - \frac{3}{2\delta_z} c_{120}^z - \frac{1}{4} c_{121}^z + \frac{3}{2\delta_z} c_{122}^z - \frac{1}{4} c_{123}^z \\ & - \frac{3}{2\delta_x} c_{021}^x - \frac{1}{4} c_{121}^x + \frac{3}{2\delta_x} c_{221}^x - \frac{1}{4} c_{321}^x . \end{aligned} \quad (\text{A.51})$$

Similarly, for the face that is in the plane $z = 0$, the node for the divergence constraint is located at $(\frac{1}{2}, \frac{1}{2}, 0)$ and the divergence constraint is

$$\begin{aligned} d_{110} = c_{111}^z & - \frac{3}{2\delta_x} c_{010}^x - \frac{1}{4} c_{110}^x + \frac{3}{2\delta_x} c_{210}^x - \frac{1}{4} c_{310}^x \\ & - \frac{3}{2\delta_y} c_{100}^y - \frac{1}{4} c_{110}^y + \frac{3}{2\delta_y} c_{120}^y - \frac{1}{4} c_{130}^y \end{aligned} \quad (\text{A.52})$$

and finally for the face that is in the plane $z = 1$ the node is located at $(\frac{1}{2}, \frac{1}{2}, 1)$ and the divergence constraint is

$$\begin{aligned} d_{112} = c_{113}^z & - \frac{3}{2\delta_x} c_{012}^x - \frac{1}{4} c_{112}^x + \frac{3}{2\delta_x} c_{212}^x - \frac{1}{4} c_{312}^x \\ & - \frac{3}{2\delta_y} c_{102}^y - \frac{1}{4} c_{112}^y + \frac{3}{2\delta_y} c_{122}^y - \frac{1}{4} c_{132}^y . \end{aligned} \quad (\text{A.53})$$

Consider the constraint in the plane $x = 1$ for the brick labeled by the integers (l, m, n) and the constraint in the plane $x = 0$ for the brick labeled by the integers $(l + 1, m, n)$.

$$\begin{aligned} d_{2,1,1,l,m,n} & = c_{3,1,1,l,m,n}^x \\ & - \frac{3}{2\delta_{y,l,m,n}} c_{2,0,1,l,m,n}^y - \frac{1}{4} c_{2,1,1,l,m,n}^y \\ & + \frac{3}{2\delta_{y,l,m,n}} c_{2,2,1,l,m,n}^y - \frac{1}{4} c_{2,3,1,l,m,n}^y \\ & - \frac{3}{2\delta_{z,l,m,n}} c_{2,1,0,l,m,n}^z - \frac{1}{4} c_{2,1,1,l,m,n}^z \\ & + \frac{3}{2\delta_{z,l,m,n}} c_{2,1,2,l,m,n}^z - \frac{1}{4} c_{2,1,3,l,m,n}^z \end{aligned} \quad (\text{A.54})$$

$$\begin{aligned} d_{0,1,1,l+1,m,n} & = c_{1,1,1,l+1,m,n}^x \\ & - \frac{3}{2\delta_{y,l+1,m,n}} c_{0,0,1,l+1,m,n}^y - \frac{1}{4} c_{0,1,1,l+1,m,n}^y \\ & + \frac{3}{2\delta_{y,l+1,m,n}} c_{0,2,1,l+1,m,n}^y - \frac{1}{4} c_{0,3,1,l+1,m,n}^y \\ & - \frac{3}{2\delta_{z,l+1,m,n}} c_{0,1,0,l+1,m,n}^z - \frac{1}{4} c_{0,1,1,l+1,m,n}^z \\ & + \frac{3}{2\delta_{z,l+1,m,n}} c_{0,1,2,l+1,m,n}^z - \frac{1}{4} c_{0,1,3,l+1,m,n}^z \end{aligned} \quad (\text{A.55})$$

The face is the same size for each brick, so $\delta_{y,l,m,n} = \delta_{y,l+1,m,n}$ and $\delta_{z,l,m,n} = \delta_{z,l+1,m,n}$. If the tangential components of the field are continuous across the face of the brick, then

$$c_{2,0,1,l,m,n}^y = c_{0,0,1,l+1,m,n}^y \quad (\text{A.56})$$

$$c_{2,1,1,l,m,n}^y = c_{0,1,1,l+1,m,n}^y \quad (\text{A.57})$$

$$c_{2,2,1,l,m,n}^y = c_{0,2,1,l+1,m,n}^y \quad (\text{A.58})$$

$$c_{2,3,1,l,m,n}^y = c_{0,3,1,l+1,m,n}^y \quad (\text{A.59})$$

$$c_{2,1,0,l,m,n}^z = c_{0,1,0,l+1,m,n}^z \quad (\text{A.60})$$

$$c_{2,1,1,l,m,n}^z = c_{0,1,1,l+1,m,n}^z \quad (\text{A.61})$$

$$c_{2,1,2,l,m,n}^z = c_{0,1,2,l+1,m,n}^z \quad (\text{A.62})$$

$$c_{2,1,3,l,m,n}^z = c_{0,1,3,l+1,m,n}^z \quad (\text{A.63})$$

If the partial derivatives of the field component that is perpendicular to the face are continuous, then $c_{3,1,1,l,m,n}^x = c_{1,1,1,l+1,m,n}^x$ and also $d_{2,1,1,l,m,n} = d_{0,1,1,l+1,m,n}$. This implies that the divergence constraints that arise at the node that is in the centre of the face common to both bricks are the same. Similar results hold for the faces that lie in the planes $y = 0$, $y = 1$, $z = 0$ and $z = 1$. Thus, there is only one independent constraint at the centre of each face in the mesh.

A.4 Centre constraint

There is a divergence constraint at the node that is found at the centre of each brick.

$$\begin{aligned} d_{111} = & - \frac{3}{2\delta_x} c_{011}^x - \frac{1}{4} c_{111}^x + \frac{3}{2\delta_x} c_{211}^x - \frac{1}{4} c_{311}^x \\ & - \frac{3}{2\delta_y} c_{101}^y - \frac{1}{4} c_{111}^y + \frac{3}{2\delta_y} c_{121}^y - \frac{1}{4} c_{131}^y \\ & - \frac{3}{2\delta_z} c_{110}^z - \frac{1}{4} c_{111}^z + \frac{3}{2\delta_z} c_{112}^z - \frac{1}{4} c_{113}^z \end{aligned} \quad (\text{A.64})$$

This constraint is the only one out of 27 that reduces the sparsity of the S and T matrices. This is because the coefficient that is eliminated links previous bricks together in a chain that is parallel to the x -axis. It is not necessary to use the x -axis, chains of bricks that are parallel to the y -axis or the z -axis are just as effective. However, it is not possible to eliminate four coefficients that make a chain of bricks forming a rectangle. If a 4×4 matrix is formed from the four divergence constraints in the rectangle using the factors that go with the four coefficients, then the rank of the matrix is three.

If the divergence is zero then $d_{1,1,1,l,m,n} = 0$ for all (l, m, n) . In that case, the divergence constraint for the brick labeled by (l, m, n) that follows by eliminating the coefficients c_{211}^x in each brick is found below.

$$\begin{aligned}
 c_{2,1,1,l,m,n}^x = c_{0,1,1,1,m,n}^x + \sum_{i=1}^l \delta_{x,i,m,n} \left(\begin{aligned}
 & \frac{1}{6} c_{1,1,1,i,m,n}^x + \frac{1}{6} c_{3,1,1,i,m,n}^x \\
 & + \frac{1}{\delta_{y,i,m,n}} c_{1,0,1,i,m,n}^y + \frac{1}{6} c_{1,1,1,i,m,n}^y \\
 & - \frac{1}{\delta_{y,i,m,n}} c_{1,2,1,i,m,n}^y + \frac{1}{6} c_{1,3,1,i,m,n}^y \\
 & + \frac{1}{\delta_{z,i,m,n}} c_{1,1,0,i,m,n}^z + \frac{1}{6} c_{1,1,1,i,m,n}^z \\
 & - \frac{1}{\delta_{z,i,m,n}} c_{1,1,2,i,m,n}^z + \frac{1}{6} c_{1,1,3,i,m,n}^z
 \end{aligned} \right) \quad (\text{A.65})
 \end{aligned}$$

Appendix B

Physical meaning of functional

The functional in equation (2.36) is related to the complex power form of Poynting's theorem [4]. In the same way that the complex power is defined in terms of phasors for the voltage V and the current I as $P = I^*V$, consider the quantity $\mathbf{J}^*(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r})$, which, apart from a factor of 2, is the complex power per volume that is dissipated at position $\mathbf{r}$.

$$\mathbf{J}^* \cdot \mathbf{E} = (\nabla \times \mathbf{H}^*) \cdot \mathbf{E} + j\omega \epsilon \mathbf{E}^* \cdot \mathbf{E} \quad (\text{B.1})$$

$$= \nabla \cdot (\mathbf{H}^* \times \mathbf{E}) + \mathbf{H}^* \cdot (\nabla \times \mathbf{E}) + j\omega \epsilon \mathbf{E}^* \cdot \mathbf{E} \quad (\text{B.2})$$

$$= \nabla \cdot (\mathbf{H}^* \times \mathbf{E}) - j\omega \mu \mathbf{H}^* \cdot \mathbf{H} + j\omega \epsilon \mathbf{E}^* \cdot \mathbf{E} \quad (\text{B.3})$$

$$\begin{aligned} &= -\frac{1}{j\omega} \nabla \cdot \left(\mathbf{E} \times \frac{1}{\mu} (\nabla \times \mathbf{E}^*) \right) \\ &+ \frac{1}{j\omega} \left(\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \mathbf{E} \right) \end{aligned} \quad (\text{B.4})$$

In equation (B.1), $\mathbf{J}^*$ was replaced using the complex conjugate of equation (1.8), Ampere's law with the Maxwell displacement current. The next line follows using the vector identity $\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B})$. Equation (B.3) is obtained using Faraday's law to eliminate $\nabla \times \mathbf{E}$. The first term is proportional to the Poynting vector for harmonic fields, $\mathbf{S} = \mathbf{E} \times \mathbf{H}^*/2$ [4]. The second and third terms, each purely imag-

inary, are proportional to the reactive power stored in the magnetic and electric fields, respectively. Equation (B.4) follows from equation (B.3) from using Faraday's law again, this time to eliminate $\mathbf{H}$. The complex power dissipated over the volume of integration is

$$\begin{aligned} \frac{1}{2} \iiint \mathbf{J}^* \cdot \mathbf{E} dV &= -\frac{1}{2j\omega} \iint (\mathbf{n} \times \mathbf{E}) \cdot \frac{1}{\mu} (\nabla \times \mathbf{E}^*) dS \\ &+ \frac{1}{2j\omega} \iiint \left(\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \mathbf{E} \right) dV \end{aligned} \quad (\text{B.5})$$

where the divergence theorem has been used to obtain the surface integral. The factor of $1/2$ is present because $\mathbf{E}$ and $\mathbf{H}$ are the amplitudes of the time-harmonic fields, that is, they do not contain a factor of $1/\sqrt{2}$ that occurs in the definition of a phasor. For a cavity with perfectly conducting walls, the only current is a surface current density on the boundary that arises because $\mathbf{H}$ is zero inside of the conductor and the tangential component is non-zero inside of the cavity at the boundary. Thus, the current is zero everywhere except on the conducting walls where it is tangential to the surface. However, here, the tangential component of the electric field is zero, and therefore $\mathbf{J}^* \cdot \mathbf{E} = 0$ everywhere. If the volume of integration includes the entire volume of the cavity, then the surface integral is also zero since $\mathbf{n} \times \mathbf{E} = 0$ at the surface and $\mathbf{E} = 0$ within the perfect conductor. The complex power form of Poynting's theorem can be simplified further in this case.

$$0 = \frac{1}{2j\omega} \iiint \left(\frac{1}{\mu} (\nabla \times \mathbf{E}^*) \cdot (\nabla \times \mathbf{E}) - \omega^2 \epsilon \mathbf{E}^* \cdot \mathbf{E} \right) dV \quad (\text{B.6})$$

$$= \frac{1}{2j\omega} F(\mathbf{E}) \quad (\text{B.7})$$

Therefore, the variational procedure amounts to finding the stationary points of the complex power form of Poynting's theorem for time-harmonic fields, apart from a factor of $2j\omega$. It has also been shown that $F(\mathbf{E}) = 0$, which can be interpreted to mean that the

energy that is stored in the cavity flows back and forth between the electric and magnetic fields.

Appendix C

Basis functions in cylindrical coordinates

The basis functions defined in equations (2.14)–(2.16) for Cartesian coordinates are modified to solve problems in cylindrical coordinates. The divergence constraints are the same in both cases. The singularity on the cylindrical coordinate system axis is discussed, followed by an example calculation of the resonant frequencies of a cylinder with annular cross-section.

C.1 Definition of basis functions in cylindrical coordinates

The divergence of a vector field $\mathbf{A}(\mathbf{r})$ in cylindrical coordinates is

$$\nabla \cdot \mathbf{A} = \frac{1}{r} \frac{\partial}{\partial r} (r A_r) + \frac{1}{r} \frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}. \quad (\text{C.1})$$

If the components B_r , B_ϕ and B_z are defined as

$$B_r = \frac{A_r}{r} \quad (\text{C.2})$$

$$B_\phi = A_\phi \quad (\text{C.3})$$

$$B_z = \frac{A_z}{r} \quad (\text{C.4})$$

then

$$\nabla \cdot \mathbf{A} = \frac{1}{r} \left(\frac{\partial B_r}{\partial r} + \frac{\partial B_\phi}{\partial \phi} + \frac{\partial B_z}{\partial z} \right). \quad (\text{C.5})$$

Multiplying both sides of equation C.5 by r results in

$$r \nabla \cdot \mathbf{A} = \frac{\partial B_r}{\partial r} + \frac{\partial B_\phi}{\partial \phi} + \frac{\partial B_z}{\partial z}, \quad (\text{C.6})$$

which is the same as the divergence in Cartesian coordinates if $B_r = A_x$, $B_\phi = A_y$ and $B_z = A_z$. Thus, if the same basis functions are used for (B_r, B_ϕ, B_z) and (A_x, A_y, A_z) then this will result in the same divergence constraints for both cases.

The basis functions in cylindrical coordinates are defined as

$$A_r(r, \phi, z) = \sum_{i=0}^3 \sum_{j=0}^2 \sum_{k=0}^2 c_{ijk}^x \Delta_{ri} \frac{H_i(r')}{r} L_j(\phi') L_k(z') \quad (\text{C.7})$$

$$A_\phi(r, \phi, z) = \sum_{i=0}^2 \sum_{j=0}^3 \sum_{k=0}^2 c_{ijk}^y \Delta_{\phi j} L_i(r') H_j(\phi') L_k(z') \quad (\text{C.8})$$

$$A_z(r, \phi, z) = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^3 c_{ijk}^z \Delta_{zk} \frac{L_i(r')}{r} L_j(\phi') H_k(z'). \quad (\text{C.9})$$

The primes denote the local coordinate system for a given brick, that is,

$$r' = (r - r_0)/\delta_r \quad (\text{C.10})$$

$$\phi' = (\phi - \phi_0)/\delta_\phi \quad (\text{C.11})$$

$$z' = (z - z_0)/\delta_z \quad (\text{C.12})$$

where $0 \leq r' \leq 1$ and $r_0 \leq r \leq r_0 + \delta_r$ within a given brick. Similar relations hold for ϕ and z . The variable Δ_{ri} is equal to 1 for $i = 0, 2$ and it is equal to δ_r for $i = 1, 3$. This results in simpler divergence constraints, similar to the Cartesian case. The variables $\Delta_{\phi j}$ and Δ_{zk} are defined similarly. Note that the factor of r in the denominator of the basis functions for A_r and A_z is the global radial coordinate, not the local coordinate that appears as an argument of the polynomials. Also note that, in the case of cylindrical coordinates, $r \nabla \cdot \mathbf{A}(r, \phi, z)$ is modelled to second order accuracy in the variables (r, ϕ, z) , whereas in Cartesian coordinates, $\nabla \cdot \mathbf{A}(x, y, z)$ is modelled to second order accuracy in the variables (x, y, z) .

C.2 Singularity on the axis of the cylindrical coordinate system

The radial and angular unit vectors are defined in terms of the Cartesian unit vectors as

$$\hat{\mathbf{r}} = \cos \phi \hat{\mathbf{x}} + \sin \phi \hat{\mathbf{y}} \quad (\text{C.13})$$

$$\hat{\phi} = -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}} \quad (\text{C.14})$$

where ϕ is the angle from the x -axis. However, at $r = 0$, the angle ϕ is not defined, and neither are the unit vectors $\hat{\mathbf{r}}$ and $\hat{\phi}$. To derive the values of A_r and A_ϕ on the coordinate axis, express $\mathbf{A}$ in terms of the Cartesian unit vectors and require that $\mathbf{A}$ be unique on the axis, that is, $\partial A_x / \partial \phi = 0$ and $\partial A_y / \partial \phi = 0$ as $r \rightarrow 0$.

$$\mathbf{A} = A_r \hat{\mathbf{r}} + A_\phi \hat{\phi} + A_z \hat{\mathbf{z}} \quad (\text{C.15})$$

$$= A_r (\cos \phi \hat{\mathbf{x}} + \sin \phi \hat{\mathbf{y}}) + A_\phi (-\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}}) + A_z \hat{\mathbf{z}} \quad (\text{C.16})$$

$$= (A_r \cos \phi - A_\phi \sin \phi) \hat{\mathbf{x}} + (A_r \sin \phi + A_\phi \cos \phi) \hat{\mathbf{y}} + A_z \hat{\mathbf{z}} \quad (\text{C.17})$$

The value of $\mathbf{A}$ does not depend on ϕ as $r \rightarrow 0$.

$$0 = \frac{\partial}{\partial \phi} (A_r \cos \phi - A_\phi \sin \phi) \quad (\text{C.18})$$

$$= \frac{\partial A_r}{\partial \phi} \cos \phi - A_r \sin \phi - \frac{\partial A_\phi}{\partial \phi} \sin \phi - A_\phi \cos \phi \quad (\text{C.19})$$

$$0 = \frac{\partial}{\partial \phi} (A_r \sin \phi + A_\phi \cos \phi) \quad (\text{C.20})$$

$$= \frac{\partial A_r}{\partial \phi} \sin \phi + A_r \cos \phi + \frac{\partial A_\phi}{\partial \phi} \cos \phi - A_\phi \sin \phi \quad (\text{C.21})$$

Multiply equation (C.19) by $\cos \phi$ and add that to equation (C.21) multiplied by $\sin \phi$ to get

$$\frac{\partial A_r}{\partial \phi} - A_\phi = 0. \quad (\text{C.22})$$

Similarly, multiply equation (C.19) by $\sin \phi$ and subtract that from equation (C.21) multiplied by $\cos \phi$ to get

$$\frac{\partial A_\phi}{\partial \phi} + A_r = 0. \quad (\text{C.23})$$

The solution of equations (C.22) and (C.23) is

$$A_r(0, \phi, z) = \alpha(z) \cos \phi + \beta(z) \sin \phi \quad (\text{C.24})$$

$$A_\phi(0, \phi, z) = -\alpha(z) \sin \phi + \beta(z) \cos \phi. \quad (\text{C.25})$$

In cylindrical coordinates,

$$\nabla \times \mathbf{A} = \hat{\mathbf{r}} \left(\frac{1}{r} \frac{\partial A_z}{\partial \phi} - \frac{\partial A_\phi}{\partial z} \right) + \hat{\phi} \left(\frac{\partial A_r}{\partial z} - \frac{\partial A_z}{\partial r} \right) + \hat{\mathbf{z}} \frac{1}{r} \left(\frac{\partial (r A_\phi)}{\partial r} - \frac{\partial A_r}{\partial \phi} \right). \quad (\text{C.26})$$

The z -component can be expanded as

$$\frac{\partial A_\phi}{\partial r} + \frac{1}{r} \left(A_\phi - \frac{\partial A_r}{\partial \phi} \right) \quad (\text{C.27})$$

and so if equation (C.22) is not satisfied then $(\nabla \times \mathbf{A})_z$ is infinite on the axis. The divergence equation (C.1) can also be expanded to give

$$\nabla \cdot \mathbf{A} = \frac{\partial A_r}{\partial r} + \frac{1}{r} \left(A_r + \frac{\partial A_\phi}{\partial \phi} \right) + \frac{\partial A_z}{\partial z} \quad (\text{C.28})$$

and so if equation (C.23) is not satisfied then $\nabla \cdot \mathbf{A}$ is infinite on the axis.

The basis functions defined in equations (C.7)–(C.9) do not solve the differential equations (C.22) and (C.23) exactly, with the exception of the trivial solution $A_r = 0$ and $A_\phi = 0$ at $r = 0$. (This follows since the basis functions are not linear combinations of $\cos \phi$ and $\sin \phi$ on the axis.) If the basis functions interpolate the solution in equations (C.24) and (C.25) then the error in equation (C.22) is of order $(\delta_\phi)^3$ and the error in equation (C.23) is of order $(\delta_\phi)^5$. Although each error goes to zero as $\delta_\phi \rightarrow 0$, in any finite element method calculation δ_ϕ is finite. The result is that the curl and divergence are each infinite at the origin. Because of the singularities at the origin in the curl and divergence equations that occur using the basis functions defined in equations (C.7)–(C.9), the method is not used to solve problems for domains containing the axis.

Note that the radial component of the curl contains the term

$$\frac{1}{r} \frac{\partial A_z}{\partial \phi} \quad (\text{C.29})$$

which would be finite provided constraints are implemented to impose

$$\frac{\partial A_z}{\partial \phi} = 0 \quad (\text{C.30})$$

at $r = 0$. This is possible with the basis functions defined in equations (C.7)–(C.9), but the constraints are not derived since the method will not be used for domains containing the axis.

C.3 Example: cylindrical cavity with annular cross-section

The resonant frequencies of a cylinder with annular cross-section are obtained using the basis functions defined in equations (C.7)–(C.9). The cavity walls are perfect conductors. This example is chosen because an exact solution exists, so it can be used to test the basis functions in cylindrical coordinates.

The height of the cavity is $h = 1$ and inner and outer radii are $a = 1/4$ and $b = 1$, respectively. The cavity is empty, which means that $\epsilon_r = 1$ and $\mu_r = 1$.

The problem is solved using the electric field formulation. The solution is periodic, which means that $\mathbf{E}(r, \phi + 2\pi, z) = \mathbf{E}(r, \phi, z)$. The boundary conditions are $E_r(r, \phi, z) = 0$ and $E_\phi(r, \phi, z) = 0$ for $z = 0$ and $z = h$, which are the bottom and top of the cylinder, respectively. As a result, $\partial E_r / \partial r = 0$ and $\partial E_\phi / \partial \phi = 0$ for $z = 0$ and $z = h$. The divergence equation (C.28) implies that $\partial E_z / \partial z = 0$ on the surfaces $z = 0$ and $z = h$. On the surfaces $r = a$ and $r = b$, $E_\phi = 0$ and $E_z = 0$, which imply that $\partial E_\phi / \partial \phi = 0$ and $\partial E_z / \partial z = 0$. On these surfaces, the divergence equation implies that

$$0 = \frac{1}{r} \frac{\partial}{\partial r} (r A_r) \quad (\text{C.31})$$

$$= \frac{1}{r} \frac{\partial B_r}{\partial r}. \quad (\text{C.32})$$

Thus, $\partial B_r / \partial r = 0$ for $r = a$ and $r = b$.

The exact solutions can be obtained using separation of variables. The solutions can be divided into three categories.

1. The first set of solutions have eigenvalue, k^2 , obtained from the solving the transcendental equation

$$J_m(a\gamma) Y_m(b\gamma) - J_m(b\gamma) Y_m(a\gamma) = 0 \quad (\text{C.33})$$

where

$$\gamma = \sqrt{k^2 - \left(\frac{p\pi}{h}\right)^2} \quad (\text{C.34})$$

$p = 1, 2, 3, \dots$, $m = 0, 1, 2, 3, \dots$, J_m is the Bessel function of the first kind of order m and Y_m is the Bessel function of the second kind of order m . When $m = 0$ the multiplicity is 1 and when $m > 0$ the multiplicity is 2.

2. The second set of solutions is similar to the first except that instead of the transcendental equation (C.33), the eigenvalues are obtained from the zeros of

$$J'_m(a\gamma) Y'_m(b\gamma) - J'_m(b\gamma) Y'_m(a\gamma) = 0 \quad (\text{C.35})$$

where the prime denotes derivative with respect to the argument.

3. The third set of solutions has eigenvalues $k^2 = (p\pi/h)^2$, with multiplicity 1.

Table C.1: Eigenvalues, k^2 , in units of L^{-2} , of cavity with annulus cross-section. The mesh is $n_r \times n_\phi \times n_z = 16 \times 24 \times 16$ with 71040 unknowns. The type of solution obtained using separation of variables is given with the eigenvalue multiplicity in parentheses.

FEM	Transcendental	Type (Multiplicity)	FEM Error (%)
9.8696	9.8696	3 (1)	0
12.5746	12.5740	2 (2)	0.0048
16.7913	16.7911	1 (1)	0.0012
18.9271	18.9255	2 (2)	0.0085
19.7806	19.7803	1 (2)	0.0015
26.6607	26.6607	1 (1)	0
27.4634	27.4559	2 (2)	0.0273
28.3024	28.3013	1 (2)	0.0039
29.6500, 29.6502	29.6499	1 (2), 2 (1)	0.0003, 0.0010
34.9146	34.9146	2 (2)	0
38.1696	38.1337	2 (2)	0.0941

The results obtained with the basis functions defined in equations (C.7)–(C.9) using an $n_r \times n_\phi \times n_z = 16 \times 24 \times 16$ with 71040 unknowns are found in table C.1. The exact solutions are also given. The lowest ten eigenvalues agree to five significant figures, while the eleventh eigenvalue agrees to four significant figures. The multiplicity is correct.

C.4 Conclusions

The definition of the basis functions is modified in equations (C.7)–(C.9) so that they can be applied to problems in cylindrical coordinates. However, these cannot model to behaviour on the coordinate system axis exactly, resulting in infinite values in the divergence and curl equations. Thus, they are not applied to problems containing the coordinate axis. The basis functions are used to obtain the eigenvalues of a cylindrical cavity with an annular cross-section. The eigenvalues obtained with the finite element method are in excellent agreement with the exact eigenvalues obtained using separation of variables.

Appendix D

Definition of S and T matrices

To define the elements of the S and T matrices for a given brick, it is first necessary to assign the order that the basis functions appear in each row and column. The basis functions have three indices i , j and k for the product of polynomials for the local x , y and z coordinates, respectively. There is not a unique order to convert the triple index notation to a single index notation. The order numbering used in this work is found in tables D.1 - D.6. The dimensions of the brick are $\delta_x \times \delta_y \times \delta_z$. The unit vectors $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$ are included in the definition of the basis functions so that the S and T matrices can be defined easily using the single index notation.

Let the basis functions in single index notation be labeled $\mathbf{b}_i(x, y, z)$. The matrix elements for the T and S matrices within a given brick are defined in equations (D.1) and (D.2), respectively.

$$T_{ij} = \iiint \epsilon \mathbf{b}_i \cdot \mathbf{b}_j dV \quad (\text{D.1})$$

$$S_{ij} = \iiint \frac{1}{\mu} (\nabla \times \mathbf{b}_i) \cdot (\nabla \times \mathbf{b}_j) dV \quad (\text{D.2})$$

The large, sparse matrices for the entire domain are then assembled in the usual way. (See, for example, Silvester and Ferrari [9].)

Table D.1: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
E_x	1	$H_0(x)L_0(y)L_0(z)\mathbf{x}$	E_x	10	$H_2(x)L_0(y)L_0(z)\mathbf{x}$
E_x	2	$H_0(x)L_0(y)L_1(z)\mathbf{x}$	E_x	11	$H_2(x)L_0(y)L_1(z)\mathbf{x}$
E_x	3	$H_0(x)L_0(y)L_2(z)\mathbf{x}$	E_x	12	$H_2(x)L_0(y)L_2(z)\mathbf{x}$
E_x	4	$H_0(x)L_1(y)L_0(z)\mathbf{x}$	E_x	13	$H_2(x)L_1(y)L_0(z)\mathbf{x}$
E_x	5	$H_0(x)L_1(y)L_1(z)\mathbf{x}$	E_x	14	$H_2(x)L_1(y)L_1(z)\mathbf{x}$
E_x	6	$H_0(x)L_1(y)L_2(z)\mathbf{x}$	E_x	15	$H_2(x)L_1(y)L_2(z)\mathbf{x}$
E_x	7	$H_0(x)L_2(y)L_0(z)\mathbf{x}$	E_x	16	$H_2(x)L_2(y)L_0(z)\mathbf{x}$
E_x	8	$H_0(x)L_2(y)L_1(z)\mathbf{x}$	E_x	17	$H_2(x)L_2(y)L_1(z)\mathbf{x}$
E_x	9	$H_0(x)L_2(y)L_2(z)\mathbf{x}$	E_x	18	$H_2(x)L_2(y)L_2(z)\mathbf{x}$

Table D.2: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
$\partial E_x/\partial x$	19	$\delta_x H_1(x)L_0(y)L_0(z)\mathbf{x}$	$\partial E_x/\partial x$	28	$\delta_x H_3(x)L_0(y)L_0(z)\mathbf{x}$
$\partial E_x/\partial x$	20	$\delta_x H_1(x)L_0(y)L_1(z)\mathbf{x}$	$\partial E_x/\partial x$	29	$\delta_x H_3(x)L_0(y)L_1(z)\mathbf{x}$
$\partial E_x/\partial x$	21	$\delta_x H_1(x)L_0(y)L_2(z)\mathbf{x}$	$\partial E_x/\partial x$	30	$\delta_x H_3(x)L_0(y)L_2(z)\mathbf{x}$
$\partial E_x/\partial x$	22	$\delta_x H_1(x)L_1(y)L_0(z)\mathbf{x}$	$\partial E_x/\partial x$	31	$\delta_x H_3(x)L_1(y)L_0(z)\mathbf{x}$
$\partial E_x/\partial x$	23	$\delta_x H_1(x)L_1(y)L_1(z)\mathbf{x}$	$\partial E_x/\partial x$	32	$\delta_x H_3(x)L_1(y)L_1(z)\mathbf{x}$
$\partial E_x/\partial x$	24	$\delta_x H_1(x)L_1(y)L_2(z)\mathbf{x}$	$\partial E_x/\partial x$	33	$\delta_x H_3(x)L_1(y)L_2(z)\mathbf{x}$
$\partial E_x/\partial x$	25	$\delta_x H_1(x)L_2(y)L_0(z)\mathbf{x}$	$\partial E_x/\partial x$	34	$\delta_x H_3(x)L_2(y)L_0(z)\mathbf{x}$
$\partial E_x/\partial x$	26	$\delta_x H_1(x)L_2(y)L_1(z)\mathbf{x}$	$\partial E_x/\partial x$	35	$\delta_x H_3(x)L_2(y)L_1(z)\mathbf{x}$
$\partial E_x/\partial x$	27	$\delta_x H_1(x)L_2(y)L_2(z)\mathbf{x}$	$\partial E_x/\partial x$	36	$\delta_x H_3(x)L_2(y)L_2(z)\mathbf{x}$

Table D.3: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
E_y	37	$H_0(y)L_0(x)L_0(z)\mathbf{y}$	E_y	46	$H_2(y)L_0(x)L_0(z)\mathbf{y}$
E_y	38	$H_0(y)L_0(x)L_1(z)\mathbf{y}$	E_y	47	$H_2(y)L_0(x)L_1(z)\mathbf{y}$
E_y	39	$H_0(y)L_0(x)L_2(z)\mathbf{y}$	E_y	48	$H_2(y)L_0(x)L_2(z)\mathbf{y}$
E_y	40	$H_0(y)L_1(x)L_0(z)\mathbf{y}$	E_y	49	$H_2(y)L_1(x)L_0(z)\mathbf{y}$
E_y	41	$H_0(y)L_1(x)L_1(z)\mathbf{y}$	E_y	50	$H_2(y)L_1(x)L_1(z)\mathbf{y}$
E_y	42	$H_0(y)L_1(x)L_2(z)\mathbf{y}$	E_y	51	$H_2(y)L_1(x)L_2(z)\mathbf{y}$
E_y	43	$H_0(y)L_2(x)L_0(z)\mathbf{y}$	E_y	52	$H_2(y)L_2(x)L_0(z)\mathbf{y}$
E_y	44	$H_0(y)L_2(x)L_1(z)\mathbf{y}$	E_y	53	$H_2(y)L_2(x)L_1(z)\mathbf{y}$
E_y	45	$H_0(y)L_2(x)L_2(z)\mathbf{y}$	E_y	54	$H_2(y)L_2(x)L_2(z)\mathbf{y}$

Table D.4: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
$\partial E_y/\partial y$	55	$\delta_y H_1(y)L_0(x)L_0(z)\mathbf{y}$	$\partial E_y/\partial y$	64	$\delta_y H_3(y)L_0(x)L_0(z)\mathbf{y}$
$\partial E_y/\partial y$	56	$\delta_y H_1(y)L_0(x)L_1(z)\mathbf{y}$	$\partial E_y/\partial y$	65	$\delta_y H_3(y)L_0(x)L_1(z)\mathbf{y}$
$\partial E_y/\partial y$	57	$\delta_y H_1(y)L_0(x)L_2(z)\mathbf{y}$	$\partial E_y/\partial y$	66	$\delta_y H_3(y)L_0(x)L_2(z)\mathbf{y}$
$\partial E_y/\partial y$	58	$\delta_y H_1(y)L_1(x)L_0(z)\mathbf{y}$	$\partial E_y/\partial y$	67	$\delta_y H_3(y)L_1(x)L_0(z)\mathbf{y}$
$\partial E_y/\partial y$	59	$\delta_y H_1(y)L_1(x)L_1(z)\mathbf{y}$	$\partial E_y/\partial y$	68	$\delta_y H_3(y)L_1(x)L_1(z)\mathbf{y}$
$\partial E_y/\partial y$	60	$\delta_y H_1(y)L_1(x)L_2(z)\mathbf{y}$	$\partial E_y/\partial y$	69	$\delta_y H_3(y)L_1(x)L_2(z)\mathbf{y}$
$\partial E_y/\partial y$	61	$\delta_y H_1(y)L_2(x)L_0(z)\mathbf{y}$	$\partial E_y/\partial y$	70	$\delta_y H_3(y)L_2(x)L_0(z)\mathbf{y}$
$\partial E_y/\partial y$	62	$\delta_y H_1(y)L_2(x)L_1(z)\mathbf{y}$	$\partial E_y/\partial y$	71	$\delta_y H_3(y)L_2(x)L_1(z)\mathbf{y}$
$\partial E_y/\partial y$	63	$\delta_y H_1(y)L_2(x)L_2(z)\mathbf{y}$	$\partial E_y/\partial y$	72	$\delta_y H_3(y)L_2(x)L_2(z)\mathbf{y}$

Table D.5: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
E_z	73	$H_0(z)L_0(x)L_0(y)\mathbf{z}$	E_z	82	$H_2(z)L_0(x)L_0(y)\mathbf{z}$
E_z	74	$H_0(z)L_0(x)L_1(y)\mathbf{z}$	E_z	83	$H_2(z)L_0(x)L_1(y)\mathbf{z}$
E_z	75	$H_0(z)L_0(x)L_2(y)\mathbf{z}$	E_z	84	$H_2(z)L_0(x)L_2(y)\mathbf{z}$
E_z	76	$H_0(z)L_1(x)L_0(y)\mathbf{z}$	E_z	85	$H_2(z)L_1(x)L_0(y)\mathbf{z}$
E_z	77	$H_0(z)L_1(x)L_1(y)\mathbf{z}$	E_z	86	$H_2(z)L_1(x)L_1(y)\mathbf{z}$
E_z	78	$H_0(z)L_1(x)L_2(y)\mathbf{z}$	E_z	87	$H_2(z)L_1(x)L_2(y)\mathbf{z}$
E_z	79	$H_0(z)L_2(x)L_0(y)\mathbf{z}$	E_z	88	$H_2(z)L_2(x)L_0(y)\mathbf{z}$
E_z	80	$H_0(z)L_2(x)L_1(y)\mathbf{z}$	E_z	89	$H_2(z)L_2(x)L_1(y)\mathbf{z}$
E_z	81	$H_0(z)L_2(x)L_2(y)\mathbf{z}$	E_z	90	$H_2(z)L_2(x)L_2(y)\mathbf{z}$

Table D.6: Single index to triple index conversion.

Field quantity	Single index	Triple index basis function	Field quantity	Single index	Triple index basis function
$\partial E_z/\partial z$	91	$\delta_z H_1(z)L_0(x)L_0(y)\mathbf{z}$	$\partial E_z/\partial z$	100	$\delta_z H_3(z)L_0(x)L_0(y)\mathbf{z}$
$\partial E_z/\partial z$	92	$\delta_z H_1(z)L_0(x)L_1(y)\mathbf{z}$	$\partial E_z/\partial z$	101	$\delta_z H_3(z)L_0(x)L_1(y)\mathbf{z}$
$\partial E_z/\partial z$	93	$\delta_z H_1(z)L_0(x)L_2(y)\mathbf{z}$	$\partial E_z/\partial z$	102	$\delta_z H_3(z)L_0(x)L_2(y)\mathbf{z}$
$\partial E_z/\partial z$	94	$\delta_z H_1(z)L_1(x)L_0(y)\mathbf{z}$	$\partial E_z/\partial z$	103	$\delta_z H_3(z)L_1(x)L_0(y)\mathbf{z}$
$\partial E_z/\partial z$	95	$\delta_z H_1(z)L_1(x)L_1(y)\mathbf{z}$	$\partial E_z/\partial z$	104	$\delta_z H_3(z)L_1(x)L_1(y)\mathbf{z}$
$\partial E_z/\partial z$	96	$\delta_z H_1(z)L_1(x)L_2(y)\mathbf{z}$	$\partial E_z/\partial z$	105	$\delta_z H_3(z)L_1(x)L_2(y)\mathbf{z}$
$\partial E_z/\partial z$	97	$\delta_z H_1(z)L_2(x)L_0(y)\mathbf{z}$	$\partial E_z/\partial z$	106	$\delta_z H_3(z)L_2(x)L_0(y)\mathbf{z}$
$\partial E_z/\partial z$	98	$\delta_z H_1(z)L_2(x)L_1(y)\mathbf{z}$	$\partial E_z/\partial z$	107	$\delta_z H_3(z)L_2(x)L_1(y)\mathbf{z}$
$\partial E_z/\partial z$	99	$\delta_z H_1(z)L_2(x)L_2(y)\mathbf{z}$	$\partial E_z/\partial z$	108	$\delta_z H_3(z)L_2(x)L_2(y)\mathbf{z}$

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