A Software Platform For The Simulation Of Light Propagation In Photonic Crystal Structures With Defects

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Contents

Chapter 1

Introduction

Preface:

Definition of the problem will be treated in chapter **??**, followed by a brief state of the art recollection where some background in the topics of photonic crystals and computational methods for physics will be mentioned. Then, fundamental concepts behind light propagation in periodic materials (chapter 3) and the model used for the finite element procedure used are presented.

Chapter 2

Problem

??

2.1 Problem statement

This project aims to develop a simulation software package that permits analysis of electromagnetic (EM) wave propagation, in the context of Photonic Crystal (PC) defects modeling and design.

2.2 Objectives

2.2.1 General objectives

- Build a software platform capable of simulating electromagnetic field propagation in perfect PC and also in PC with defects such as cavities and inclusions.
- The platform architecture must be structured in a way that facilitates future upgrading, possible optimization schemes, and integration with other kinds of simulations like confinement of electrons in potential wells and crystals.

Specific objectives

1. Apprehend the theory behind EM fields and its applications in photonics. Particularly:
   (a) general overview of computational methods in electromagnetism and deeper understanding of methods that fit the problem statement.
   (b) Photonic crystals and the mathematical tools for modeling periodicity, as well as

(c) technological applications of defects in photonic crystals and common case studies.

2. Define a set of implementation requirements and constraints, in terms of the numerical method, and expected functionality.

3. Implement algorithms to solve problems that relate to technological applications studied in the appropriation stage.

   (a) Solve simple scalar-static 2D problems

   (b) Implement vector field solver for stationary non periodic conditions (this may qualify as spectral solution or not)

   (c) Vector field solutions for time dependent problems

   (d) Introduce periodic conditions

4. Document and share the results of the simulations making an analysis of the relevance and feasibility of the platform.

2.3 Justification

Most of the artificial environment we as a society have built to live in, is in one way or another a consequence of our ability to understand and transform materials present in nature. This understanding is so important that human history studies have come to address cultural stages of our evolution from: the Stone Age through Bronce Age, as the materials we used to overcome survival challenges [13]. Even in recent years, extraordinary changes in the way we evolve as a species can be attributed to achievements only possible by improvements on our understanding of material properties. Take for example the paradigm change caused by the discovery of electronic properties of materials such as semiconductors [17]. And the ever growing stream of technological applications derived from it.

The next frontier in the context of material science, relies in a level of understanding that allows us to not only use and transform materials, but to design them. This is the field of metamaterials, a field in which by means of manipulating the microscopical structure and geometry of a crystal-like solid, we can obtain macroscopic properties that are otherwise impossible to find in nature [7, 4]. One of the sub domains of the metamaterials frontier is that of media capable of molding and manipulating electromagnetic waves. The ability to harness light has the prospect to support a new technological revolution of a scale similar to that of transistor revolution [13]. Advances in engineered optical materials will benefit the development of areas such as high speed computing, spectroscopy, laser engineering, biomedicine and quantum computing [17]. This project concerns about one candidate of optical metamaterial set known as photonic crystals, and particularly, the light guiding properties that arise when taking advantage of lattice cavities. Photonic crystals are:

> *"Artificially created periodic low-loss dielectric medium in which electromagnetic waves of certain frequencies cannot propagate [9]".*

Light in that certain frequency gap is virtually stopped because of periodicity of dielectric dispersers and the destructive interference that arises from it. This property is used in technical application for many forms of technological developments. For example Kärtner's et al. developed high resolution PC based Analogic-Digital (AD) conversion circuits [8] that are showing all-optical circuits which outperform electronic based components. Telecommunications also benefit from technologies such as ultra low loss photonic crystal fibers [2]. As well as low cost, and high definition spectroscopy technologies that take advantage of spectral selectivity in PCs; Pervez [18] has used a phenomenon called outcoupling to fabricate cheap PC based spectrometers. On the other hand, a lot of effort has been made to exploit the light confinement properties of PCs to make micro laser cavities and even single-photon sources. Theoretical background and numerical studies on spontaneous emission using microcavities in PCs has been undertaken by many researchers including works from Yablonovich and Vileneuve [30, 29, 27]. Experimental meassures of ultrafast nanocavity lasers was performed by Hatice [1] in 2006, and Moore [16] in 2008. Even state of the art quantum computing experiments are being possible by using PC based waveguides and cavities as shown by Wolters in [28].

The nature of most PC application problems, is of such complexity that very often numerical tools are the only way of modeling new designs and performance. Figure 2.1 shows some of the fields that benefit from electromagnetic numerical simulations as stated by Jin [12]. Computational methods such as: Plane Wave Expansion (PWE) [25, 14], Finite Difference Time Domain (FDTD) [2, 3], Method of Moments (MoM) or Boundary Element Method (BEM) and Finite Element Methods (FEM)[23, 15], have had their share in the modeling of electromagnetic fields under many different scenarios. Every one of them having their own strengths and weaknesses in terms of: ease of implementation, precision, and computational resources.

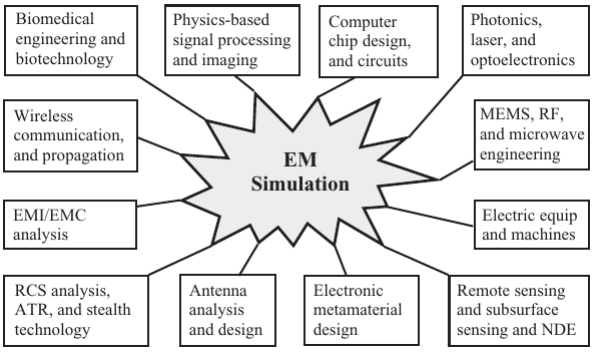

Figure 2.1: Maxwell equations by the hand of numerical methods have the power to impact many scientific and technological areas. Taken from Jin et al [12]

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In the context of Universidad EAFIT, and specifically of Engineering Physics, we see a growing research background in computational physics that goes from modeling seismic waves [11], and resonant modes in musical instruments [22]; passing through quantum mechanics like relativistic phenomena in graphene [26], and quantum potential wells and crystals [6]; to finally address a computational module for digital holography and speckle [24], and research on Plane Wave Methods for calculation of bandgap structures in photonic crystals [14]. It can be stated that this trend in numerical methods applied to crystal-like materials has been embraced and supported by the Computational and Theoretical Physics Research Initiative of engineering physics students (SFTyC). This work will expand and continue the initiative towards strengthening undergraduate research and software development abilities.

Chapter 3

Electromagnetic waves in periodic media

3.1 Maxwell equations

Give an introduction to Maxwell equations in both their Integral and Diferntial forms.

$$\oint_C \mathbf{E} \cdot d\mathbf{l} = -\frac{d}{dt}\int_S \mathbf{B} \cdot d\mathbf{S} \qquad \text{(Faraday)} \tag{3.1}$$

$$\oint_C \mathbf{H} \cdot d\mathbf{l} = \frac{d}{dt}\int_S \mathbf{D} \cdot d\mathbf{S} + \int_S \mathbf{J} \cdot d\mathbf{S} \qquad \text{(Ampere-Maxwell)} \tag{3.2}$$

$$\int_S \mathbf{D} \cdot d\mathbf{S} = \int_V \rho dV \qquad \text{(Gauss)} \tag{3.3}$$

$$\int_S \mathbf{B} \cdot d\mathbf{S} = 0 \qquad \text{(Gauss for magnetism),} \tag{3.4}$$

In differential form we have

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \text{(Faraday)} \tag{3.5}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \qquad \text{(Ampere-Maxwell)} \tag{3.6}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Gauss)} \tag{3.7}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss for magnetism)} \tag{3.8}$$

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t} \qquad \text{(Continuity),} \tag{3.9}$$

Describe the current Continuity Equation

$$\int_S \mathbf{J} \cdot d\mathbf{S} = -\frac{d}{dt} \int_V \rho dV. \tag{3.10}$$

from 3.5 to (3.9) we can get just 3 independent set of vectorial equations. Define the meaning of each variable in that expression and continue with the definition of constitutive relations (Electric polarization and Magnetization):

In both set of equation we have

- **E**: Electric field intensity (volts/meter),
- **D**: Electric flux density (coulombs/meter^2),
- **H**: Magnetic field intensity (amperes/meter),
- **B**: Magnetic flux density (webers/meter),
- **J**: Electric current density (amperes/meter^2),
- ρ: Electric charge density (coulombs/meter^3).

$$\mathbf{D} = \epsilon_0 \cdot \mathbf{E} + \mathbf{P} \tag{3.11}$$

$$\mathbf{B} = \mu_0 \cdot \mathbf{H} + \mathbf{M}, \tag{3.12}$$

P is the polarization vector that tell us information about the response of the material to the external field due to orientation of the molecules inside of it, and **M** is the magnetization vector that is the analogous of the polarization for the magnetic case. If the fields are small enough the behavior of the material is linear and we can express the polarization and magnetization vectors as linear functions of **E** and **H**

$$\mathbf{D} = \bar{\bar{\epsilon}} \cdot \mathbf{E} \tag{3.13}$$

$$\mathbf{B} = \bar{\bar{\mu}} \cdot \mathbf{H}, \tag{3.14}$$

where the double bar refers to a second order tensor, $\cdot$ is a tensor-vector product.

This may be a good place to talk about classification of media and or boundary conditions, Jianmings book: Theory and computation of electromagnetic fields might be a good source for that.

3.2 Wave equation for electric fields

If we take the curl to (3.5), we get

$$\nabla \times \nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\nabla \times \mathbf{B} = -\frac{\partial}{\partial t}\nabla \times (\bar{\bar{\mu}} \cdot \mathbf{H}) \ ,$$

assuming a (piecewise) homogeneous material

$$\begin{aligned}\nabla \times \nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\nabla \times \mathbf{B} = \frac{\partial}{\partial t}(\bar{\bar{\mu}} \cdot \nabla \times \mathbf{H}) \\ = -\frac{\partial}{\partial t}\left(\bar{\bar{\mu}} \cdot \left[\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}\right]\right) \ ,\end{aligned}$$

if the polarization and magnetization do not vary with time –there is not hysteresis–

$$\begin{aligned}\nabla \times \nabla \times \mathbf{E} &= -\bar{\bar{\mu}} \cdot \left[\frac{\partial^2 \mathbf{D}}{\partial t^2} + \frac{\partial \mathbf{J}}{\partial t}\right] \\ \nabla \times \nabla \times \mathbf{E} &= -\bar{\bar{\mu}} \cdot \left[\bar{\bar{\epsilon}} \cdot \frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{\partial \mathbf{J}}{\partial t}\right] \ .\end{aligned} \tag{3.15}$$

Similarly, we take the curl to (3.6), and under the same assumptions, we get

$$\begin{aligned}\nabla \times \nabla \times \mathbf{H} &= \frac{\partial \nabla \times \mathbf{D}}{\partial t} + \nabla \times \mathbf{J} \\ &= \frac{\partial \nabla \times (\bar{\bar{\epsilon}} \cdot \mathbf{E})}{\partial t} + \nabla \times \mathbf{J} \\ &= \frac{\partial \bar{\bar{\epsilon}} \cdot \nabla \times \mathbf{E}}{\partial t} + \nabla \times \mathbf{J} \\ &= \frac{\partial \bar{\bar{\epsilon}} \cdot \left(-\frac{\partial \mathbf{B}}{\partial t}\right)}{\partial t} + \nabla \times \mathbf{J} \ ,\end{aligned}$$

finally

$$\begin{aligned}\nabla \times \nabla \times \mathbf{H} &= -\bar{\bar{\epsilon}} \cdot \frac{\partial^2 \mathbf{B}}{\partial t^2} + \nabla \times \mathbf{J} \\ \nabla \times \nabla \times \mathbf{H} &= -\bar{\bar{\epsilon}} \cdot \bar{\bar{\mu}} \cdot \frac{\partial^2 \mathbf{H}}{\partial t^2} + \nabla \times \mathbf{J} \ .\end{aligned} \tag{3.16}$$

If we apply the vector identity $\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$, and assume that we do not have electrical charges[1] we can rewrite (3.15) and (3.16) as

$$\nabla^2 \mathbf{E} = \bar{\bar{\mu}} \cdot \bar{\bar{\epsilon}} \cdot \frac{\partial^2 \mathbf{E}}{\partial t^2} - \bar{\bar{\mu}} \cdot \frac{\partial \mathbf{J}}{\partial t} \tag{3.17}$$

$$\nabla^2 \mathbf{H} = \bar{\bar{\epsilon}} \cdot \bar{\bar{\mu}} \cdot \frac{\partial^2 \mathbf{H}}{\partial t^2} - \nabla \times \mathbf{J} \tag{3.18}$$

[1] This identity always hold for the magnetic field since it is divergence free. WHAT ABOUT THE ELECTRICAL CASE?? Maybe this is why Joannopolous treats the problem for the magnetic field case instead of the electric one

If we neglect the terms $\frac{\partial \mathbf{J}}{\partial t}$ and $\nabla \times \mathbf{J}$ –the source terms in the equations– and assume isotropy –assuming isotropy the material tensors could be represented as simple scalars– we get the well known expressions

$$\left(\nabla^2 - \mu\epsilon\frac{\partial^2}{\partial t^2}\right)\mathbf{E} = \mathbf{0} \tag{3.19}$$

$$\left(\nabla^2 - \mu\epsilon\frac{\partial^2}{\partial t^2}\right)\mathbf{H} = \mathbf{0} \ , \tag{3.20}$$

that are vectorial wave equations with phase speed $c = \sqrt{\epsilon\mu}$.

This form of (3.15) is relevant for us because the program is currently based on this approximation. This particular topic will be treated furthermore in the implementation section **??**.

3.3 Time harmonic fields, reciprocal space and Fourier transform

Linearity of Maxwell equations, and a restriction to time harmonic variations permits the separation of time and spatial dependencies in the form:

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

This is known as a phasorial notation, and from here on, when dealing with time harmonic fields we will be interested only on the unknown phasor function $\mathbf{E}(\mathbf{r})$ which will represent the field distribution at a fixed time.

Considering a single harmonic wave propagating with angular frequency ω we get:

$$\nabla \times \nabla \times \mathbf{E} = -\omega^2\bar{\bar{\mu}} \cdot \bar{\bar{\epsilon}} \cdot \mathbf{E} - i\omega\bar{\bar{\mu}} \cdot \mathbf{J} \tag{3.21}$$

$$\nabla \times \nabla \times \mathbf{H} = -\omega^2\bar{\bar{\epsilon}} \cdot \bar{\bar{\mu}} \cdot \mathbf{H} + \nabla \times \mathbf{J} \ , \tag{3.22}$$

that are the expressions for the frequency domain.

$$\bar{\bar{\mu}} = \mu_0 \bar{\bar{\mu_r}} \tag{3.23}$$

$$\bar{\bar{\epsilon}} = \epsilon_0 \bar{\bar{\epsilon_r}} \tag{3.24}$$

$$\mu_0 = \sqrt{\mu_0 \epsilon_0} \sqrt{\frac{\mu_0}{\epsilon_0}} \tag{3.25}$$

$$k_0 = \omega \sqrt{\mu_0 \epsilon_0} \tag{3.26}$$

$$Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}} \tag{3.27}$$

$$c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \tag{3.28}$$

where $\bar{\bar{\mu_r}}$,$\bar{\bar{\epsilon_r}}$ are the relative permeability and permitivity, respectively, k_0, Z_0, and c are the free space wave number intrinsic impedance, and speed of light in free space. Using this:

$$\bar{\bar{\mu_r}}^{-1} \nabla \times \nabla \times \mathbf{E} = -\omega^2 \mu_0 \epsilon_0 \bar{\bar{\epsilon_r}} \cdot \mathbf{E} - i\omega\mu_0 \mathbf{J} \tag{3.29}$$

$$\bar{\bar{\mu_r}}^{-1} \nabla \times \nabla \times \mathbf{E} = k_0^2 \bar{\bar{\epsilon_r}} \cdot \mathbf{E} - ik_0 Z_0 \mathbf{J} \tag{3.30}$$

3.4 Electromagnetism as an eigenvalue problem

The current section treats the harmonic wave equation in a formalism similar to that of quantum mechanics. It might be seen as a sumarized version of the treatment of Joannopoulos [13], and Johnson.

Going back to equation 3.30, and assuming no sinks or sources ($\mathbf{J} = 0$), we can see that the form of the equation is one of a eigenvalue problem. Where a series of operations on a function $\mathbf{E}$ (eigenfunction or eigenvector) gives us the same function multiplied by a constant scalar (eigenvalue). In this case we will label the operator acting on $\mathbf{E}$ as $\hat{\Theta}$ in order to make the equation look like a simpler-looking eigenvalue problem:

$$\hat{\Theta}\mathbf{E} = \left(\frac{\omega}{c}\right)^2 \mathbf{E} \tag{3.31}$$

Where:

$$\hat{\Theta}\mathbf{E} \triangleq \bar{\bar{\mu_r}}^{-1} \nabla \times \nabla \times \mathbf{E} \tag{3.32}$$

Here the eigenvectors or phasors $\mathbf{E}$ represent spatial patterns of the harmonic modes, and eigenvalues $\left(\frac{\omega}{c}\right)^2$ give information about the frequency ω (and thus wave number k_0) of such modes.

3.4.1 Hermiticity

As in Quantum Mechanics with the Hamiltonian, some key properties of the eigenfunctions that satisfy equation 3.31 are:

- Have real eigenvalues,
- are orthogonal,
- can be obtained by a variational principle
- and can be catalogued by symmetry properties .

All of these properties rely on the fact that the linear operator is from a kind known as **Hermitian operator**.

To understand why $\hat{\Theta}$ is Hermitian we need first to understand the inner product of two wavefunctions $\mathbf{F}(\mathbf{r})$ and $\mathbf{G}(\mathbf{r})$:

$$(\mathbf{F}(\mathbf{r}), \mathbf{G}(\mathbf{r})) \triangleq \int \mathbf{F}^*(\mathbf{r}) \cdot \mathbf{G}(\mathbf{r}) \tag{3.33}$$

where * denotes complex conjugation. From definition 3.33 we can see that: $(\mathbf{F}, \mathbf{G}) = (\mathbf{G}, \mathbf{F})^*$ for and $\mathbf{F}$ and $\mathbf{G}$. Also, $(\mathbf{F}, \mathbf{F})$ is always real and non-negative, and $(\mathbf{F}, \mathbf{F})$ is known as the L^2 norm of $\mathbf{F}$. A normalized wavefunction is one where $(\mathbf{F}, \mathbf{F}) = 1$.

Having defined an inner product for two wavefunctions, we say that any operator $\hat{\Theta}$ is **Hermitian** if $\left(\mathbf{F}, \hat{\Theta}\mathbf{G}\right) = \left(\hat{\Theta}\mathbf{F}, \mathbf{G}\right)$ for any fields $\mathbf{F}$ and $\mathbf{G}$.

Now using this we can check that the operator in equation 3.30 is Hermitian and derive nice properties around that conclusion:

$$\begin{aligned}
\left(\mathbf{F}, \hat{\Theta}\mathbf{G}\right) &= \int \mathbf{F}^* \cdot \frac{1}{\bar{\bar{\mu}}_r} \nabla \times \nabla \times \mathbf{G} \\
&= \int (\nabla \times \mathbf{F})^* \cdot \frac{1}{\bar{\bar{\mu}}_r} (\nabla \times \mathbf{G}) + \int \nabla \cdot \left(\mathbf{F} \times \frac{1}{\bar{\bar{\mu}}_r} \nabla \times \mathbf{G} \right) \\
&= \int \left[\nabla \times \left(\frac{1}{\bar{\bar{\mu}}_r} \nabla \times \mathbf{F} \right) \right]^* \cdot \mathbf{G} + \int \nabla \cdot \left(\nabla \times \mathbf{F} \times \frac{1}{\bar{\bar{\mu}}_r} \nabla \times \mathbf{G} \right) + \int \nabla \cdot \left(\mathbf{F} \times \frac{1}{\bar{\bar{\mu}}_r} \nabla \times \mathbf{G} \right) \\
&= \int \left[\nabla \times \left(\frac{1}{\bar{\bar{\mu}}_r} \nabla \times \mathbf{F} \right) \right]^* \cdot \mathbf{G} \\
&= \left(\hat{\Theta}\mathbf{F}, \mathbf{G} \right)
\end{aligned}$$

Here the vector cross product identity[2] is used twice and surface terms that derive from using the Divergence Theorem are neglected.

The importance of knowing that the operator in the left side of 3.30 is hermitian resides in the fact that Hermitian operators have real numbers as eigenvalues. This can be seen by taking the inner product $\left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right)$ and observing that operation of $\hat{\Theta}$ on one of its eigenvectors $\mathbf{E}$ produces the same eigenvector multiplied by the eigenvalue as shown in 3.31. Then:

$$\left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right) = \left(\frac{\omega}{c}\right)^2 (\mathbf{E}, \mathbf{E})$$

Given that $(\mathbf{E}, \mathbf{E})$ is real, as we mentioned before, when taking the complex conjugate of that product we have:

$$\left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right)^* = \left(\frac{\omega^2}{c^2}\right)^* (\mathbf{E}, \mathbf{E})$$

and being Hermitian:

$$\begin{aligned} \left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right)^* &= \left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right)^* \\ \left(\frac{\omega^2}{c^2}\right)^* (\mathbf{E}, \mathbf{E}) &= \left(\frac{\omega^2}{c^2}\right) (\mathbf{E}, \mathbf{E}) \end{aligned}$$

Speed of light c is real, so $\omega^2 = \left(\omega^2\right)^*$ must be real.

3.4.2 Symmetry groups

As in Quantum Mechanics and any other eigen-problems, we must introduce the concept of orthogonality in order to understand other operations. We say that two wavevectors are **orthogonal** if $(\mathbf{E}, \mathbf{E}) = 0$, and this happens whenever they have different frequencies. This can be seen as a product of Hermiticity of operator $\hat{\Theta}$ by the following operation on two different modes $\mathbf{E}_1$ and $\mathbf{E}_1$:

$$\begin{aligned} c^2 \left(\mathbf{E}_2, \hat{\Theta}\mathbf{E}_1\right) &= c^2 \left(\hat{\Theta}\mathbf{E}_2, \mathbf{E}_1\right) \\ \omega_1^2 \left(\mathbf{E}_2, \mathbf{E}_1\right) &= \omega_2^2 \left(\mathbf{E}_2, \mathbf{E}_1\right) \\ \left(\omega_1^2 - \omega_2^2\right) \left(\mathbf{E}_2, \mathbf{E}_1\right) &= 0 \end{aligned}$$

From this one can see that if two eigenfunctions have different frequencies $(\omega_1^2 - \omega_2^2 \neq 0)$ then $(\mathbf{E}, \mathbf{E}) = 0$ must be true and they are orthogonal. Now, if $\left(\omega_1^2 - \omega_2^2\right) = 0$ then $\mathbf{E}_1$ and $\mathbf{E}_1$ are not necessarily orthogonal, and the value is known as a **degenerate** frequency because there is more than one state or wavefunction with eigenvalue $\left(\frac{\omega^2}{c^2}\right)$. In this section we will see that degeneracy is related with symmetries of the domain, and that will be useful for the solution of periodic problems.

[2] $\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B})$ With $\mathbf{A} = \mathbf{F}$ and $\mathbf{B} = \nabla \times \mathbf{G}$, first and then $\mathbf{A} = \nabla \times \mathbf{F}$ and $\mathbf{B} = \mathbf{G}$

Symmetry operations are operations that do not transform the wavefunction of a mode. Symmetries of a problem are such that if a symetry operation is applied to the wavefunction, it remains the same but multiplied by a scalar. This is called being invariant under the operation. So rotation, inversion, and reflections, are common symmetry operations that can be applied to systems that are symmetric under rotation, inversion and reflection, respectively. Probably the most immediate symmetry operation one can think of is the identity operation: $\hat{E}\mathbf{E}(\mathbf{r}) = \mathbf{E}(\mathbf{r})$, that transform a system into itself.

Another interesting operation is that of Inversion ($\hat{O_I}$), which takes a function $\mathbf{E}(\mathbf{r})$ and inverts its argument: $\hat{O_I}\mathbf{E}(\mathbf{r}) = \mathbf{E}(-\mathbf{r})$. If $\mathbf{E}(-\mathbf{r}) = \mathbf{E}(\mathbf{r})$ we say that the mode is invariant under inversion, or invertible. Finally, the translation operator is one where the argument gets shifted in space by a given displacement $\mathbf{d}$: $\hat{T}_d\mathbf{E}(\mathbf{r}) = \mathbf{E}(\mathbf{r} - \mathbf{d})$. One function that is invariant over translation operations is a plane wave like e^{ikz}, because operation of $\hat{T}$ over the planewave gives the same wavefunction by a scalar $e^{-ik\mathbf{d}}$:

$$\hat{T}e^{ikz} = e^{ik(z-\mathbf{d})} = e^{-ik\mathbf{d}}e^{ikz}$$

We can see here that this is an eigenvalue problem with eigenfunctions of the form e^{ikz} and complex eigenvalues $e^{-ik\mathbf{d}}$. Now, operators can act on other operators, and they can also be invariant under symmetry operations. If we have an operator $\hat{\Theta}$ whose intrinsic medium properties are characterized by $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$, and those properties are homogeneous in space, we will be acting on a system with translational symmetry. That is, the operator is the same at different points in space. So, if we have a wave function $\mathbf{E}(\mathbf{r})$ displace it with $\hat{T}_d$, then act on it with $\hat{\Theta}$ and displace it back with an inverted translation operator $\hat{T_d}^{-1}$ we will get the same result as if only $\hat{\Theta}$ was used:

$$\hat{\Theta}\mathbf{E}(\mathbf{r}) = \hat{T_d}^{-1}\hat{\Theta}\hat{T}_d\mathbf{E}(\mathbf{r})$$
$$\hat{\Theta} = \hat{T_d}^{-1}\hat{\Theta}\hat{T}_d$$

Whenever that happens with operators, we can write it in the form:

$$\hat{T}_d\hat{\Theta} - \hat{\Theta}\hat{T}_d = 0$$

and bring the definition of **commutator** between two operators as in Quantum Mechanics:

$$\left[\hat{A}, \hat{B}\right] \triangleq \hat{A}\hat{B} - \hat{B}\hat{A} \tag{3.34}$$

If $\left[\hat{A}, \hat{B}\right] = 0$ we say that $\hat{\Theta}$ commutes with $\hat{T}_d$, and that implies that that there are wavefunctions common to both. This is useful because sometimes eigenvalues and eigenfunctions of simple symmetry operators are easier to determine than those of $\hat{\Theta}$. The set of symmetry operators that commute with $\hat{\Theta}$ forms the symmetry group of the problem.

The fact that plane wave solutions are a solution of the problem is a consequence of them being solution to a symmetry operation that commutes with the operator of the problem. "When one has commuting operators, one can choose simultaneous eiigenvectors of both operators" [13]

The shared eigenfunctions transform as irreducible representations of the symmetry group. Examples of operators that belong to the symmetry group of a given crystal lattice are Translation (both continous and discrete), Rotation, and mirror operations.

Bloch-Floquet theory results from the special case of discrete translation operators. Also from quantum mechanics we can import the concept of commuting and commutators between operators.

3.4.3 Conservation of energy for waves in source less media

We define the energy of a field $\mathbf{w}$ as its norm $||\mathbf{w}||^2 = (\mathbf{w}, \mathbf{w})$. Conservation of energy in time in a source less problem like that of equation 3.15 is obtained when $||\mathbf{w}||^2$ variation in time is zero, thus:

$$\frac{\partial ||\mathbf{w}||^2}{\partial t} = \frac{\partial (\mathbf{w}, \mathbf{w})}{\partial t} = (\dot{\mathbf{w}}, \mathbf{w}) - (\mathbf{w}, \dot{\mathbf{w}}) = \left(\hat{\Theta}\mathbf{w}, \mathbf{w}\right) + \left(\mathbf{w}, \hat{\Theta}\mathbf{w}\right) = \left(\hat{\Theta}\mathbf{w}, \mathbf{w}\right) - \left(\hat{\Theta}\mathbf{w}, \mathbf{w}\right) = 0 \quad (3.35)$$

Remembering that in a problem that is not harmonic we have $\hat{\Theta}\mathbf{E} = \frac{\partial^2 \mathbf{E}}{\partial t^2}$This means that under Hermitic operators such as $\hat{\Theta}$ the energy of the field is conserved

3.4.4 Energy functional of electromagnetic waves

By means of the **electromagnetic variational theorem** we can formulate an energy functional to to be minimized. This functional is defined as a normalized inner product between the function and the function multiplied by the operator:

$$U_f(\mathbf{E}) \triangleq \frac{\left(\mathbf{E}, \hat{\Theta}\mathbf{E}\right)}{(\mathbf{E}, \mathbf{E})} \quad (3.36)$$

It is similar to other formulations used in fields like Quantum Mechanics and Classical mechanics such as expectation values, and energy Lagrangians. The process of finding solutions that minimize such a potential is the core of what methods like Galerkin do for solving differential equations. In chapter 4 we will use a similar expression in order to solve the wave equation using Galerkin with Finite Elements.

Chapter 4

Finite element method

El cálculo variacional es una disciplina que se encarga de encontrar el mínimo de un funcional. En donde un funcional es una mapeo de un espacio evectorial a los reales. esta es la ec diferencial Lu = f sí o qué? Entonces el residuo es esto R = Lu - f o mejor dicho esto R(v) = Lv - f Y cuando se evalúa en la solución R(u) = 0 Entonces minimizar un residuo no tiene gracia, porque es encontrar la solución exacta Que es lo que no sabemos hacer Pero entonces uno puede decir Minimicemos un residuo "promediado" Por, ej, la norma del error Entonces definimos un Residuo ponderado Rp(u,v) = int(v*Lu - v*f) (weighting en españoll es ponderar) Uno propone una solución con una forma que uno conoce: senos y cosenos, polinomios, Gaussianas.... Y encuentra encuentra la combinación lineal de esas funciones que minimiza Rp (Ya estamos hablando de métodos aproximados para la ecuación diferencial)

The Finite Element Method approximate an integral formulation that is –in some sense– equivalent with a differential equation. This integral (weak) formulation could be obtained from a variational principle, such as the Principle of Virtual Works, or the Integral of Action [10], but could also be obtained from a more general approach like the Weigthed Residue Method [31, 20]. In the cas of electromagnetic waves, we can formulate a variational principle where the functional to be minimized is the energy carried by the electric and magnetic fields (FALTA REFERENCIA).

This project uses the Galerkin Finite Element Method to construct an approximate solution of initial-boundary value problems involving the wave equation of electromagnetic fields 3.30.

Galerkin's method converts a continuous operator problem like a differential equation to a discrete problem by stating it as a weighted residual formulation.

4.1 Weak formulation of the problem

In a weighted residual formulation weight functions are used in order to minimize a functional that is stated as the integral of the operator problem over the simulation domain4.1.

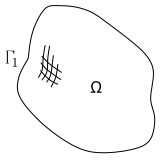

Figure 4.1: Abstract simulation domain and boundary

Galerkin method involves weight functions that belong to the same space as the solution. integration over the domain:

My weight functions wanna be called $\mathbf{W}$ instead. They will belong to the same function space as $\mathbf{E}$.

$\int_\Omega \mathbf{W}\cdot$(3.30):

$$\int_\Omega \mathbf{W}\cdot\left[\nabla\times\ \left(\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)-k_0^2\bar{\bar{\epsilon_r}}\cdot\mathbf{E}\right]=-ik_0Z_0\int_\Omega \mathbf{W}\cdot\mathbf{J} \tag{4.1}$$

$$\int_\Omega \mathbf{W}\cdot\nabla\times\ \left(\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)-k_0^2\int_\Omega \mathbf{W}\cdot\bar{\bar{\epsilon_r}}\cdot\mathbf{E}=-ik_0Z_0\int_\Omega \mathbf{W}\cdot\mathbf{J} \tag{4.2}$$

Now lets focus on the first integral on the left hand side of the equation. Here we will invoke the vector identity: $\mathbf{A}\cdot\nabla\times\mathbf{B}=\mathbf{B}\cdot\nabla\times\mathbf{A}-\nabla\cdot(\mathbf{A}\times\mathbf{B})$ Where $\mathbf{A}=\mathbf{W}$ and $\mathbf{B}=\bar{\bar{\epsilon_r}}\nabla\times\mathbf{E}$ To express it as:

$$\int_\Omega \mathbf{W}\cdot\nabla\times\ \left(\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)=\int_\Omega \bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\cdot\nabla\times\mathbf{W}-\int_\Omega \nabla\cdot\left(\mathbf{W}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right) \tag{4.3}$$

The Divergence Theorem allows us to transform the volume integral on the second term of the right hand side to a closed surface integral:

$$\int_\Omega \nabla\cdot\left(\mathbf{W}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)=\oint_\Gamma \hat{n}\cdot\left(\mathbf{W}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right) \tag{4.4}$$

And we will have two kinds of boundaries, Dirichlet and Newman (Reference some textbook), thus $\oint_\Gamma=\int_{\Gamma_D}+\int_{\Gamma_N}$. The Dirichlet contribution will be zero because the weight functions have also been chosen to be zero at Dirichlet boundaries ($\mathbf{W}\mid_{\Gamma_D}=0$). One last step is to apply the triple product identity to the argument inside the Newman integral so that:

$$\hat{n}\cdot\left(\mathbf{W}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)=\mathbf{W}\cdot\left(\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\times\hat{n}\right)=-\mathbf{W}\cdot\left(\hat{n}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right)$$

Substituting everything:

$$\int_\Omega \bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\cdot\nabla\times\mathbf{W} - k_0^2\mathbf{W}\cdot\bar{\bar{\epsilon_r}}\cdot\mathbf{E} + \int_{\Gamma_N}\mathbf{W}\cdot\left(\hat{n}\times\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right) = -ik_0Z_0\int_\Omega\mathbf{W}\cdot\mathbf{J} \tag{4.5}$$

4.2 Boundary conditions

Look for a nice reference that explain the situation on the boundaries and why is it important to define both the field at the boundary or the ratio of the field at the boundary. Maybe something related to the uniqueness of the solution. Pending to include.

$$\hat{n}\times\mathbf{E} = \mathbf{P} \quad on\ \Gamma_D \tag{4.6}$$

$$\hat{n}\times\left(\bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\right) = \mathbf{K}_N \quad on\ \Gamma_N \tag{4.7}$$

$\mathbf{P}$ is the value for tangential electric field on Dirichlet boundaries Γ_D, η_r is the normalized surface impedance and $\mathbf{K}_N$ is a function that represents boundary sources or electric field flux on Γ_N.

Replacing equation 4.7 in 4.5:

$$\begin{aligned}\int_\Omega \bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\cdot\nabla\times\mathbf{W} - k_0^2\mathbf{W}\cdot\bar{\bar{\epsilon_r}}\cdot\mathbf{E} &= -ik_0Z_0\int_\Omega\mathbf{W}\cdot\mathbf{J} \\ &\quad -\int_{\Gamma_N}\mathbf{W}\cdot\mathbf{K}_N\end{aligned} \tag{4.8}$$

$$\begin{aligned}\int_\Omega \bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\cdot\nabla\times\mathbf{W} - k_0^2\mathbf{W}\cdot\bar{\bar{\epsilon_r}}\cdot\mathbf{E} &= -ik_0Z_0\int_\Omega\mathbf{W}\cdot\mathbf{J} \\ &\quad -\int_{\Gamma_N}\mathbf{W}\cdot\mathbf{K}_N\end{aligned} \tag{4.9}$$

Using:

$$-\mathbf{W}\cdot(\hat{n}\times(\hat{n}\times\mathbf{E})) = (\hat{n}\times\mathbf{W})\cdot(\hat{n}\times\mathbf{E})$$

4.3 Abstract form of the equation

Time to introduce bi linear operators. These operators are meant to ease mathematical manipulations. Let's do some definitions first: $\mathbb{V}$ is a vector space of square integrable functions that vanishes at Dirichlet boundaries.

$$\mathbb{V} = \left\{v\in L^2(a,b) : a(v,v) < \infty \wedge v(\Gamma_D) = 0\right\}$$

$$L^2 = \left\{v : \Omega\to\mathbb{R} \quad such\ that \quad \int_\Omega v^2 d\Omega = 0\right\}$$

$$\begin{aligned} a(\mathbf{W},\mathbf{E}) &: \mathbb{V}\times\mathbb{V}\to\mathbb{R} \\ a(\mathbf{W},\mathbf{E}) &= \int_\Omega \bar{\bar{\mu_r}}^{-1}\nabla\times\mathbf{E}\cdot\nabla\times\mathbf{W}d\Omega \end{aligned} \tag{4.10}$$

$$\begin{aligned} m(\mathbf{W},\mathbf{E}) &: \mathbb{V}\times\mathbb{V}\to\mathbb{R} \\ m(\mathbf{W},\mathbf{E}) &= \int_\Omega k_0^2\mathbf{W}\cdot\bar{\bar{\epsilon_r}}\cdot\mathbf{E}d\Omega \end{aligned} \tag{4.11}$$

$$\begin{aligned} q(\mathbf{W}) &: \mathbb{V}\to\mathbb{R} \\ q(\mathbf{W}) &= \int_{\Gamma_N}\mathbf{W}\cdot\mathbf{K}_N \end{aligned} \tag{4.12}$$

$$\begin{aligned} f(\mathbf{W}) &: \mathbb{V}\to\mathbb{R} \\ f(\mathbf{W}) &= ik_0Z_0\int_\Omega\mathbf{W}\cdot\mathbf{J} \end{aligned} \tag{4.13}$$

Where $\mathbf{J}$ and $\mathbf{K}_N$ are known field and boundary conditions.

These operators take vectors as inputs and return scalars.

$$a(\mathbf{W},\mathbf{E}) - m(\mathbf{W},\mathbf{E}) = -f(\mathbf{W}) - q(\mathbf{W}) \tag{4.14}$$

4.4 Base functions and discretization

For 2D:

$$\mathbf{E} = E(x,y)_x\hat{a}_x + E(x,y)_y\hat{a}_y$$

The domain will be split in elements defined by relations between nodes (Add a figure and explain better how is it that you split a domain). The approximate solution will be computed using interpolations applied to nodal values. Lets say that the set of nodes that represent values of the field in the domain is called η. On nodes belonging to Dirichlet boundaries we will know the value of the field and it is convenient to split the set of nodes into its known and unknown elements $\eta_D \cup \eta \setminus \eta_D = \eta$. Each physical node will contain two components of the field, one for x and the other for y. So the number of evaluation nodes gets doubled.

If N is the total number of values:

$$N = n_x + n_y$$

.

Where n_x and n_y are the number of evaluation nodes associated to fields in x and y . When programming it is convenient to distinguish where does a node belongs, so I will treat n_x and n_y as sets as well in order to build a notation for the sums based on how an iterator surfs a set.

$$n_x = n_x \in \eta_D + n_x \in \eta \setminus \eta_D$$

$$n_y = n_y \in \eta_D + n_y \in \eta \setminus \eta_D$$

If I say:

$$i : n_x \in \eta_D$$

That will mean that the iteration will occur on the indexes that belong to the set of nodes in the Dirichlet region associated to x component of the field.

$$E(x,y)_x \approx \sum_{i:\ n_x \in \eta_D} h_i E_i^x + \sum_{i:\ n_x \in \eta \setminus \eta_D} h_i E_i^x$$
$$E(x,y)_y \approx \sum_{i:\ n_y \in \eta_D} h_i E_i^y + \sum_{i:\ n_x \in \eta \setminus \eta_D} h_i E_i^y$$

Left side is known values and right side is unknowns.

In the same way but without knowing W on the boundary:

$$\mathbf{W} = W(x,y)_x \hat{a}_x + W(x,y)_y \hat{a}_y$$

$$W(x,y)_x \approx \sum_{i:\ n_x \in \eta_D} h_i W_i^x + \sum_{i:\ n_x \in \eta \setminus \eta_D} h_i W_i^x$$
$$W(x,y)_y \approx \sum_{i:\ n_y \in \eta_D} h_i W_i^y + \sum_{i:\ n_x \in \eta \setminus \eta_D} h_i W_i^y$$

I believe that with source terms and boundaries the expansion can be made either with only the known values on nodes, or with interpolation functions such as those before. Right here I think I will ommit interpolation of $\mathbf{J}$ and $\mathbf{K}_N$.

$$\mathbf{J} = J(x,y)_x \hat{a}_x + J(x,y)_y \hat{a}_y$$

$$J(x,y)_x \approx \sum_{i:\ n_x \in \eta_D} h_i J_i^x + \sum_{i:\ n_x \in \eta \setminus \eta_D} h_i J_i^x$$
$$J(x,y)_y \approx \sum_{i:\ n_y \in \eta_D} J_i^y + \sum_{i:\ n_x \in \eta \setminus \eta_D} J_i^y$$

$$\mathbf{K}_N = K(x,y)_x \hat{a}_x + K(x,y)_y \hat{a}_y$$

$$K(x,y)_x \approx \sum_{i:\ n_x \in \eta_D} h_i K_i^x + \sum_{i:\ n_x \in \eta \setminus \eta_D} 0$$
$$K(x,y)_y \approx \sum_{i:\ n_y \in \eta_D} h_i K_i^y + \sum_{i:\ n_x \in \eta \setminus \eta_D} 0$$

Definition of h_i is left for later because its complicated.

Substitution of **E** and **W**, into **??** is a mess. To make it easier lets use the operators and their nice properties. To be bilinear is to be linear in both arguments, to be linear means to satisfy additivity and homogeneity. An illustration of this:

$$a(\alpha u + \beta v, w) = \alpha a(u,w) + \beta a(v,w)$$

$$a(u, \alpha v + \beta w) = \alpha a(u,v) + \beta a(u,w)$$

The rotational and dot product inside the integrals defined in the abstract forms are linear. A proof which I am pending to do will show that the operators themselves are bi linear. Also, it remains to be prooved if the following is true:

$$a(u,v) = a(v,u)$$

$$m(u,v) = m(v,u)$$

So the following can happen:

$$\begin{aligned} a\left(W_x, E_x\right) = \quad & a\left(\sum_{i:\ n_x \in \eta_D} h_i W_i^x, \sum_{j:\ n_x \in \eta_D} h_j E_j^x\right) + a\left(\sum_{i:\ n_x \in \eta \setminus \eta_D} h_i W_i^x, \sum_{j:\ n_x \in \eta \setminus \eta_D} h_j E_j^x\right) \\ = \quad & \sum_{i:\ n_x \in \eta_D} W_i^x a\left(h_i, \sum_{j:\ n_x \in \eta_D} h_j E_j^x\right) + \sum_{i:\ n_x \in \eta \setminus \eta_D} W_i^x a\left(h_i, \sum_{j:\ n_x \in \eta \setminus \eta_D} h_j E_j^x\right) \\ = \quad & \sum_{i:\ n_x \in \eta_D} W_i^x \sum_{j:\ n_x \in \eta_D} E_j^x a\left(h_i, h_j\right) + \sum_{i:\ n_x \in \eta \setminus \eta_D} W_i^x \sum_{j:\ n_x \in \eta \setminus \eta_D} E_j^x a\left(h_i, h_j\right) \\ = \quad & \sum_{j:\ n_x \in \eta_D} a\left(h_i, h_j\right) E_j^x \sum_{i:\ n_x \in \eta_D} W_i^x + \sum_{j:\ n_x \in \eta \setminus \eta_D} a\left(h_i, h_j\right) E_j^x \sum_{i:\ n_x \in \eta \setminus \eta_D} W_i^x \end{aligned} \tag{4.15}$$

$$\sum_{j:\ n_x \in \eta_D} E_j^x = \vec{g}_j^x$$

$$\sum_{i:\ n_x \in \eta \setminus \eta_D} W_i^x = \vec{W}^x$$

$$\sum_{j:\ n_x \in \eta \setminus \eta_D} E_j^x = \vec{E}^x$$

$$\vec{g}_i = \vec{g}_j^x + \vec{g}_j^y \qquad j = 1..N$$

$\vec{g}_j$ is a vector of size N that holds values of E on each Dirichlet boundary node for both x, and y components. Vector $\hat{g}_i^y$ follows from a simmilar procedure on E_y. It is of importance for me as the one to program to say that: even though the sets defined under the summation are subsets of the set of all nodes, when programming, their associate vectors will span the whole domain. In other words this notation stands for entries to indexes to vectors that may be defined full of zeroes. Or in a different approach: j in $j:\ n_x \in \eta_D$ can be indexes 1 and N meaning that the first and last nodes belong to Dirichlet boundary points on x All other elements of the vector are undefined and hold their initiation value zero.

Changing the indexes i,j and using the definition of dot product in a matrix notation we can translate the abstract form as:

$$a\left(W_x, E_x\right) = \langle \mathbb{A}\vec{g}^x, \vec{W}^x \rangle + \langle \mathbb{A}\vec{E}^x, \vec{W}^x \rangle$$

Where A is a matrix whose elements contain the indexed integration over the basis functions h_i, and h_j, these are known values because we know the form of the functions and can easily calculate the integrals by numerical or analytic means.

$$\mathbb{A} = \mathbb{A}^x + \mathbb{A}^y$$

$$\mathbb{A}^x = \sum_{i,j}^{n_x \in \eta \setminus \eta_D} a(h_i, h_j) + \sum_{i,j}^{n_y \in \eta \setminus \eta_D} a(h_i, h_j)$$

The product $\mathbb{A}^x \vec{g}^x = \vec{d}^x$ will be called the Dirichlet vector.

$$a\left(W_x, E_x\right) = \langle \vec{d}^x, \vec{W}^x \rangle + \langle \mathbb{A}^x \vec{E}^x, \vec{W}^x \rangle \tag{4.16}$$

In a very similar way but now substituting the approximate functions into the kinetic operator $m(\mathbf{W}, \mathbf{E})$ we get:

$$\begin{aligned} m\left(W_x, E_x\right) &= \langle \mathbb{M}^x \vec{g}^x, \vec{W}^x \rangle + \langle \mathbb{M}^x \vec{E}^x, \vec{W}^x \rangle \\ m\left(W_x, E_x\right) &= \langle \vec{b}^x, \vec{W}^x \rangle + \langle \mathbb{M}^x \vec{E}^x, \vec{W}^x \rangle \end{aligned} \tag{4.17}$$

With:

$$\mathbb{M} = \mathbb{M}^x + \mathbb{M}^y$$

$$\mathbb{M} = \sum_{i,j}^{n_x \in \eta \setminus \eta_D} m(h_i, h_j) + \sum_{i,j}^{n_y \in \eta \setminus \eta_D} m(h_i, h_j)$$

And the same follows with operators q and f:

$$f(W_x) = \langle \vec{f}^x, \vec{W}^x \rangle \tag{4.18}$$

$$q(W_x) = \langle \vec{q}^x, \vec{W}^x \rangle \tag{4.19}$$

$$\vec{f}_i^x = ik_0 Z_0 \sum_{i:\ n_x \in \eta} \int_\Omega h_i J_i^x$$

$$\vec{q}_i^x = \sum_{i:\ n_x \in \eta_N} \int_{\Gamma_N} h_i K_i^x$$

Where I introduced a subset of the set $\eta \setminus \eta_D$ called η_N which represents nodes on Newman boundaries.

Substituting definitions: 4.16,4.17, 4.19, 4.18 in equation 4.14, we get:

$$\langle \vec{d}^x, \vec{W}^x \rangle + \langle \mathbb{A}^x \vec{E}^x, \vec{W}^x \rangle - \langle \vec{b}^x, \vec{W}^x \rangle - \langle \mathbb{M}^x \vec{E}^x, \vec{W}^x \rangle = -\langle \vec{f}^x, \vec{W}^x \rangle - \langle \vec{q}^x, \vec{W}^x \rangle$$

$$\langle \mathbb{A}^x \vec{E}^x - \mathbb{M}^x \vec{E}^x, \vec{W}^x \rangle = \langle \vec{b}^x - \vec{d}^x - \vec{q}^x - \vec{f}^x, \vec{W}^x \rangle \tag{4.20}$$

Being $\vec{W}^x$ an arbitrary function, the following linear system of equations appear:

$$\left(\mathbb{A}^x - \mathbb{M}^x\right) \vec{E}^x = \vec{b}^x - \vec{d}^x - \vec{q}^x - \vec{f}^x \tag{4.21}$$

Similarly and following exactly the same procedure:

$$\left(\mathbb{A}^y - \mathbb{M}^y\right) \vec{E}^y = \vec{b}^y - \vec{d}^y - \vec{q}^y - \vec{f}^y \tag{4.22}$$

And right now I guess those can be summed. I really don't get why I chose to separate them in the first place. Guess it was in order to make it clear that the components where independent.

So, Matrices and vectors are of the same size (N) for both equations, and the places where one has zeros has values in the other. I don't see any impediment to sum 4.21 and 4.22:

$$\left(\mathbb{A}^x - \mathbb{M}^x\right) \vec{E}^x + \left(\mathbb{A}^y - \mathbb{M}^y\right) \vec{E}^y = \vec{b} - \vec{d} - \vec{q} - \vec{f}$$

A system that I really don't know if can be brought to the form

$$\mathbb{K}\vec{E} = \vec{v}$$

Something that I've seen happening in many books is to remove rows and columns associated to Dirichlet positions of E in the matrices and vectors of the equation. This is done because we already know the values of E for those points and their information is already saved in vector $\vec{d}$. I will add the symbol $\backslash D$ before the symbols to note that Dirichlet rows and columns should be deleted.

$$^{\backslash D}\left[\left(\mathbb{A}^x - \mathbb{M}^x\right)\vec{E}^x + \left(\mathbb{A}^y - \mathbb{M}^y\right)\vec{E}^y = \vec{b} - \vec{d} - \vec{q} - \vec{f}\right]$$

4.5 Vectorial vs scalar formulation

4.6 Edge elements vs Node Elements

4.7 Second order elements, shape functions.

4.8 Numerical integration and Gauss quadrature

4.9 Mass matrices

¿What is the meaning of Mass matrices in EM?

discrete representation of a continuous distribution of something that multiplies the second time derivative of the field.

Mass matrices are cataloged as consistent or diagonal. Consistent mass matrices use the same shape functions as the ones used to generate the element stiffness matrix. All reference to mass matrices mentioned before, were consistent. [21] The other way to formulate mass matrices is the lumped mass matrix. Which is made by avoiding the interpolation and simply placing particle masses m_i at nodes i of an element such that $\sum m_i$ is the total element mass.

The great advantage of lumped mass matrices is that they are diagonal and the solution of the system of equations can be performed in a explicit manner convenient for big computational domains. However, precision is lost by not stating mass as functions to be interpolated.

To form a lumped mass matrix one can use the HRZ Lumping scheme which consist on the following algorithm [21]:

1. Compute the diagonal coefficients of the consistent mass matrix.
2. Compute the mass for each element m.
3. Compute the trace of the matrix s.
4. scale all the diagonal coefficients by multiplying them by the ratio $\frac{m}{s}$.

4.10 Explicit formulation

central-difference method Aproximates the second order derivative of $\mathbf{E}$ by expanding $\mathbf{E}_{n+1}$ and $\mathbf{E}_{n-1}$ in taylor series about time $n \triangle t$:

$$\mathbf{E}_{n+1} = \mathbf{E}_n + \delta t \dot{\mathbf{E}}_n + \frac{\delta t^2}{2}\ddot{\mathbf{E}}_n + \frac{\delta t^3}{6}\dddot{\mathbf{E}}_n + O(\delta t^4) \tag{4.23}$$

$$\mathbf{E}_{n-1} = \mathbf{E}_n - \delta t \dot{\mathbf{E}}_n + \frac{\delta t^2}{2}\ddot{\mathbf{E}}_n - \frac{\delta t^3}{6}\dddot{\mathbf{E}}_n + O(\delta t^4) \tag{4.24}$$

Restricting to fourth-order accuracy ($O(\delta t^4)$) and adding 4.23 to 4.24 one can easily solve for $\mathbf{E}_{n+1}$:

$$\ddot{\mathbf{E}}_n = \frac{1}{\delta t^2}\left(\mathbf{E}_{n+1} - 2\mathbf{E}_n + \mathbf{E}_{n-1}\right) \tag{4.25}$$

subscript n denotes time $n\delta t$ with δt being the selected timestep.

Replacing into our general formulation one gets (fix details):

$$\frac{1}{\delta t^2}\mathbb{M}\mathbf{E}_{n+1} = \frac{1}{\delta t^2}\mathbb{M}\left[2\mathbf{E}_n - \mathbf{E}_{n-1}\right]\mathbb{A}\mathbf{E}_n \tag{4.26}$$

Nice concluding remarks in page 424 of the book.

Chapter 5

Results

As mentioned in the introduction, a software platform able to simulate propagation of electromagnetic waves in photonic crystals was developed. In chapter 3 the equations that rule the problem where stated, and background behind one method of solution for them using FEA has been discussed in chapter 4. In this chapter the solutions obtained by applying these concepts are presented and compared with either their analytic solutions or numerical solutions from the literature.

5.1 Electrostatic benchmark tests

Now, platform PeyeQM was built in a bottom-up process that started by making a FE solver that could handle static scalar problems of electron confinement in 2D potential wells for application in Quantum Mechanics. This project involved an upgrade of that platform that began with the implementation of support for vector formulations, and a transition to Object Oriented Paradigm that could improve flexibility and maintenance.

The first section of this chapter shows the results obtained for Electrostatic benchmark tests, and were made in order to assert the accuracy of the static vectorial solver, and routines for the construction of stiffness matrices.

5.1.1 Electric field due to charged elements

Parallel plate capacitor

The first experiment was to simulate the most basic field we could think of, this is, that inside a parallel plate capacitor, where field lines go straight from one plate to the other.

Electric fields satisfy equation 3.5. If there are no sources or sinks ($-\frac{\partial \mathbf{B}}{\partial t} = 0$), then the field $\mathbf{E}$ is said to be *irrotational* and by an identity of vector calculus we know that there must exist a scalar field V whose gradient is a valid Electrostatic vector field:

$$\nabla \times \nabla V = 0 \tag{5.1}$$

Scalar equations are easier to solve and are very useful when the medium is homogeneous and isotropic, this is the reason why many books stick with scalar problems and leave the process of obtaining $\mathbf{E}$ as performing on V the derivations in operator ∇. Using the scalar potential as an intermediate step for the solution of $\mathbf{E}$ stops being a good idea when interfaces between mediums and sharp geometries appear, and a direct solution using vector fields gains relevance.

In a parallel plate capacitor like that in figure 5.1, we consider two (infinite, parallel, plane, perfectly conducting, charged) plates that occupy the planes $x = 0$ and $x = d$ kept at potentials $V = 0$ and $V = V_0$ respectively. With plates of very large dimensions compared to the spacing between them, the potential becomes a function of x only, and equation 5.1 becomes:

$$\frac{d^2V}{dx^2} = 0$$

Integrating twice, we get:

$$V(x) = Ax + B \tag{5.2}$$

Where A and B are constants of integration solved by using boundary conditions.

$$V(0) = A0 + B = 0 \quad or \quad B = 0$$

$$V(d) = Ad + B = V_0 \quad or \quad A = \frac{V_0}{d}$$

Making the particular solution for the potential:

$$V = \frac{V_0}{d}x \quad for \quad 0 < x < d$$

The field is then obtained by taking the gradient of V, and we add a $-$ sign taking into account that $\mathbf{E}$ is a conservative field.

$$\mathbf{E} = -\nabla V = -\frac{dV}{dx}\hat{a}_x = -\frac{V}{d}\hat{a}_x \tag{5.3}$$

This means that the field is uniform and directed from the higher potential plate to the lower potential plate as shown in 5.1 **??**.

A rectangular region was meshed and Dirichlet boundary condition were applied in the bottom and top plates as a field pointing down. Separation d is taken unitary and the result is shown in figure 5.2.

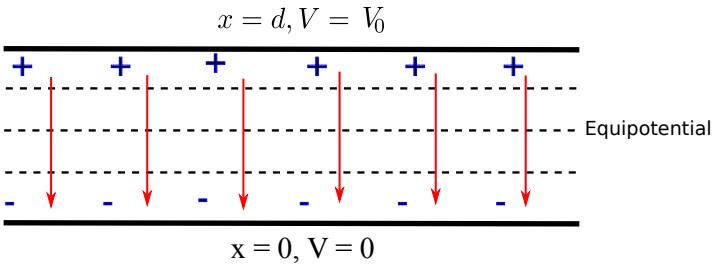

Figure 5.1: Cross sectional view of parallel plate capacitor.

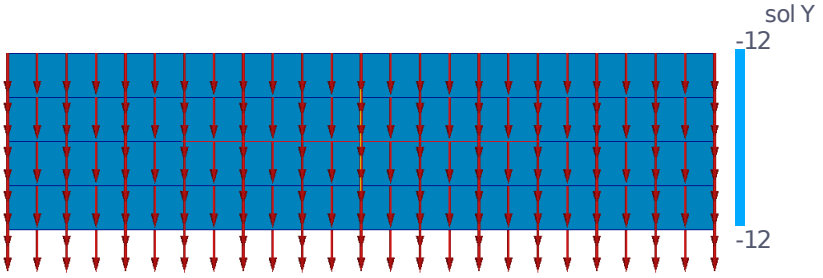

Figure 5.2: Solution of electric field in parallel plate capacitor.

It can be seen that the lines don't change in either magnitude or direction, and go from the charged plate wit potential V_0 to the bottom plate as expected.

This test showed that the routines for assembling stiffness matrices are capable of continuing a simple field over a distance between to boundaries.

The script for producing this simulation and the necessary input files can be seen in the *repository*.

Charged cylinder

The next field problem to solve in order to test PeyeQM was one with circular geometry. The solution for the field due to a point charge or a charged cylinder was used to compare the precision of the method for representing fields with two components.

Gauss law 3.3 in spherical coordinates, assuming a homogeneous medium with scalar permittivity is:

$$\epsilon \int_S \mathbf{E} \cdot d\mathbf{S} = \int_V \rho dV \tag{5.4}$$

Where $\int_V \rho dV = q$ is the charge of the particle. If that charge is distributed uniformly, then there are no preferred directions and the electric field must be radial [5] and have constant intensity over

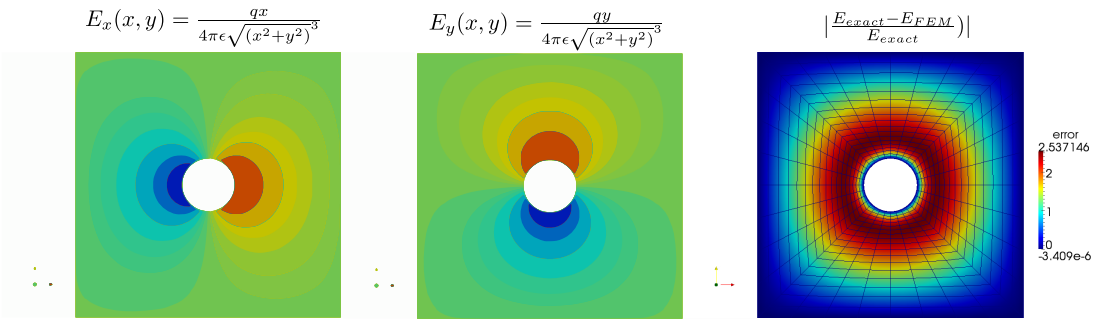

Figure 5.3: Whole simulation of Electric field due to a charged cylinder. Left, Numerical result for the x component of the field. Middle, x component of the solution, and, right, mesh and error calculated between analytic formula and results.

spherical shells. So for an arbitrary spherical shell of radius r:

$$\epsilon \mathbf{E} \int_\theta \int_\phi r^2 sin(\theta) d\phi = q$$
$$\mathbf{E}_r(r) = \frac{q}{4\pi\epsilon r^2}\hat{r}$$

Now, this has to be transformed into Cartesian coordinates in order to input boundary conditions. If we consider r as the magnitude of vector $\vec{r}$ in the unitary direction $\hat{r}$ then we can transform it to a linear combination of unitary vectors $\hat{x}$ and $\hat{y}$ by the following:

$$\vec{r} = rcos(\theta)\hat{x} + rsin(\theta)\hat{y} \tag{5.5}$$

And by trigonometry we know that $cos(\theta) = \frac{x}{r}$ and $sin(\theta) = \frac{y}{r}$. Making the necessary substitutions we get to:

$$\mathbf{E}_r(r) = \mathbf{E}_x(x,y) + \mathbf{E}_y(x,y) = \frac{qx}{4\pi\epsilon\sqrt{(x^2+y^2)}^3}\hat{x} + \frac{qy}{4\pi\epsilon\sqrt{(x^2+y^2)}^3}\hat{y} \tag{5.6}$$

So, a plot the solution after simulating should match a representation of this analytic result. We initially proposed a model where the charged cylinder or point source is modeled as a whole circle inside a square domain, the results of the simulation (figure 5.3) showed that for this kind of problem where the field decays in the form $\frac{1}{r^2}$ it was better to use finer meshes and take advantage of symmetries to reduce the computational cost. Taking just an eight of the model, and reshaping the outer boundary to a circle improved the quality of the elements and allowed us to use a finer mesh. figure 5.4 shows the y and x components of the field as well as the error between the simulation and the analytic solution. For the simulation factor $\frac{q}{2\pi\epsilon}$ has been normalized to 1, and the mesh was done done using 1996 QUAD8 elements with 5525 nodes, thus 11050 degrees of freedom. As a comparison, the simulation of the whole circle involved 2432 elements and 7040 nodes with 14080 degrees of freedom, but it solved for a domain that was eight times bigger.

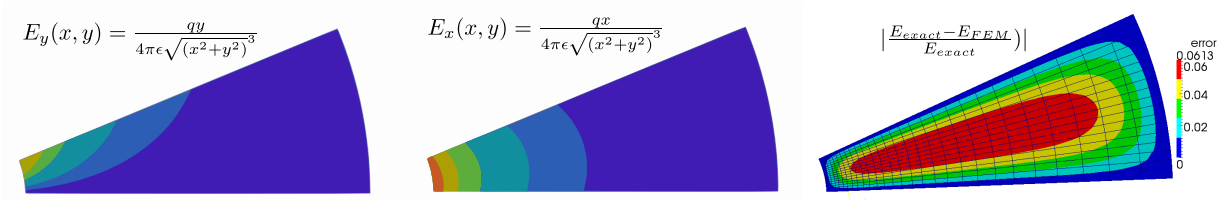

Figure 5.4: Segment of the simulation for Electric field due to a charged cylinder. a) Numerical result for the y component of the field, b) x component of the solution, c) Mesh and error calculated between analytic formula and results.

Electric Dipole, two charged spheres.

A similar simulation was performed using two semicircular surfaces, taking advantage of inversion symmetry along x axis. Boundary conditions are Dirichlet conditions over the circles and the rectangular boundaries on top, and Neumann conditions set to 0 on bottom lines. The analytic solution is simply the overlapping of the field due to charge 1 and charge 2, having one of them centered in the origin, and the other displaced by a distance d. The field everywhere can be expressed as:

$$\mathbf{E}_1(x,y) = x\left(x^2+y^2\right)^{-\frac{3}{2}}\hat{x} + y\left(x^2+y^2\right)^{\frac{3}{2}}\hat{y} \tag{5.7}$$

$$\mathbf{E}_2(x,y) = -(x-4)\left((x-4)^2+y^2\right)^{-\frac{3}{2}}\hat{x} - y\left((x-4)^2+y^2\right)^{\frac{3}{2}}\hat{y} \tag{5.8}$$

$$\mathbf{E}_x = \left[x\left(x^2+y^2\right)^{-\frac{3}{2}} - (x-4)\left((x-4)^2+y^2\right)^{-\frac{3}{2}}\right]\hat{x} \tag{5.9}$$

$$\mathbf{E}_y = \left[y\left(x^2+y^2\right)^{\frac{3}{2}} - y\left((x-4)^2+y^2\right)^{\frac{3}{2}}\right]\hat{y} \tag{5.10}$$

Where again $\frac{q}{2\pi\epsilon} = 1$ for the left charged circle and -1 for the one on the right at a distance $d = 4$. Figure 5.5 shows components x and y of the resulting field as obtained from the FE solver. The direction of the field lines can be observed by means of arrow glyphs in figure 5.6, where field lines go outwards in the positively charged cylinder and inwards in the negative. In the same way as before, a comparison between analytic and numerical solutions was performed (figure 5.7) and error appeared to be magnified in the region between cylinders. This value keeps being higher than expected, and different meshing schemes were tested in order to improve accuracy. Less error was observed using adaptative meshing methods than structured grids. The current mesh for this simulation has 510 elements and 1622 degrees of freedom, a future simulation is proposed with finer meshes using a PC with bigger RAM.

$$\mathbf{E}_x = \left[x\left(x^2+y^2\right)^{-\frac{3}{2}} - (x-4)\left((x-4)^2+y^2\right)^{-\frac{3}{2}} \right] \qquad \mathbf{E}_y = \left[y\left(x^2+y^2\right)^{\frac{3}{2}} - y\left((x-4)^2+y^2\right)^{\frac{3}{2}} \right]$$

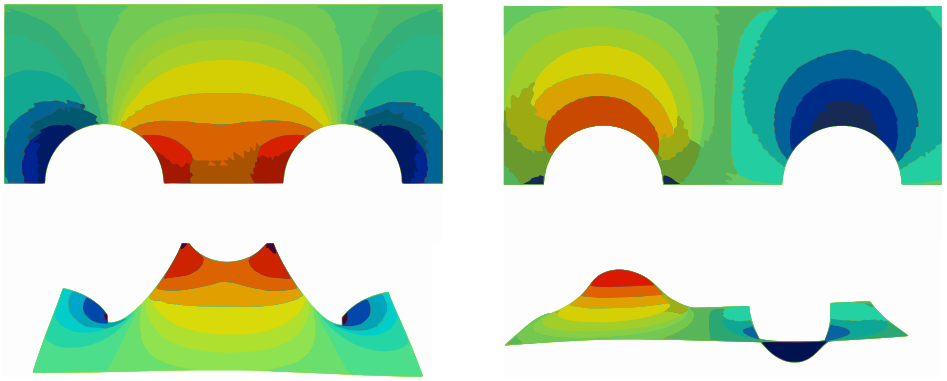

Figure 5.5: Components of the electric field after simulating a problem of two cylinders with opposite charges.

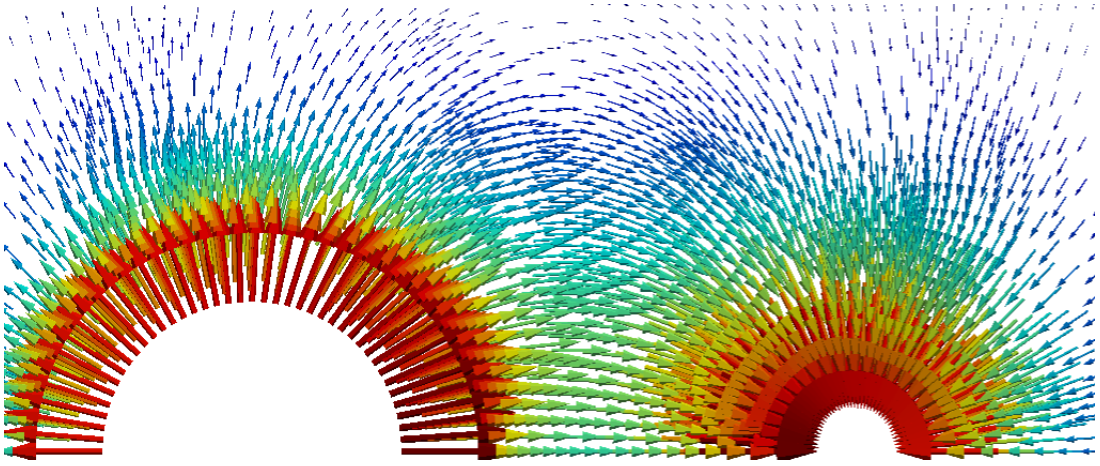

Figure 5.6: Arrow glyphs of the solution for the dipole problem. Lenght and color of the arrow indicate magnitude of the field. As expected, the field points from the positively charged cylinder to the negative.

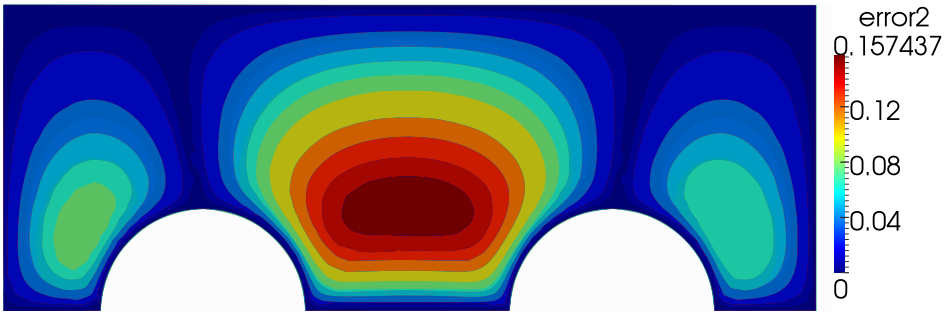

Figure 5.7: Error calculation of simulation against exact solution. The method reproduces the nature of the problem, but a finer mesh is needed to obtain precise results.

5.2 Harmonic benchmark tests

The second section regards solutions of eigenvalue problems, either for closed domains or infinite and periodic ones. The first part will deal with simulation of resonant modes in wave guides, and the second with free waves and periodic crystals.

5.2.1 Eigenvalues and modes in waveguides

Ideal wave guides can be modelled by a source-less version of the wave equation for time harmonic fields 3.21 in arbitrary 2D domains closed by a metallic boundary that guarantees Dirichlet condition $\mathbf{E} = 0 \quad at \quad \Gamma$. This problem is relevant in electromagnetism and telecommunications because it is the principle behind many applications such as data transmission in fiber optics, and microwaves. Here, the 2D domain represents a cross section of a metallic structure that guides waves along its axis. We are particularly interested in knowing two things:

1. The modes or wave functions that are solution to the equation for a particular shape.
2. The frequencies associated to those modes or shapes.

And will start by introducing the analytic solution behind simple wave guides such as rectangular and circular guides.

Rectangular waveguides

In transverse magnetic fields (TM) that travel inside a waveguide whose axis is over z, we have $\mathbf{H}_z = 0$ and solve for $\mathbf{E}$ components. Solutions of equation 3.30 where the medium inside the wave guide is a perfect dielectric, and for eigenvalues $\vec{k}^2 = \omega^2\mu\epsilon$ is a lengthy but straightforward process that involves separation of variables and use of boundary conditions:

$$\mathbf{E}_x = 0 \quad for \quad y = 0,\ 0 < x < a \tag{5.11}$$
$$\mathbf{E}_x = 0 \quad for \quad y = b,\ 0 < x < a \tag{5.12}$$
$$\mathbf{E}_y = 0 \quad for \quad x = 0,\ 0 < y < b \tag{5.13}$$
$$\mathbf{E}_y = 0 \quad for \quad x = a,\ 0 < y < b \tag{5.14}$$

A description of the solution process is left for the reader to look up in references such as Rao [19] or Jianming [12]. What is found in the process is that only certain discrete frequencies are allowed inside the waveguide, and they are given by:

$$\omega_{n,m} = \frac{1}{\sqrt{\mu\epsilon}}\sqrt{\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2} \qquad m, n = 0, 1, 2, ... \quad (m = n \neq 0) \tag{5.15}$$

Where ω is indexed by integers n, m and the trivial solution $\omega = 0$ is excluded. a is the width of the rectangular cross section and b is its height. The wave functions that are solution to this eigenproblem for each component of the field are in the following general form:

$$\mathbf{E}_z = A \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{b} e^{\mp j k_z z} \tag{5.16}$$

$$\mathbf{E}_x = \mp j B \frac{m\pi}{a} \cos \frac{m\pi x}{a} \sin \frac{n\pi x}{b} e^{\mp j k_z z} \tag{5.17}$$

$$\mathbf{E}_y = \mp j C \frac{n\pi}{b} \sin \frac{m\pi x}{a} \cos \frac{n\pi x}{b} e^{\mp j k_z z} \tag{5.18}$$

For our comparisons we will only look at how closely the shapes of the simulated solution represent $\mathbf{E}$ in 5.16, and how similar are the analytic and numeric natural frequencies of the guide ω.

Comparison of ω^2 for square wave-guide				
m,n	1,1	1,2	2,2	3,1
FEM	4.93480857	12.33721117	19.73961759	24.6763011
Anlytic	4.93480220	12.33700550	19.73920880	24.67401100

Comparison of ω^2 for rectangular waveguide $a = 2b$				
m,n	1,1	2,1	3,1	1,2
FEM	3.08425459	4.93480795	8.0190859	12.33717191
Anlytic	3.08425137	4.93480220	8.0190535	12.33700550

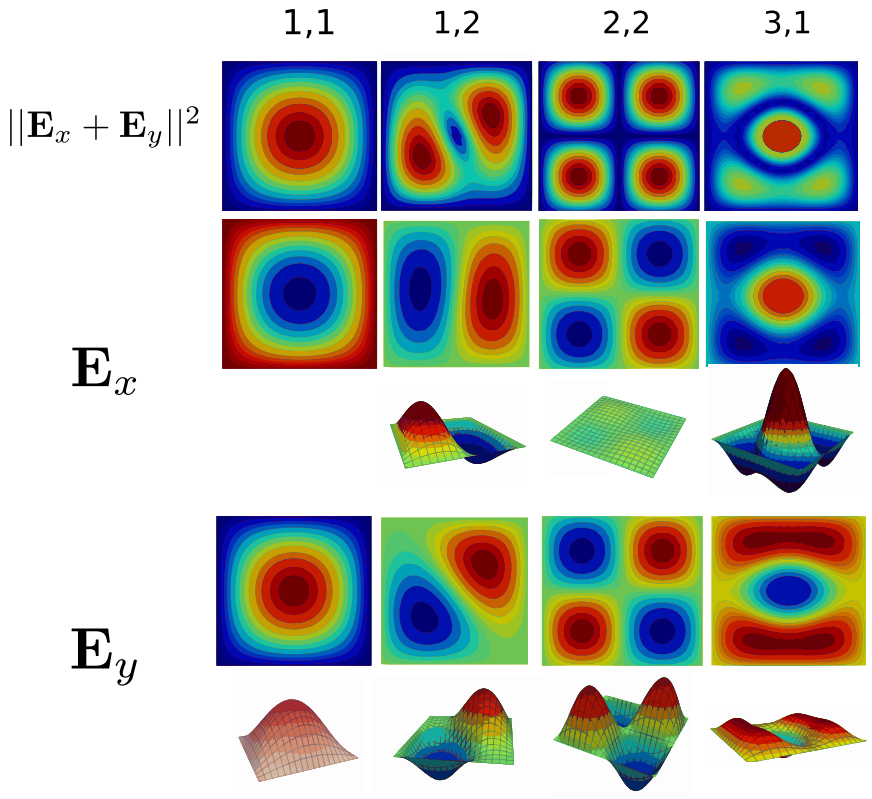

Figure 5.8: Results for three different modes from the simulation of a square shaped waveguide with side $a = b = 2$

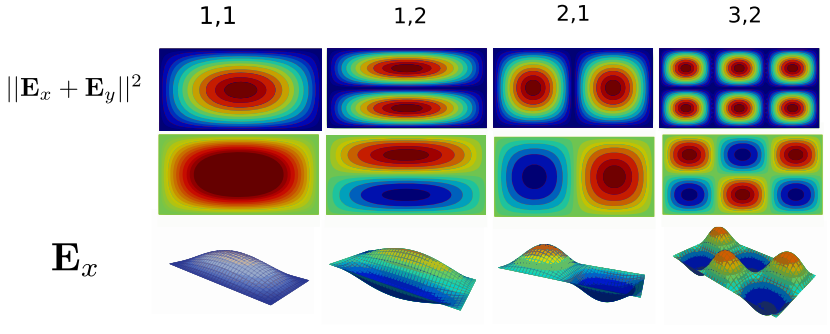

Figure 5.9: Results for three different modes from the simulation of a rectangle shaped waveguide with sides $a = 4$ and $b = 2$.

Chapter 6

Implementation

6.1 Object Oriented Paradigm

6.2 Classes, Diagrams and flow charts of PeYeQM

Chapter 7

Conclusions and future work

7.1 Conclusions

The objectives were met.

7.2 Future work

- Define vectorial triangular elements and scalar quadrilateral elements.
- Consider adding regions with Perfectly Matched Layers (PML) for the simulation of open domains.
- Evaluate convergence of the method for the problems described in chapter 5 using finer spatial and spectral meshes.
- Perform more simulations of time dependent problems involving deffects in finite crystals. And compare the results of Q factor and efficiency with other publications.
- Integrate the CAD and solver into a optimization algorithm that maximizes transmission or confinement by inducing variations in position and shape of defects in the lattice.
- Consider parallelization schemes to be implemented in order to make bigger simulations plausible.

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