Exploring Heterogeneous Time-Varying Materials for Photonic Applications, *Towards Solutions for the Manipulation and Confinement of Light*

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ABSTRACT

Exploring Heterogeneous Time-Varying Materials for Photonic Applications

Damián Pablo San-Román-Alerigi

Over the past several decades our understanding and meticulous characterization of the transient and spatial properties of materials evolved rapidly. The results present an exciting field for discovery, and craft materials to control and re-shape light that we are just beginning to fathom. State-of-the-art nano-deposition processes, for example, can be utilized to build stratified waveguides made of thin dielectric layers which put together result in a material with effective abnormal dispersion. Moreover, materials once deemed well-known are revealing astonishing properties, verbi gratia chalcogenide glasses undergo an atomic reconfiguration, when illuminated with electrons or photons, that results in a modification of its permittivity and permeability, up to \( \approx 40\% \). Moreover, these changes can be modulated in time.

This work revolves around the characterization and model of spacetime-varying materials and their applications, revisits Maxwell’s equations in the context of non-linear spacetime-varying media, and based on them introduces a numerical scheme that can be used to model waves in this kind of media, finally some interesting applications for light confinement and beam transformations are shown.
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LIST OF ABBREVIATIONS

EELS  Electron Energy Loss Spectroscopy
FDTD  Finite Difference Time Domain
FEM   Finite Element Method
FVM   Finite Volume Method
FWHM  full-width-half-maximum
ODE   Ordinary Differential Equation
PDE   Partial Differential Equation
PICs  Photonic Integrated Circuits
PSM   [Pseudo–]Spectral Method
WENO  Weighted Essentially Non-Oscillatory
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Introduction

I must had been five or four years old the first time I heard that light moved so fast, that it would go around the planet eight times before I could count one second. I was marveled, light could traverse all lands, go anywhere, transform and break in colorful errant streaks that met here and there in flaring beans on the kitchen floor. I began to play with mirrors and concocted an intricate plan to catch it, as if light was a firefly. The system would barter the bright light of Summer days into dozen glaring drops that I could use later to lit the night. Time passed, college came, and with it new knowledge and ideas. Light is ubiquitous and restless, our modern world relies on it and on its interactions with matter. Tailoring these interactions might be the key to stop light, to harvest it and transfigure it into the tiny beads I once imagined.

Materials can change our perception of light, take for example a straw half-submerged in a glass with water. The straw appears to be broken, and yet we know that is not the case; rather, it is the refraction of light rays traversing water what creates the illusion. Refraction is the underlying principle to understand the path followed by light rays as they traverse any material. One may wonder, then, if a skillful craftsmen could not join different liquids together to render an unimaginable illusion. What if this could be done in ever so small scales? And what if this imagined artifact could change also in time as light traverses it? What would happen then?

This manuscript is an attempt to solve some of these questions. As such It encompasses a set of discussions, journal publications, conferences, and white-papers
concerned with spacetime-varying materials and their photonic applications. My
intention has been to build a platform to study and model light propagation in
these media, one that can be expanded and used to design photonic devices and
explore new physical phenomena.

Fresnel, Fizeau, and time-varying media

Refraction and reflection were the starting knot in a thread of wave phenomena
originating in the interaction of light with matter: interference, refraction, po-
larization, birefringence, dispersion... In the XIX century Maxwell’s work, sum-
marized in his famed equations, together with Hertz’ experiments, showed that
light can be described as an electromagnetic wave [1–4]. Their discovery laid the
ground for many of our modern technologies. It changed forever our understand-
ing of light-matter interactions, and in turn originated theories and methods that
revolutionize our comprehension about the electromagnetic properties of materials
and the fundamental building blocks of light itself.

Yet, in the context of spacetime-varying media light-matter interactions remain
a matter of debate and discovery. To illustrate, let us go back to refraction. In
a letter to Arago, Fresnel posited that light rays traversing a moving fluid would
experience a change in their velocity that could not be accounted for solely by
refraction [5–8]. He calculated that light rays would be dragged by the moving
medium by a factor that depended on the medium’s velocity,

\[ V = \frac{v \left(1 - \frac{1}{n^2}\right)}{1 + \frac{v}{cn}} \]  

(1)

where \( v \) is the velocity of the medium and \( V \) the speed of light in it.

Moved by Fresnel’s work, Fizeau conceived an experiment using a moving fluid
and mirrors to measure the speed of light in flowing water (see Figure 1). He found
that the velocity of light in the liquid was lessened by a factor that matched Fres-
nel’s predictions. To explain the result, Fizeau and Fresnel posited a theory that
Figure 1: Fizeau’s experimental setup to observe the change in the speed of light propagating in moving water.

conjured the existence of a stationary \( \textit{æther} \) which dragged along moving substances but not air. However, the existence of æther was refuted by Michelson’s and Morley’s experiment \[9\], contradicting Fizeau’s and Fresnel’s hypothesis and experimental results. The conundrum was brought to terms by Lorentz, he proposed a mechanism of time-space contraction co-linear to the direction of motion that correctly explained Fresnel’s results \[10\]. This work, in turn, was the basis of Einstein’s general description of the electrodynamics of moving bodies \[11\], followed by the demonstration of the invariance of Maxwell’s equations under Lorentz transformations, ultimately leading to the derivation of the Minkowsky–Maxwell equations \[12–14\].

In special relativity, the paraxial approximation of the Minkowsky–Maxwell equations predicts Fizeau’s result. In particular, Laue showed that in Fresnel’s experiment the wave velocity would be given by \[15\]:

\[
V = \frac{v \left(1 - \frac{1}{n^2}\right)}{1 + \frac{v}{c} \frac{1}{n^2}} \approx v \left(1 + \frac{1}{n^2}\right)
\]

These results demonstrated a fascinating side of spacetime-varying media and wave interactions. Yet, until recently they were seldom revisited in applied science and engineering, perhaps owing to the many complications of creating [meta]materials with time-varying properties.

The panorama, however, is rapidly changing. As technology has evolved, so did
our comprehension of the inter- and intra-atomic laws governing material properties; leading the design of sophisticated characterization and fabrication methods, that give us the ability to craft materials that can be used to control light in ways that were unthinkable before. State-of-the-art nano-deposition processes, for example, can be employed in building stratified waveguides; made of dozen thin dielectric layers, each $\geq 10\text{nm}$, these waveguides show an effective abnormal dispersion with huge potential applications for telecommunications. That being said, meticulous characterizations of transient and spatial properties of materials, are revealing that these can be modulated in time at rates akin to electromagnetic wave oscillations, see \textit{e.g.} \cite{16,17}. Known as spacetime-varying or time-varying media, they present fascinating challenges and opportunities in all areas of research. In particular, wave-matter interactions, numerical models and applications remain a matter of debate and are largely unexplored. Notwithstanding, some novel effects have been identified: trapping, confinement, ultra-short pulse coupling, beam transformation, negative refraction, eigen-polarization, and the optical Bohm–Aharonov effect \cite{18–26}.

In terms of modeling, until not long ago only one general numerical scheme had been proposed for linear time-varying materials \cite{27}. This work presents, to the best of my knowledge, the first non-linear, full wave, numerical solver for Maxwell’s equations in spacetime-varying media. Furthermore, the numerical scheme described in this thesis can be readily extended to other wave phenomena \cite{28}.

Within the realm of photonic applications, spacetime-varying materials could open the door to manipulate light in new and exciting ways. Hence the need to introduce a platform that can be used to elucidate and model novel technologies to control light for \textbf{Photonic Integrated Circuits (PICs)} applications. The results of such model could be used to test diverse [meta]materials to enable myriad photonic devices, either feasible or imagined. In turn, these technologies could become the
heart of the next generation PICs [all-optical] super-computer processors, optical memories, ultra-high bandwidth telecommunications, non-invasive therapies and scanners for medicine, and even Alcubierre’s like warp drives [29].

**Abridged chronology**

This text is organized into self-contained parts that discuss the fundamentals and photonic applications of spacetime-varying media. The first introduces the fundamental physics and numerical methods. The second presents the applications. Finally, the third advances a material platform to build them. This order is intended to introduce the reader progressively to the subject –time-varying materials. However, historically this text began to forge in the search for time-varying materials. The choice, ultimately fell on Chalcogenide glasses, because it is easy to incorporate in traditional nano-fabrication methods. Moreover, spectroscopic analysis revealed an unknown feature: its refractive index decreased by as much as \( \approx 40\% \) when illuminated with electrons. This reversible change can be modulated at a pace akin to the frequency of electromagnetic radiation [17].

Moved by these results, and given the raising interest in PICs, I designed a beam transformation system based in a linear refractive index mapping. The device could be one day fabricated using chalcogenides and used as the light source in hand held tomography scanners [30]. Further, given the rising interest in all-optical computers, I investigated the possibility of crafting a time delay systems based on similar premiss. The result was a set of centro-symmetrical refractive index mappings that can trap light in perennial orbits redolent of celestial mechanics [31].

Concomitantly, to these findings I began working with David Ketcheson on a fullwave numerical scheme to model light propagation in non-linear, heterogeneous and time-varying media. The results premier in this work [28].
The full list of publications and conferences related to this project can be found in Appendix C.
Part I

Prolegomena
Chapter 1

Revisiting Maxwell’s electromagnetics

Maxwell’s equations are a set of non-linear hyperbolic Partial Differential Equations (PDEs) that describe the propagation of electromagnetic radiation and its interaction with materials or vacuum. Usually, materials are thought to vary in space, but time-varying materials have seldom been considered in the literature.

In the last decade interest in time-varying materials surged as a result of advances in characterization techniques and material sciences. Recent publications have demonstrated that there exists a wide miscellany of materials where electromagnetic properties can be modulated in time, with rates akin to electromagnetic wave oscillations \[16,17\]. The physical consequences and the practical applications ensuing from these discoveries are just beginning to be explored. Effects stemming from wave propagation in spacetime-varying media include: trapping, confinement, ultra-short pulse coupling, beam transformation, negative refraction, eigen–polarization, and optical Bohm–Aharonov \[14,18,26\].

The advent of these materials paves the way to control and manipulate light in ways yet to be imagined. PICs where light confinement and trapping is crucial, could become a reality through these media; enabling the next generation of computers and optical data systems, and even Alcubierre’s like warp drives \[29\].
Whence derives the need to create numerical schemes that can incorporate transient material properties and allow us to further the realm of photonics.

We begin this chapter by deriving Maxwell’s equations in spacetime-varying, heterogeneous, anisotropic and non-linear media, followed by a discussion on [semi–]analytical solutions for elementary configurations. It is our objective, however, to go beyond the scope of the rather modest set of analytical solutions. Thus, in the next chapter we describe a numerical scheme to model wave propagation in these settings. Later, we elaborate on the paraxial approximation to this problem using the formalism provided by Lagrange-Euler equations for spacetime geometries; introduce the notion of the inverse problem for paraxial equations, and discuss how it can be used to develop trapping refractive index conditions. To conclude these prolegomena we study a solution the primordial description of the inverse scattering problem in electromagnetics, and use it to craft a Gauss to Bessel beam converter.

1.1 Frames of reference, notation and definitions

Since we are concerned with spacetime-varying materials it is useful to define some frames of reference:

1. **laboratory frame**, it is the one where the laboratory is at rest, usually it is the frame of reference used to make measurements,

2. **co-moving frame**, it is the one attached to the object being measured. Consequently, in this frame the object is stationary.

*Proper frames can be *inertial* or *non-inertial*. An *inertial frame* is a frame of reference that describes time and space homogeneously, isotropically, and in a time-independent manner. All *inertial frames* do not accelerate with respect to one another. Therefore, measurements in one inertial frame can be transformed to another by means of Lorentz’ transformations.
Unless otherwise stated, we will assume that all derived quantities are measured from the laboratory frame. Noting that in the co-moving frame these quantities can be obtained using either Minkowsky–Maxwell constitutive equations or through Lorentz transformation [32].

For simplicity, throughout this manuscript we adopt the following convention when referring to spacetime coordinates: time will be denoted by either \( t \) or \( x^0 \), while space will be represented by either \( x, y, z \), or \( x^i, i \geq 1 \).

Second-rank tensors will be indicated by \( \Box \). The electric and magnetic fields will be denoted by \( q_e \) and \( q_h \), respectively. And vacuum properties are comprised in the diagonal tensor \( \bar{\eta}^0_l \in \mathbb{R}^{m \times m} \), with diagonal entries \( \varepsilon_o \in \mathbb{R} \) for \( l = e \), and \( \mu_o \in \mathbb{R} \) for \( l = h \).

Finally, let us introduce the vector \( q \) to represent the conserved quantities; particular to electromagnetics it takes the form:

\[
q \equiv \begin{pmatrix} q_e \\ q_h \end{pmatrix},
\]

where \( q_{e,h} : \mathbb{R}^m \times \mathbb{R}^{3+1} \rightarrow \mathbb{R}^m \) and \( q : \mathbb{R}^n \times \mathbb{R}^{3+1} \rightarrow \mathbb{R}^n \), with \( n = 2m \).

### 1.2 Maxwell’s equations

Maxwell’s equations in a charge– and current free space are given by:

\[
D_t - \nabla \times q_h = 0,
\]

\[
B_t + \nabla \times q_e = 0,
\]

where the relation between \( D \), \( B \) and \( q_{e,h} \) is governed by the constitutive equations [32]:

\[
D = \zeta_e (\bar{\eta}_e, q_e),
\]

\[
B = \zeta_h (\bar{\eta}_h, q_h).
\]
where \( \bar{\eta} : \mathbb{R}^{m \times m} \times \mathbb{R}^{3+1} \to \mathbb{R}^{m \times m} \), with \( l = e, h \), is a symmetrical second-rank tensors with non-zero off-diagonal entries. Whereas, \( \zeta : \mathbb{R}^{m \times m} \times \mathbb{R}^{m} \times \mathbb{R}^{3+1} \to \mathbb{R}^{m} \) is a nonlinear, real-valued, function. Note that \( \bar{\eta}_{e,h} \) describes the electric, \( l = e \), or magnetic, \( l = h \) properties of the material; customarily referred to as permittivity and permeability, respectively.

Substituting relations (1.2) into (1.1), using the chain rule and grouping similar terms reduces the latter to the homogeneous system:

\[
\zeta(\bar{\kappa}, q)_t + f_i(q, r)_{x^i} = 0,
\]

(1.3)

where \( \zeta : \mathbb{R}^{n \times n} \times \mathbb{R}^{n} \times \mathbb{R}^{3+1} \to \mathbb{R}^{n} \) is the column vector with entries \((\zeta_e, \zeta_h)\), and \( \bar{\kappa} : \mathbb{R}^{n \times n} \times \mathbb{R}^{3+1} \to \mathbb{R}^{n \times n} \) is a second-rank tensor whose entries are the electric and magnetic properties of the material.

In some cases one might be interested in dealing with the field \( q \) direction, i.e. the non-homogeneous version of (1.3). Expanding the time derivative and simplifying we obtain:

\[
\bar{\kappa}(q, r, t) \cdot q_t + f_i(q; r)_{x^i} = \psi(q, r, t),
\]

(1.4)

where we have used Einstein’s summation rules; as described earlier, \( q \) refers to the the fields \( q_{e,h} \), i.e. the conserved quantities; and \( f : \mathbb{R}^{n} \times \mathbb{R}^{3} \to \mathbb{R}^{n} \) described the spatial derivatives of the field, i.e. the fluxes. The factor \( \bar{\kappa} : \mathbb{R}^{n \times n} \times \mathbb{R}^{3+1} \to \mathbb{R}^{n \times n} \) is commonly known as the capacity function, it comprises the material properties \( \bar{\eta}_{l} \). Finally, \( \psi : \mathbb{R}^{n} \times \mathbb{R}^{3+1} \to \mathbb{R}^{n} \) is known as the source term, contains the time derivatives of the material properties \( \bar{\eta}_{l} \), i.e. the non-hyperbolic terms. Note that \( \bar{\kappa} \) and \( \psi \) may be nonlinear in \( q \), but do not depend on derivatives of \( q \).

Equation (1.4) is a non-linear hyperbolic PDE whose solution describes wave propagation in heterogeneous, anisotropic, non-linear, and time-varying media: given some initial condition \( q(r, t = 0) \).

\[\text{Notice that the term } \bar{\kappa} \text{ may also be understood as the change in metric of the discretization space} \ [33,34].\]
Let \( \{l, m\} = \{e, h\} \cong \{-1, 1\} \). Then the terms in (1.4) can expanded explicitly using (1.2), so that \( \bar{\kappa} \) encompasses:

\[
\bar{\kappa} = \partial_{q_i} \zeta_i^l.
\] (1.5)

The \( i \)-th element of the flux function \( f_i \) is defined by:

\[
f_i^l = \epsilon_{ijk} \{ \partial_x^k q_{m \neq l}^j - \partial_x^j q_{m \neq l}^k \} \text{sgn}(l) = -\partial_t \psi_i^l.
\] (1.6)

And the source term, \( \psi_i \), is defined by:

\[
\psi(q, r, t) = -\partial_t \zeta_i^l \partial_t \eta_i^l.
\] (1.7)

Where again, for compactness, we have used Einstein’s summation convention.

1.2.1 Constitutive relations

The constitutive relations (1.2) in general can take any form based on the response of the material to the electromagnetic field and vice-versa. Because of this, it is customary in classical electromagnetics to expand the constitutive relations in a power series around some constant field \( q_0 \), to obtain:

\[
\zeta_k = \bar{\eta}_k^l \cdot \left( q_l + \bar{\chi}^{(i)}_l \cdot q_i^l \right), \quad i = 1, \ldots
\] (1.8)

where \( \bar{\eta}_k^l \) here represents the vacuum electromagnetic tensor, and \( \bar{\chi}^{(n)}_l \), the \( n \)-th order susceptibility tensor. This expansion results convenient to segregate the material response into a linear and non-linear terms,

\[
\zeta_l = \bar{\eta}_l^0 \cdot \left( \bar{I} + \bar{\chi}^{(1)}_l \right) q_l + \bar{\eta}_l^0 \left( \bar{\chi}^{(i)}_l \cdot q_i^l \right) \quad i \geq 2
\]

\[
= \bar{\eta}_l^0 \cdot \bar{\eta}_l^0 \cdot q_l + \bar{\eta}_l^0 \cdot \bar{\xi}_l^n,
\] (1.9)

where \( \bar{\xi}_l^n \) is the sum over \( \bar{\chi}^{(n)}_l \), with \( n \geq 2 \). The first term on the righthand-side of (1.9), \( \bar{\eta}_l^0 \), is known as the relative permittivity, \( l = e \), and permeability, \( l = m \). It represents the linear response of the medium to the propagation of
electromagnetic radiation. The second term, $\xi$, contains the non-linear electric and magnetic susceptibility tensors, they describe the material non-linear response to electromagnetic radiation [1].

Consequently, the capacity function, $\bar{\kappa}$, takes the form:

$$\bar{\kappa}(q, r, t) = \bar{\eta}_l \cdot \left( \bar{\eta}_l^r + \partial_q \xi \right)$$

$$= \bar{\eta}_l^0 \cdot \left( \bar{\eta}_l^r + \bar{\chi}^{(k)}_l \cdot q^{k-1}_l \right), \quad k \geq 2. \quad (1.10)$$

and the source term becomes:

$$\psi(q, r, t) = \bar{\eta}_l^0 \left( \partial_t \bar{\eta}_l^r + \partial_t \bar{\chi}^{(k)}_l \cdot q^{k-1}_l \right) \cdot q_l \quad (1.11)$$

Theoretically it is possible to imagine a material with time-varying $\chi^{(i)}_l$, however, until this moment, it remains uncertain whether time-varying susceptibilities, electric or magnetic, are possible in naturally occurring or manmade materials. Thus, in our calculations in Part II we reduce to zero the second righthand-side term in (1.11).

### 1.2.2 Twofold electromagnetic problem

Two family of problems ensue from equation (1.4): (i) forward problems, describe the time evolution of the field $q$; and (ii) the inverse [electromagnetic] problem, they depart from known fields at input and output to determine the material properties that transformed the field.

In (i) the material properties, $\bar{\eta}$ and initial condition, $q_o$, are known at all points in time and space. The evolution of $q$ at every time step is then calculated through various methods raging from [semi] analytical solutions for the full or paraxial approximation and numerical discretization. In general, an analytical solution is rarely trivial and often numerical methods are required. Multiple methods have been developed in this area, most dealing with non-linear and space heterogeneity. However, numerical methods that encompass time-varying coefficients (capacity
function and source term) to the best of our knowledge have not been derived for a generalized scenario. Our goal, henceforth, is to develop a multi-dimensional numerical solver to (1.4) in the most general case possible. As part of this development, we will also discuss the paraxial approximation to (1.4) and use it to find possible solutions to problems in light trapping and concentration.

In (ii) the field \( q \) is known at different points in time and space, and the material properties are unknown. This is the starting point for the inverse electromagnetic problem which we will discuss later in the text. The inverse problem in heterogeneous media is ill-defined, and hence unique solutions, if any, are not guaranteed. For the purpose of light reshaping this problem can be used to explore beam transformation systems, optical cloaks, concentrators, etc. [22, 30, 35–38].

1.3 Analytic solution

In order to provide a general panorama of the complexity and opportunities of spacetime-varying media, we turn our attention to solving the general nonlinear problem posed in (1.4).

To decrease the complexity of the nonlinear equation (1.4), consider an isotropic medium in one spatial dimension,

\[
\bar{\kappa}(q, x, t) \cdot q_t + f(q; x, t)_x = \psi(q, x, t), \tag{1.12}
\]

In this context \( q \) encompasses:

\[
q(x, t) = \begin{pmatrix} q^0 \\ q^1 \end{pmatrix} \equiv \begin{pmatrix} q_e \\ q_h \end{pmatrix}, \tag{1.13}
\]

where \( q^i : \mathbb{R}^{1+1} \to \mathbb{R} \). Accordingly, the flux function, \( f \), takes the form:

\[
f(q; x, t) = \begin{pmatrix} \frac{\partial q^1}{\partial e} \\ \frac{\partial q^0}{\partial h} \end{pmatrix}. \tag{1.14}
\]
Following from definition (5), $\bar{\kappa}$ is given by:

$$\bar{\kappa} = \begin{pmatrix}
\eta_e^r + k \chi_e^{(k)} (q^0)^{k-1} & 0 \\
0 & \eta_h^r + k \chi_h^{(k)} (q^1)^{k-1},
\end{pmatrix}, \quad k \geq 2,$$

(1.15)

with $\eta^r_i : \mathbb{R}^{1+1} \rightarrow \mathbb{R}$ and constant $\chi^{(k)} \in \mathbb{R}$. Next, we can use (1.11) to determine the source term,

$$\psi(q; x, t) = -\bar{\kappa}_t \cdot q,$$

(1.16)

where we have assumed that $\partial_t \chi^{(i)}_l = 0$ for $i \geq 2$.

Substituting (1.13)–(1.16) into (1.12), and simplifying yields the 1D nonlinear PDE

$$q_t + \bar{\beta} \cdot (A \cdot q_x) = (\ln (\bar{\beta}))_t \cdot q,$$

(1.17)

where $\bar{\beta} = \kappa^{-1}$, and $A$ is the Jacobian of $f$, i.e. $A = \partial_q f$.

Equation (1.17) together with the initial condition $q(x, t = 0) = g(x)$, describe wave propagation in one spatial dimension space filled with a nonlinear isotropic medium with spacetime-varying permittivity and permeability.

### 1.3.1 Characteristic curves

Equation (1.17) is a quasilinear PDE of hyperbolic type, therefore we can use the method of characteristics to find $q$ [39]. In this method we consider the time rate of change of $q(x(t), t)$ as measured by a co-moving observer, $x = X(t)$. Thus, by virtue of the chain rule we have:

$$\frac{d}{dt} q(X(t), t) = \partial_t q + \frac{dX}{dt} \partial_X q$$

(1.18)

Consequently (1.17) reduces to a set of two coupled Ordinary differential equations (ODEs)

$$\frac{dq}{dt} = (\ln (\bar{\beta}))_t \cdot q,$$

(1.19a)

$$\frac{dX}{dt} = \bar{\beta} \cdot A \equiv c(x, t).$$

(1.19b)
where, \( c(x, t) : \mathbb{R}^{1+1} \to \mathbb{R} \) is the wave velocity.

That is, the solution to (1.17) can be found by solving (1.19a) along the trajectory defined by (1.19b), known as the characteristic curve.

The propagation velocity of an initial point will be given by the righthand-side of (1.19b), which is the characteristic velocity, or the local wave velocity.

In general an analytic solution to either (1.19a) and (1.19b) can rarely be found. Nevertheless, we can approximate the solution by means of a semi-analytic scheme. In this context we can use a Runge Kutta method to first integrate (1.19b) and obtain the characteristic curves, afterwards we can integrate (1.19a) along the characteristic curves to find the value of \( q \). This procedure can be implemented in Matlab using \texttt{ode45} and a linear interpolation to find arbitrary points within the characteristic’s path.

In the next section we use an updated version of Fizeau’s and Fresnel’s experiment to study the comportment of characteristics in a medium with a flowing perturbation. Using Lagrangian mechanics, Cacciatori et al. showed that a moving Gaussian perturbation in the refractive index can trap light in co-moving singularities, noting that this could be optical analogues to black-holes \[25\]. A constrain of their method is that the results are only valid in the paraxial approximation to electromagnetics. A fullwave solution to this problem is of interest to PICss, where moving perturbations could be used for energy harvesting, coupling and optical delay lines.

1.3.2 Lorentz transformations

In view that we are studying time-varying media it is useful to introduce Lorentz’ transformations to move between the laboratory frame of reference and a co-
moving frame of reference. In one dimension they take the form:

$$\gamma = \frac{1}{\sqrt{1 - v^2}},$$  \hspace{1cm} (1.20a)

$$t' = \gamma (t - vx),$$  \hspace{1cm} (1.20b)

$$x' = \gamma (x - vt),$$  \hspace{1cm} (1.20c)

1.4 Analytic results: Media in motion

Now, we introduce a succinct example solutions to (1.17) for a traveling perturbation in \( \eta \). This compendium is intended to acquaint the reader with benchmark examples of light propagation in time-varying media; and produce a test solution to study convergence in the numerical model described in the next chapter.

Due to its complexity and to secure a unique solution to the PDE (1.19), for the remaining part of this chapter we assume propagation in a linear medium, \( \bar{\chi}^i = 0, i \geq 2 \).

1.4.1 Moving jump

Let us begin by studying the dynamics of the characteristics in (1.19) when we introduce a perturbation of the form:

$$\eta(x, t) = \begin{cases} \eta_o & x + x_o < v \cdot t + x_o, \\ \frac{\delta \eta}{\sigma} (x - vt - x_o) + \eta_o & vt + x_o \leq x \leq vt + \sigma + x_o, \\ \eta_o + \delta \eta & x > vt + \sigma + x_o, \end{cases}$$  \hspace{1cm} (1.21)

where \( \eta_o \) is the background relative permittivity or permeability, \( \delta \eta \) is the perturbation shift, \( \sigma \) its width, \( x_o \) the offset in the \( x \)-direction, and \( v \) the perturbation’s velocity.
Figure 1.1: Plot of characteristic curves for a wave propagating in a medium with a linear moving jump in $\bar{\eta}$, as measured from the laboratory frame of reference. Seeding points lie in the range $x_o - \sigma \leq x_i \leq x_o + \sigma$, and the perturbation parameters are set to varying velocity $v$, $\eta_o = 1.5$, $\delta \eta = 0.15$, $\sigma = 5$ and $x_o = 10$.

In this case (1.19b) has an analytical solution:

$$x(t) = \begin{cases} 
\frac{\eta_o x_o + l}{\eta_o} & \text{if } x < vt, \\
\sigma \left(1 - \eta_o v + \frac{\delta \eta^2 x}{v^2} + \mathcal{L}_w \left[\left(-1 + \eta_o v + \frac{\delta \eta x}{v}\right) x^{1 - \eta_o v + \frac{\delta \eta (x v - vt)}{v}}\right]\right) & \text{if } vt \leq x \leq vt + \sigma, \\
\frac{x_o (\eta_o + \delta \eta) + l}{\eta_o + \delta \eta} & \text{if } x > vt + \sigma,
\end{cases}$$

(1.22)

where $\mathcal{L}_w$ is the principal solution to Lambert’s W function, also called omega.
function. It is defined as the inverse function of \[40\]:

\[ f(W) = We^w. \]  

(1.23)

The inverse can be obtained by virtue of Lagrange inversion theorem as \[40,41\]:

\[ W(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!} z^n. \]  

(1.24)

Diverse numerical toolboxes like Matlab or Mathematica can compute the principal solution to Lambert’s W function. Thus we can sketch the solution to the characteristics for the moving jump, and use these to calculate the values of \( q \).

Figure 1.1 shows a plot of some characteristic curves for different perturbation velocities, \( v \). Observe that when the velocity of the moving perturbation lies in the range \( v < 1/(\eta_o + \delta\eta) \) the dynamic of the solution is fairly simple: characteristics passing through it will be refracted, change their speed and continue to propagate otherwise unperturbed.

The characteristic curves become more interesting as the speed of the perturbation becomes comparable to the speed of the wave in the medium, \( u \). Observe Figures 1.1c and 1.1b, they depict the case when \( 1/(\eta_o + \delta\eta) < v < 1/\eta_o \). In this scenario the characteristics beginning at the left side of the perturbation, \( u_l = 1/\eta_o \), move faster than the perturbation; hence they will eventually catch to it. As the waves and the perturbation interact, the speed of the waves decreases owing to the raise in \( \eta \) (see equation (1.19b)). Because of this, as the left-side waves evolve their velocity will asymptotically converge to \( v \). Their characteristic path will converge to one parallel to the perturbation’s own characteristic. Physically, this entails that the waves are trapped into a singularity; a point that co-moves with the perturbation. An observer sitting on the perturbation would see that from his vantage point the waves slowdown until they eventually stop.

In Figure 1.2 we have plotted some characteristic curves as seen by an observer in the co-moving frame. See, in particular Figures 1.2c and 1.2b, they depict the case when the characteristics converge to a line with slope zero, i.e. trapping.
Figure 1.2: Plot of characteristic curves for a wave propagating in a medium with a linear moving jump in $\bar{\eta}$, as measured from the co-moving frame of reference. Seeding points lie in the range $x_0 - \sigma \leq x_i \leq x_0 + \sigma$, and the perturbation parameters are set to varying velocity $v$, $\eta_0 = 1.5$, $\delta\eta = 0.15$, $\sigma = 5$ and $x_0 = 10$.

1.4.2 Gaussian moving perturbation

As we will from the material characterization in Chapter 8, it is possible to create small perturbations that move in a medium by using an electron or laser beam. Because the shape of the perturbation is inherited from the energy distribution of said beam we consider in this section a small Gaussian perturbation [16][17].

Let $\eta$ take a Gaussian shape,

$$\eta(x, t) = \eta_0 + \delta\eta e^{-(x-ut)^2/\sigma^2}$$  \hspace{1cm} (1.25)

In this case there is no analytical solution to (1.19). However, we can inte-
grate (1.19b) numerically. Some of these characteristic curves, as seen from the laboratory frame, for different perturbation velocities are plotted in Figure 1.3.

![Characteristic Curves](image)

(a) $v = 0.00$  
(b) $v = 0.61$

(c) $v = 0.63$  
(d) $v = 0.75$

Figure 1.3: Plot of characteristic curves for a wave propagating in a medium with a Gaussian-like moving perturbation in $\bar{\eta}$, as measured from the laboratory frame of reference. Seeding points lie in the range $x_o - \sigma \leq x_i \leq x_o + \sigma$, and the perturbation parameters are set to varying velocity $v$, $\eta_o = 1.5$, $\delta\eta = 0.15$, $\sigma = 5$ and $x_o = 10$.

Once again observe that when the velocity of the perturbation is $v < 1/(\eta_o + \delta\eta)$ characteristics passing through it will be refracted and change their speed momentarily. Because the speed of the perturbation is smaller compared to the wave’s speed the characteristics eventually pass it. As they do their velocity goes back to their original speed and continue to propagate otherwise unperturbed.

As the speed of the perturbation becomes comparable to the speed of the wave in the medium, $u$, some conditions for trapping appear. If $1/(\eta_o + \delta\eta) < v < 1/\eta_o$, characteristics initially starting to the left side of the perturbation, $u_l = 1/\eta_o$, ...
move faster than the perturbation and catch it. As they do, their speed decreases due to the change in $\eta$; this velocity continues until their speeds are equal, and the waves’ light path asymptotically converge to a singularity.

Points starting to the right of the perturbation propagate at a speed $1/(\eta_0 + \delta \eta) \leq u_r < 1/\eta_0$. There are two possibilities: (i) $u_r < v$, (ii) $u_r = v$, and (iii) $u_r > v$. Points in (i) will be caught in the perturbation and converge to a singularity located radially-opposed to the points that began to the left. In (ii) there is only one characteristic, it will remain unperturbed and co-move with the perturbation.

Physically, this means that the waves are begin trapped into singularities; a point that co-moves with the perturbation. An observer sitting on the perturbation would see that, from his vantage point, waves approaching to the perturbation slowdown until they eventually halt in two symmetrical points.

As with the previous case, transforming to the co-moving frame can bring a clearer picture. See, for example, Figures 1.4b and 1.4c they illustrate the case when the curves converge to a line with slope zero.
Figure 1.4: Plot of characteristic curves for a wave propagating in a medium with a Gaussian-like moving perturbation in $\bar{\eta}$, as measured from the co-moving frame of reference. Seeding points lie in the range $x_o - \sigma \leq x_i \leq x_o + \sigma$, and the perturbation parameters are set to varying velocity $v$, $\eta_o = 1.5$, $\delta\eta = 0.15$, $\sigma = 5$ and $x_o = 10$. 

(a) $v = 0.00$  
(b) $v = 0.61$  
(c) $v = 0.63$  
(d) $v = 0.75$
Chapter 2

Numerical modeling

We now turn our attention to the numerical approximation to the solution of (1.4). As described in Section 1.2, this equation is a non-linear hyperbolic PDE with spacetime-varying coefficients. It describes the wave propagation problem on heterogeneous, isotropic, non-linear and time-varying media.

To model time-independent media several numerical methods have been developed over the years: Finite Difference Time Domain (FDTD), Finite Element Method (FEM), Pseudo–Spectral Method (PSM) and FVM. FDTD was the first efficient method to numerically solve Maxwell’s equations in multiple dimensions and has remained widely popular ever since. It uses two staggered grids to split Maxwell’s equations into a semi-discrete system of ODEs and integrates in time using a leap-frog scheme. FEM has been widely used to calculate time-independent solutions to Maxwell’s equations with relative success, and lately explorations into PSMs and FVM for Maxwell’s are being conducted.

Notwithstanding these advances, numerical solvers for Maxwell’s equations with time-varying media have been rarely attempted. In most cases schemes have been developed to fathom out solutions to specific problems in homogeneous media with time dependent conductivity, e.g.: sudden ionization, laser pulse excitation of materials or electric arc discharge. Furthermore, Analytic solutions are possible only in a handful of cases; for example found that by variable
separation it was possible to find a solution in two dimensions when studying Transverse Magnetic cylindrical waves.

To the best of our knowledge, only a numerical scheme to model time-dependent linear media has been demonstrated \cite{27}. Based on FDTD, Faragó et al. showed that it is possible to expand the scheme in \cite{42} to account for linear heterogeneous time-dependent media. They achieve this by applying an operator splitting method and Magnus’ series expansion \cite{27}. Because of splitting the scheme needs to recompute iteration matrices at every time step. Moreover, the scheme can only account for linear materials.

When a wave travels along a time-dependent medium every change in the material acts like a boundary between two regions that have different material properties, thus the incident wave can be split into right and left going waves. An approach is to think about the solution in terms of a flux across the interface between the two regions, which is the idea behind FVM schemes. FVM methods are ideal for heterogeneous media, where every grid cell is assigned an average of the material properties enclosed by it, and the solution is found in terms of the flux across the interfaces of the cell \cite{33}.

In this chapter we extend the method proposed in \cite{50} for the solution of (1.4) to incorporate time-dependent fluctuations, capacities and sources. In particular we use a high order discretization based on the method of lines, as described in \cite{50}. This scheme allows us to use different reconstruction methods, such as Weighted Essentially Non-Oscillatory (WENO) or piecewise-polynomial reconstruction; and sundry time integrators; thus adding to its versatility, scalability and application range.

Because (1.4) is a general non-linear algebraic PDE the method described in this chapter can be applied to other wave phenomena. Thus in the ensuing sections we will focus on developing a general numerical scheme to solve (1.4) and later apply it to Maxwell’s equations.
2.1 A finite volume method for non-linear hyperbolic PDEs with spacetime-varying coefficients

Let us consider (1.4) in one spatial dimension

$$\bar{\kappa}(q, x, t) \cdot q(x, t)_t + f(q)_x = \psi(q, x, t),$$

(2.1)

where $q: \mathbb{R}^{1+1} \rightarrow \mathbb{R}^n$ is the vector of conserved quantities, $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$ corresponds to the flux, $\bar{\kappa}: \mathbb{R}^n \times \mathbb{R}^{1+1} \rightarrow \mathbb{R}^{n \times n}$ is the capacity function, and $\psi: \mathbb{R}^n \times \mathbb{R}^{1+1} \rightarrow \mathbb{R}^n$ includes any non-hyperbolic term.

If the coefficients in (2.1) are independent of time, then it can be reduced to the more familiar set of hyperbolic conservation laws:

$$\bar{\kappa}(x) \cdot q(x, t)_t + f(q)_x = \psi(q, x),$$

for which higher order numerical methods have been developed, see e.g. [33,50–52].

A method for high resolution wave propagation was initially introduced by LeVeque [53], and extended to higher order by Ketcheson et al. [50]. In this chapter we extend the latter to include capacity functions that depend on $q$ and $t$.

2.1.1 Finite Volume schemes

A finite volume approach is based on subdividing the spatial domain into finite volumes, often called grid cells or cells for short; and calculating an approximation to the integral of $q$ over each of these volumes. For example, the cell average $Q_i(t)$ is given by

$$Q_i(t) = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x, t) dx,$$

(2.2)

where the index $i$ denotes the cell number and $\Delta x$ its size.

*The method described in this section is one dimensional and can be easily extended to higher dimensions based on the solution to the 1D problem [33,50].

†Remember that $\bar{\kappa}$ and $\psi$ are in general nonlinear in $q$, but do not depend on derivatives of $q$.
Rearranging (2.1), using definition (2.2), integrating the former over $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [t, t + \Delta t]$ and dividing by $\Delta x$ we obtain:

$$Q_{n+1}^i = Q_n^i - \frac{1}{\Delta t} \int_t^{t+\Delta t} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \bar{\kappa}^{-1} \cdot (f(q)_x - \psi(q, x, t)) \, dx \, dt.$$  (2.3)

where

$$Q_i(t + \Delta t) \approx Q_{n+1}^i, \quad \text{and} \quad Q_i(t) \approx Q_n^i.$$

Equation (2.3) tell us how the cell average $Q_n^i$ gets updated at every time step, $t^n$. To have a fully discrete scheme we need to find an adequate approximation to the integral in (2.3) in terms of $Q_n^i$.

### 2.1.2 Notation, Riemann problem and high order reconstruction

We use the notation for the Riemann solution from [50, 53]. It originates from the consideration of the hyperbolic system:

$$q_t + \bar{A} \cdot q_x = 0,$$  (2.4)

where $\bar{A} \in \mathbb{R}^{n \times n}$. Equation (2.4) is hyperbolic if $\bar{A}$ is diagonalizable with real eigenvalues; hereafter we assume this to be the case. Let $s^p$ and $r^p$ denote the eigenvalues and corresponding eigenvectors of $A$ for $1 \leq p \leq n$. Hereinafter we assume the eigenvalues to be sequenced in ascending order, i.e. $s^1 \leq \ldots \leq s^n$.

The Riemann problem consists of (2.4) and the initial data:

$$q(x, 0) = \begin{cases} q_l, & x < 0, \\ q_r, & x > 0. \end{cases}$$  (2.5)
Its solution for $t > 0$ is a piecewise-constant function with jumps proportional to $r^p$, each moving at speed $s^p$ along the ray $x = s^p t$. These waves, denoted by $W$, can be obtained in terms of the initial jump in $q$:

$$q_r - q_l = \sum_p \alpha^p r^p = \sum_p W^p. \tag{2.6}$$

Since we are interested in a finite volume discretization, it is convenient to specify notation for the net effect of all right- and left-going waves:

$$A^+ \Delta q \equiv \sum_p (s^p)^+ W^p, \quad \tag{2.7a}$$

$$A^- \Delta q \equiv \sum_p (s^p)^- W^p, \quad \tag{2.7b}$$

where the values $A^\pm \Delta q$ are known as fluctuations, and the terms $(s^p)^\pm$ denote the positive or negative part of $s^p$ [33][53]:

$$(s^p)^- = \min(s^p, 0) \quad (s^p)^+ = \max(s^p, 0).$$

To be concise we will refer to the Riemann problem with initial left state $q_l$ and right state $q_r$ as the Riemann problem with initial states $(q_l, q_r)$. Accordingly, we will sometimes use the notation $W^p(q_l, q_r)$ to represent the $p$th wave in the solution of the Riemann problem with initial states $(q_l, q_r)$.

Now, we integrate (2.4) over $[x_{i - \frac{1}{2}}, x_{i + \frac{1}{2}}] \times [t, t + \Delta t]$ and divide by $\Delta x$, to obtain:

$$Q_i(t + \Delta t) - Q_i(t) = -\frac{1}{\Delta x} \int_{t}^{t + \Delta t} \int_{x_{i - \frac{1}{2}}}^{x_{i + \frac{1}{2}}} A q_x(x, t) \, dx \tag{2.8}$$

In [50] a piecewise-polynomial approximation, accurate to order $n$, is used to approximate the solution $q(x, t)$; that is at $t = t_o$

$$\hat{q}(x, t_o) = \hat{q}_i(x), \quad \text{for} \quad x \in \left( x_{i - \frac{1}{2}}, x_{i + \frac{1}{2}} \right), \tag{2.9}$$

where

$$\hat{q}_i(x) = q(x, t_o) + O(\Delta x^{n+1}). \tag{2.10}$$
At each interface $x_{i-\frac{1}{2}}$, this approximation is discontinuous, so we must solve the Riemann problem with:

$$q(x, 0) = \begin{cases} \hat{q}_{i-1}, & x < x_{i-\frac{1}{2}}, \\ \hat{q}_i, & x > x_{i-\frac{1}{2}}. \end{cases} \quad (2.11)$$

The solution to this problem is a set of waves obtained by decomposing the jump in $Q$ in terms of the eigenvalues of $A$. If, then, we integrate (2.4) over $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [t, t + \Delta t]$ and divide by $\Delta x$, we obtain:

$$Q_i(t + \Delta t) - Q_i(t) = -\frac{\Delta t}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} A \hat{q}_x (x, t + \Delta t) \, dx \quad (2.12)$$

where $\hat{q}(x, t_o + \Delta t)$ is the exact evolution of $\hat{q}$ after a time increment $\Delta t$.

Let us define

$$s^L = \min \left( s_{i+\frac{1}{2}}^l, 0 \right), \quad s^R = \max \left( s_{i-\frac{1}{2}}^m, 0 \right), \quad (2.13)$$

and

$$q_{i-\frac{1}{2}}^R = \lim_{x \to x_{i-\frac{1}{2}}^+} \hat{q}_i(x), \quad q_{i+\frac{1}{2}}^L = \lim_{x \to x_{i+\frac{1}{2}}^-} \hat{q}_i(x) \quad (2.14)$$

where the superscripts $L$ and $R$ indicate, respectively, to the left and the right state of the interface considered.

Coming back to (2.12), taking the limit as $\Delta t \to 0$ leads to a general semidiscrete scheme [50]:

$$\frac{\partial Q_i}{\partial t} = -\frac{1}{\Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} A \hat{q}_x dx \right),$$

$$= -\frac{1}{\Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + A \Delta q_i \right) \quad (2.15)$$

where the fluctuations, $A^\pm \Delta q$, at $x_{i-\frac{1}{2}}$ are defined as

$$A^\pm \Delta q_{i-\frac{1}{2}} = \sum_p \left( s^p \left( q_{i-\frac{1}{2}}^L, q_{i-\frac{1}{2}}^R \right) \right) \pm W^p \left( q_{i-\frac{1}{2}}^L, q_{i-\frac{1}{2}}^R \right) \quad (2.16)$$

and $A \Delta q_i$, the total fluctuation, takes the form:

$$A \Delta q_i = \sum_p \left( s^p \left( q_{i-\frac{1}{2}}^R, q_{i+\frac{1}{2}}^L \right) \right) \pm W^p \left( q_{i-\frac{1}{2}}^R, q_{i+\frac{1}{2}}^L \right) \quad (2.17)$$
2.1.3 Flux: \textit{f-wave} Riemann solvers

Now we can return to (2.1). Ideally we seek a semidiscrete scheme akin to (2.15), so that we can use the algorithms developed to solve Riemann problems with varying fluxes that are employed in Clawpack \[50,52,54,55\].

Let us recall the scheme developed in \[50\] for the homogeneous system
\[q_t + f(q)_x = 0, \quad (2.18)\]

There the solution to the Riemann problem at \(x_{i-\frac{1}{2}}\) was obtained by computing a flux-based wave decomposition, where the flux difference is given in terms of the eigenvectors:
\[f\left(q_{L_{i-1/2}}^R\right) - f\left(q_{L_{i-1/2}}^L\right) = \sum_p \beta_p r_p = \sum_p Z^p_{i-1/2} \quad (2.19)\]

Here the vectors \(Z^p\) are called \textit{f-waves} \[50,52\]; and \(r^p\) are the eigenvectors of the flux jacobian, \(f_q(q) \equiv A_i(q)\). Once again, if \(\hat{q}(x,t + \Delta t)\) is the exact evolution of \(\hat{q}\) after a time increment \(\Delta t\) we obtain:
\[Q_i(t + \Delta t) - Q_i(t) = -\frac{\Delta t}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} A_i \hat{q}_x(x,t + \Delta t) dx \quad (2.20)\]

Dividing by \(\Delta t\) and taking the limit as \(\Delta t \to 0\) we obtain:
\[\frac{\partial Q_i}{\partial t} = -\frac{1}{\Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + \int_{x_{i-1/2}}^{x_{i+1/2}} A_i \hat{q}_x dx \right) \quad (2.21)\]

where the fluctuations \(A^\pm q_{i+1/2}\) are given in term of the \textit{f-waves}, \(Z\), as:
\[A^+ \Delta q_{i-\frac{1}{2}} = \sum_{p : s^{p}_{i-\frac{1}{2}} > 0} Z^p_{i-\frac{1}{2}} \quad A^- \Delta q_{i+\frac{1}{2}} = \sum_{p : s^{p}_{i+\frac{1}{2}} < 0} Z^p_{i+\frac{1}{2}} \quad (2.22)\]

Note that in the case of conservative systems the integral in (2.21) can be calculated through the flux difference:
\[\int_{x_{i-1/2}}^{x_{i+1/2}} A_i \hat{q}_x dx = f(q_{i+\frac{1}{2}}^L) - f(q_{i-\frac{1}{2}}^R) = A \Delta q_i \quad (2.23)\]

\(^4\)Note that \(f(q)_x = \partial_x f(q(x,t)) = f_q(q,x,t)q_x\).
Then (2.21) can be rewritten as:

$$\frac{\partial Q_i}{\partial t} = -\frac{1}{\Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + A \Delta q_i \right), \quad (2.24)$$

which together with (2.22) and (2.23) is the semidiscrete scheme for (2.18).

This scheme can be used to approximate the solution to (1.3), in the understanding that the conserved quantity now is $\zeta$ instead of $q$.

### 2.1.4 Spacetime-varying sources

A source terms appears in many physical problems where an external force acts on the system; it can be included through a non-hyperbolic term, $\psi$:

$$q_t + f(q)_x = \psi(q, x, t). \quad (2.25)$$

Following an analogous derivation to (2.12) ensues in

$$Q_i(t + \Delta t) - Q_i(t) = -\frac{1}{\Delta x} \left( \int_{t}^{t+\Delta t} \int_{x_i-\frac{1}{2}}^{x_i+\frac{1}{2}} (A_i \tilde{q}_x - \psi(\tilde{q}, x, t)) dxdt \right)$$

$$= -\frac{\Delta t}{\Delta x} \left( \int_{x_i-\frac{1}{2}}^{x_i+\frac{1}{2}} A_i \tilde{q}_x(x, t + \Delta t)dx - \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \int_{x_i-\frac{1}{2}}^{x_i+\frac{1}{2}} \psi(\tilde{q}, x, t)dxdt \right) \quad (2.26)$$

Once more dividing $\Delta t$ and taking the limit as $\Delta t \to 0$ results in a semidiscrete scheme:

$$\frac{\partial Q_i}{\partial t} = -\frac{1}{\Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + A \Delta q_i - A \Delta x \Psi_i \left( q^R_{i-\frac{1}{2}}, q^L_{i+\frac{1}{2}}, t \right) \right). \quad (2.27)$$

where $\Psi_i \left( q^R_{i-\frac{1}{2}}, q^L_{i+\frac{1}{2}}, t \right)$ is a suitable spatial average of $\psi(\tilde{q}, x, t)$\textsuperscript{50,52}. Equation (2.27) together with (2.22), and (2.23) approximates the solution to (2.25).

\textsuperscript{5}Notice that in electromagnetics the average of the electromagnetic coefficients is the harmonic average, defined as: $\tilde{f} = \frac{\Delta x}{\int_{x_i}^{x_i+\Delta x} f(x)}$
2.1.5 Spacetime-varying capacity functions

Our problem includes a nonlinear and spacetime-varying capacity function, leading to:

\[ \bar{\kappa}(q, x, t) \cdot q_t + f(q)_x = \psi(q, x, t), \]

If \( \bar{\kappa} \) varies smoothly, then we can discretize it as:

\[ \bar{K}_i \approx \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \bar{\kappa}(q, x, t) dx, \]  

(2.28)

notice that in certain problems \( \bar{K}_i \) is derived using the harmonic average instead.

Then, we can add it into the schemes (2.21) and (2.27) following [50]:

\[ \frac{\partial Q_i}{\partial t} = -\frac{1}{\bar{K}_i \Delta x} \left( A^+ \Delta q_{i-\frac{1}{2}} + A^- \Delta q_{i+\frac{1}{2}} + A \Delta q_i - \Delta x \psi_i \left( q_{i-\frac{1}{2}}, q_{i+\frac{1}{2}}, t \right) \right). \]  

(2.29)

Therefore, the full scheme to approximate the solution to (2.1) consists of (2.29), together with (2.28), (2.23) and (2.22).

2.2 Implementation

To integrate the semidiscrete scheme (2.29) we use the ten-stage fourth-order strong-stability-preserving Runge-Kutta scheme described in [56]. This method has large stability allowing us to use high CFL numbers, in particular for all the examples in this thesis we used a CFL number of 1.0. For reconstructing the values of \( q \) we use fifth-order \text{WENO} reconstruction [57]. Finally, the algorithm described below is implemented in the software \textit{Clawpack} [54,55].

Traditionally, methods based on finite differences use several points per wavelength to correctly model the high-frequency waves that occur in electromagnetics. We use \text{WENO} or a high-degree polynomial to reconstruct the values of \( q \) at the edges of the cells because it allow us to keep a high level of accuracy with relatively coarser grids.
2.2.1 Algorithm

At every Runge-Kutta stage the numerical implementation of (2.29) follows the steps:

1. Set cell averages of the capacity $\bar{K}_i^n$, source $\Psi_i^n$ (see Section 2.2.3).

2. Reconstruction, using fifth-order WENO compute the piecewise elements of $q$ to get states $q_{i-\frac{1}{2}}^R, q_{i+\frac{1}{2}}^L$.

3. Solve the Riemann problem with initial states $(q_{i-\frac{1}{2}}^L, q_{i+\frac{1}{2}}^R)$ to compute the fluctuations, $A^\pm \Delta q_{i-\frac{1}{2}}$ (see Equation (2.22)).

4. Using (2.23) calculate the total fluctuation $A\Delta q_i$, use states $q_{i+\frac{1}{2}}^L, q_{i-\frac{1}{2}}^R$.

5. Compute $\partial Q_i/\partial t$ using the semidiscrete scheme (2.29).

2.2.2 1D $f$-wave Riemann solver for Maxwell’s equations

For Maxwell’s equation in 1D we set (see Section 1.3):

$$q = \begin{pmatrix} q_e \\ q_h \end{pmatrix}, \quad f = \begin{pmatrix} \frac{q_h}{\eta_e} \\ \frac{q_e}{\eta_h} \end{pmatrix}$$

with,

$$\bar{\kappa} = \begin{pmatrix} \eta_e(x,t) & 0 \\ 0 & \eta_h(x,t) \end{pmatrix}$$

\footnote{Recall that in electromagnetics $\bar{\kappa}$ can be split into a linear and nonlinear terms in $q$, see Section 1.2. Therefore, at every stage the corresponding linear terms are calculated before the Riemann solves; whereas the nonlinear terms $\bar{K}_i^n$ are introduced in the Riemann solves and in the total fluctuation calculation. The source term is subtracted in the total fluctuation routine. In either case the averages are approximated by the trapezoidal rule; higher order approximations are ongoing.}

\footnote{We do not incorporate the effect of the source on this step, rather we will subtract it from the flux difference in the total fluctuation}
and considering linear materials $\psi = \partial_t \bar{K} \cdot q^{*\ast}$

To calculate the fluctuations, $A^\pm \Delta q_{i-\frac{1}{2}}$, we solve the Riemann problem at $x_{i-\frac{1}{2}}$ with flux Jacobian

$$f_q = A = \begin{pmatrix} 0 & 1/\eta_0^h \\ 1/\eta_0^h & 0 \end{pmatrix}. \quad (2.30)$$

With eigenvectors and eigenvalues:

$$r^1 = \begin{pmatrix} -Z_{i-1} \\ 1 \end{pmatrix}, \quad s^1 = -c_{i-1}, \quad (2.31a)$$

$$r^2 = \begin{pmatrix} +Z_i \\ 1 \end{pmatrix}, \quad s^2 = c_i, \quad (2.31b)$$

where $Z_k$ is the impedance,

$$Z_k = \sqrt{\frac{\eta_0^h}{\eta_k}} \quad (2.32)$$

and $c_k$ is the speed of the waves

$$c_k = \frac{1}{\sqrt{\eta_0^h \eta_k^0}}. \quad (2.33)$$

For the Riemann problem between the cells $i - 1$ and $i$, the $f$-waves, $Z^{1,2}_{i-\frac{1}{2}}$, are:

$$Z^{1}_{i-\frac{1}{2}} = \beta^1 r^1, \quad Z^{2}_{i-\frac{1}{2}} = \beta^2 r^2. \quad (2.34)$$

Let $R = [r^1 r^2]$; then we can determine the values of $\beta^i$ in (2.22) by solving the system

$$R\beta = \Delta f_{i-\frac{1}{2}};$$

to obtain

$$\beta^1 = \frac{-\Delta f^1_{i-\frac{1}{2}} + \Delta f^2_{i-\frac{1}{2}} Z_i}{Z_i + Z_{i-1}}, \quad (2.35a)$$

$$\beta^2 = \frac{\Delta f^1_{i-\frac{1}{2}} + \Delta f^2_{i-\frac{1}{2}} Z_{i-1}}{Z_i + Z_{i-1}}. \quad (2.35b)$$

Then the waves, $Z^{1,2}_{i-\frac{1}{2}}$, can be calculated and we can obtain the value of the fluctuations.

---

**Notice that we can use the same Riemann solver for a nonlinear medium; this is possible because the nonlinear terms are added to the capacity function and non-hyperbolic terms**
2.2.3 Averages of capacity function and source term

Let $\tilde{\eta}_i$ be a suitable average of an element of $\bar{\kappa}$ across the $i$th cell at some time $t^n$. Then, at the interface $x_{i-\frac{1}{2}}$ we can approximate $K_{i-\frac{1}{2}}$ using the trapezoidal rule,

$$K^n_{i-\frac{1}{2}} \approx \frac{\tilde{\eta}_i^R + \tilde{\eta}_i^L}{2} + \frac{p}{2^p} \chi^{(p)} \left( q_{i-\frac{1}{2}}^R + q_{i-\frac{1}{2}}^L \right)^{p-1}, \quad p \geq 2, \quad (2.36)$$

where we have assumed the nonlinear parameters, $\chi^{(n)}$ to be homogeneous and independent of time.

Consequently, by the trapezoidal rule the averaged source term in the $i$th cell takes the form

$$\Psi^n_i \approx \frac{\dot{\eta}_i^R q_{i-\frac{1}{2}}^R + \dot{\eta}_i^L q_{i+\frac{1}{2}}^L}{2}. \quad (2.37)$$

where for readability $\dot{\eta} = \eta_t$.

2.3 Convergence and benchmark test

Here we study the error and rate of convergence of the scheme (2.29) with respect to the exact solution in one spatial dimension, and the error with respect to a subsequent numerical solutions calculated on refined grids for one and two spatial dimensions. In future referred to as analytic and self error or convergence rate, respectively.

Table 2.1 summarizes the simulation parameters for the problems used in the convergence tests. We consider linear and isotropic materials in all cases, i.e. $\bar{\kappa}$ is diagonal with entries $\kappa^{ii} = \eta(x,t)$; finally we se the initial condition to be the Gaussian pulse in (2.39).

For brevity let us denote by

- **Problem 1** Maxwell’s equation (1.4) in 1D with time-varying capacity function and source term

- **Problem 2** Maxwell’s equation (1.4) in 1D with spacetime-varying capacity function and source term
Problem 3 Maxwell’s equation (1.4) in 2D with spacetime-varying capacity function and source term

For Problem 1 and Problem 2, \( q \) and \( f(q) \) are defined in Section 2.2.2 whereas for Problem 3 these are defined in Appendix A.1.

As announced, in Problem 1 and Problem 2, we calculate the error with respect to the analytic solution; to obtain it, we solve (1.17) through the method of characteristics as described in Section 1.3. Because the semi-analytic solution along characteristics can be calculated with high accuracy, hereafter we will refer to it as the exact solution.

Recall that Maxwell’s equations in 1D with linear spacetime-varying coefficients is the PDE

\[
\bar{\kappa}(x,t) \cdot q_t + f_1(q)_x = \bar{\kappa}(x,t)_t,
\]
while in 2D it takes the form

\[
\bar{\kappa}(x,y,t) \cdot q_t + f_1(q)_x + f_2(q)_y = \bar{\kappa}(x,y,t)_t.
\]

The Gaussian-like material profile of Problem 2 and Problem 3 is set by

\[
\eta = \eta_o + \delta \eta \exp \left( - \left( \frac{x^i - v^i t - x^i_o}{\sigma^i} \right)^2 \right), \tag{2.38}
\]
where again we use Einstein’s summation rule, \( \eta_o \in \mathbb{R} \) is the background material parameter, \( \delta \eta \in \mathbb{R} \) is the perturbation amplitude, \( v^i \in \mathbb{R} \) is the velocity, \( x^i_o \in \mathbb{R} \) is the offset, and \( \sigma^i \in \mathbb{R} \) is the width of the pulse. Similarly, the source in all analysis is given by the right-moving Gaussian-like pulse profile

\[
q_o(x,y,x_o,\sigma) = g(y) \exp \left( - \left( \frac{x - x_o}{\sigma^2} \right)^2 \right), \tag{2.39}
\]
where \( x_o \in \mathbb{R} \) is the offset in the \( x \)-direction, and \( g : \mathbb{R} \rightarrow \mathbb{R} \) is the transversal profile.

Note that we choose a Gaussian profile for the initial condition because its quadrature is a known analytic function,

\[
\frac{1}{\Delta u} \int_{u_{i-\frac{1}{2}}}^{u_{i+\frac{1}{2}}} e^{-u^2} du \equiv \frac{\sqrt{\pi}}{2\Delta u} \left( \text{erf} \left( u_{i+\frac{1}{2}} \right) - \text{erf} \left( u_{i-\frac{1}{2}} \right) \right), \tag{2.40}
\]
where \( \text{erf}(u) \) is the error function. Therefore, we can calculate cell averages of the initial condition \((Q_i)\) with high accuracy.

### 2.3.1 Measure of error

Let \( E_e(h) \) denote the error of the numerical solution with respect to the exact solution for some grid spacing \( h \); then, using the grid-function norm we can estimate the error as:

\[
E_e(h) = ||e||_1 = h \sum_{i=1}^{N} |e_i| = h \sum_{i=1}^{N} |Q_i^n - q(x_i, t_n)|, \tag{2.41}
\]

where the values are measured at some time step \( t_n \).

If the scheme is \( p \text{th} \) order accurate, then as \( h \to 0 \) we would expect the error to the analytic solution to become:

\[
E(h) = Ch^p + o(h^p), \tag{2.42}
\]

where \( C \) is some constant. Thus if \( h \) is small then,

\[
E(h) \approx Ch^p. \tag{2.43}
\]

If the grid is refined by a factor of 2 we would observe

\[
E(h/2) \approx C(h/2)^p. \tag{2.44}
\]

Let the error ratio, \( R(h) \) be

\[
R_e(h) = \frac{E(h)}{E(h/2)} \approx \frac{Ch^p}{C(h/2)^p} = 2^p. \tag{2.45}
\]

Similarly, denote by \( E_s(h) \) the error of the numerical solution on a grid with spacing \( h \) with respect to the numerical solution obtained on refined grid, \( h/2 \),

\[
E_s(h) = ||e||_1 = h \sum_{i=1}^{N} |e_i| = h \sum_{i=1}^{N} |Q_i^n - \hat{Q}_i^n|, \tag{2.46}
\]

where \( \hat{Q}_i^n \) is the solution on the refined grid with spacing \( h/2 \).
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Table 2.1: Model parameters for 1D and 2D convergence analysis.
We can calculate the error ratio $R(h)$ once again to find \[53\],

$$R_s(h) = \frac{E_s(h)}{E_s(h/2)} \approx 2^p. \quad (2.47)$$

This result tells us that the error approximated by using successively finer grids decreases by the same factor as the one observed for the exact solution.

Then we can estimate the order, $p_k$, of the method as \[53\]:

$$p_k \approx \log_2(R_k(h)), \quad k = e, s \quad (2.48)$$

where $p_e$ and $p_s$, respectively, denote the $p$th order of convergence of $E_e(h)$ and $E_s(h)$.

### 2.3.2 1D Convergence

The initial condition for the problems in this section is the right moving Gaussian pulse \[2.39\],

$$q^0(x, 0) = Zq_o(x, x_o, \sigma), \quad (2.49)$$

$$q^1(x, 0) = q_o(x, x_o, \sigma), \quad (2.50)$$

where $Z$ is the impedance \[2.32\], $x_o = -5.0$, and $\sigma = 2.0$.

For the exact solution we divide the space in $m_x = 131072$ cells, and calculate the solution along each characteristics in the time range $t \in [0, t_f]$ following the process described in Section 1.3.

**Time-varying coefficients**

We solve \textit{Problem 1} in the interval $x \in [0, 100]$ and $t \in [0, 100]$. Table 2.2 shows the error and convergence rates for propagation in this problem.

Figure 2.2 shows $E_e(h)$ for the \textit{Problem 1} as a function of $m_x = L/h$, where $L = 100$ is the length of the simulation space. Using a least-square method we can
Table 2.2: Errors and rate of convergence for Problem 1.

<table>
<thead>
<tr>
<th>$m_x$</th>
<th>$\frac{100}{m_x}$</th>
<th>$E_e(h)$</th>
<th>$p_e(h)$</th>
<th>$E_s(h)$</th>
<th>$p_s(h)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>7.812e-01</td>
<td>3.093e-01</td>
<td>3.517</td>
<td>2.632e-01</td>
<td>3.300</td>
</tr>
<tr>
<td>256</td>
<td>3.906e-01</td>
<td>2.701e-02</td>
<td>4.966</td>
<td>2.672e-02</td>
<td>4.970</td>
</tr>
<tr>
<td>1024</td>
<td>9.766e-02</td>
<td>6.004e-06</td>
<td>5.976</td>
<td>5.814e-06</td>
<td>5.976</td>
</tr>
<tr>
<td>2048</td>
<td>4.883e-02</td>
<td>9.538e-08</td>
<td>5.990</td>
<td>9.238e-08</td>
<td>5.991</td>
</tr>
<tr>
<td>4096</td>
<td>2.441e-02</td>
<td>1.501e-09</td>
<td>5.963</td>
<td>1.453e-09</td>
<td>5.993</td>
</tr>
<tr>
<td>8192</td>
<td>1.221e-02</td>
<td>2.406e-11</td>
<td>3.703</td>
<td>2.281e-11</td>
<td>5.982</td>
</tr>
<tr>
<td>16384</td>
<td>6.104e-03</td>
<td>1.848e-12</td>
<td>1.072</td>
<td>3.609e-13</td>
<td>—</td>
</tr>
</tbody>
</table>

Figure 2.2: Convergence of the finite volume solution to the analytic solution, $E_e(h)$, for Problem 1 (blue-dashed); and liner fit with slope $p_e \approx -5.789$ (red).

approximate the slope of the line in the asymptotic convergence region of $E_e(h)$ and find $p_e \approx 5.789$.

Similarly, Figure 2.3 shows $E_s(h)$ for the Problem 1. Using a least square
method we approximate the slope of the linear fit to the data in asymptotic region
of $E_s(h)$ ($2^{10} \leq mx \leq 2^{13}$) and obtain $p_s \approx 5.775$.

![Figure 2.3: Convergence of the finite volume solution to subsequent refined finite volume
solution, $E_s(h)$, for Problem 1 (blue-dashed); and liner fit with slope $p_s \approx -5.776$ (red).](image)

**Spacetime-varying coefficients**

We solve Problem 2 in the interval $x \in [0, 300]$ and $t \in [0, 274.5]$. Table 2.3 shows
the errors and convergence rates for propagation in this problem.

Figure 2.4 shows $E_e(h)$ for the Problem 2 as a function of $mx = L/h$, where
$L = 300$ is the length of the simulation space. Using a least-square method we can
approximate the slope of the line in the asymptotic convergence region of $E_e(h)$
and find $p_e \approx 3.481$.

Similarly, Figure 2.5 shows $E_s(h)$ for the Problem 2. Using a least square
method we approximate the slope of the linear fit to the data in asymptotic region
of $E_s(h)$ ($2^{10} \leq mx \leq 2^{14}$) and obtain $p_s \approx 3.441$. 
<table>
<thead>
<tr>
<th>$m x$</th>
<th>$\frac{300}{m x}$</th>
<th>$E_{e}(h)$</th>
<th>$p_{e}$</th>
<th>$E_{s}(h)$</th>
<th>$p_{s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>2.344</td>
<td>3.758</td>
<td>1.356</td>
<td>1.461</td>
<td>1.136</td>
</tr>
<tr>
<td>256</td>
<td>1.172</td>
<td>1.468</td>
<td>1.423</td>
<td>6.645e-01</td>
<td>0.973</td>
</tr>
<tr>
<td>512</td>
<td>5.859e-01</td>
<td>5.477e-01</td>
<td>1.591</td>
<td>3.86e-01</td>
<td>1.259</td>
</tr>
<tr>
<td>1024</td>
<td>2.930e-01</td>
<td>1.818e-01</td>
<td>2.790</td>
<td>1.414e-01</td>
<td>2.518</td>
</tr>
<tr>
<td>2048</td>
<td>1.465e-01</td>
<td>2.629e-02</td>
<td>4.381</td>
<td>2.469e-02</td>
<td>4.363</td>
</tr>
<tr>
<td>4096</td>
<td>7.324e-02</td>
<td>1.262e-03</td>
<td>5.058</td>
<td>1.199e-03</td>
<td>5.035</td>
</tr>
<tr>
<td>8192</td>
<td>3.662e-02</td>
<td>3.787e-05</td>
<td>5.653</td>
<td>3.658e-05</td>
<td>5.783</td>
</tr>
<tr>
<td>16384</td>
<td>1.831e-02</td>
<td>7.526e-07</td>
<td>3.114</td>
<td>6.642e-07</td>
<td>—</td>
</tr>
</tbody>
</table>

Table 2.3: Errors and rate of convergence for Problem 2.

Figure 2.4: Convergence of the finite volume solution to the analytic solution, $E_{e}(h)$, for Problem 2 (blue-dashed); and liner fit with slope $p_{e} \approx -3.481$ (red).

To explain the difference in the rate of convergence between Problem 1 and Problem 2 recall that in the former the material is only time dependent, which
Figure 2.5: Convergence of the finite volume solution to subsequent refined finite volume solution, $E_s(h)$, for Problem 2 (blue-dashed); and liner fit with slope $p_s \approx -3.441$ (red).

 together with the results of Problem 2 would suggest that the discrepancy is due to the second-order approximation to $\Psi_i$ and $K_i$ within each cell $i$ for spacetime-varying media (see equation (2.37)). Because of this we would expect the convergence rate to be second-order accurate, the higher degree of convergence ensues from using high order WENO interpolation and Runge-Kutta methods.

It could be argued that in practice the the linear terms in $K_i$ can be averaged with high precision in space using an adequate quadrature method (see equation (2.36)). However, the same cannot be done with the source term, since it depends explicitly on the value of $q$ within each cell. An alternative, currently under investigation, is to use high-order polynomial interpolation to approximate the values of the source in the cell edges and later do numerical quadrature.
2.3.3 2D Convergence

We solve Problem 3 in the interval \(\{x, y\} \in [0, 180] \times [0, 180]\) with varying grid space. The initial condition is a purely right-moving Gaussian pulse:

\[
q^0(x, 0) = 0.0,
q^1(x, 0) = Zq_o(x, x_o, \sigma),
q^2(x, 0) = q_o(x, x_o, \sigma),
\]

where \(Z\) is the impedance (2.32), \(x_o = 5.0\), and \(\sigma = 2.0\).

We use the 2D Gaussian of (2.38) to set the material parameters, as described in the beginning of this section. The Riemann solver used and the derivation of the equations is summarized in Appendix A. Table 2.4 presents a summary of the errors and rate of convergence for subsequent grid refinement.

<table>
<thead>
<tr>
<th>mx/my</th>
<th>h</th>
<th>(E_s(h))</th>
<th>(p_s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>1.978</td>
<td>1.981e-01</td>
<td>2.231</td>
</tr>
<tr>
<td>256</td>
<td>4.944e-01</td>
<td>4.222e-02</td>
<td>2.980</td>
</tr>
<tr>
<td>512</td>
<td>1.236e-01</td>
<td>5.349e-03</td>
<td>2.210</td>
</tr>
<tr>
<td>1024</td>
<td>3.090e-02</td>
<td>1.156e-03</td>
<td>2.008</td>
</tr>
<tr>
<td>2048</td>
<td>7.725e-03</td>
<td>2.875e-04</td>
<td>2.004</td>
</tr>
<tr>
<td>4096</td>
<td>1.931e-03</td>
<td>7.168e-05</td>
<td>—</td>
</tr>
</tbody>
</table>

Table 2.4: Errors and rate of convergence for Problem 3.

Figure 2.6 shows \(E_s(h)\) for Problem 3. Again, using a least square linear fit we find the rate of convergence in the asymptotic region to be \(p_s \approx 2.524\).

These results suggest that our method is second-order accurate for these problems.
Figure 2.6: Convergence of the finite volume solution to subsequent refined finite volume solution, $E_s(h)$, for Problem 3 (blue-dashed); and linear fit with slope $p_s \approx -2.313$ (red).
Chapter 3

Paraxial approximation and light paths

In this section we study light as ray, and hence our interest is on its trajectory manifold when propagating in spacetime-varying media. This approximation is useful when the area of interest is several times larger than the wavelength, for in this instance a fullwave solution to (1.4) may be unfeasible to calculate. This comes at the expense of losing the wave nature of light, in return we obtain a set of ODEs that describe the path that light would follow as it traverses a material with refractive index $\bar{n}(r,t)$.

We begin this chapter deriving the light path equations by means of Lagrange-Euler formalism, and hint the relation between time-space geometry and the refractive index, Finally we postulate the inverse problem in the context of stationary media aimed at light confinement.

3.1 Light paths and Lagrange-Euler equation

From general relativity we know that each point in spacetime can be described by a quadrivector $\{x^0 : x^1, x^2, x^3\}$, where $x^0$ corresponds to time, $t$; and the rest, $x^i$, to the three-dimensional space. Every space has associated to it a metric tensor, $g_{ij}$, and, consequently, an infinitesimal length element, $ds^2 = g_{ij}dx^i dx^j$. From general
relativity we also learn that the path described by any particle, a photon in our case, in spacetime can be parametrized by a function $x(\tau)$, where $\tau$, the proper time, is an affine parameter. This path can be found by solving Lagrange-Euler equations, recalling that the Lagrangian in this case takes the form:

$$\mathcal{L} = \frac{1}{2} \left[ g_{ij} \frac{\partial x^i}{\partial \tau} \frac{\partial x^j}{\partial \tau} \right],$$

where the derivatives are taken in respect to the affine parameter $\tau$.

The physical description in (3.1) states that if the metric is related to the electromagnetic tensors, $\bar{\eta}$, then it becomes possible to write the path of light in the ray approximation as a function of the material properties or the metric tensor $ds$.

Allow us to make a brief parenthesis. In the ray approximation it is convenient to define a dimensionless quantity the encompasses the combined effect of the electric and magnetic properties of materials. Customarily known as refractive index, it is defined as:

$$\bar{n} = \sqrt{\bar{\eta}_e \cdot \bar{\eta}_h}$$

where $\bar{n} : \mathbb{R}^{3+1} \to \mathbb{R}^3$. The refractive index was first introduced by Snell in his famed relation for the refraction of light between two media \[4\],

$$n_1 \sin \theta_1 = n_2 \sin \theta_2,$$

where $\theta_i$ are the angles of incidence and refraction. In Snell’s view the refractive index is a measure of the degree of refraction a ray of light will endure when traversing a material.

An alternative view comes from (1.19b) for linear materials, where the magnitude of $\bar{\beta}$, together with definition (3.2), tell us that the refractive index measures the fraction the wave speed and the wavelength are reduced compared to background when traversing a material with refractive index $n$.

* A conserved quantity parameter that serves to link spacetime variables through each inertial reference frame.
Coming back to Lagrange-Euler equations (3.1), if the equivalence between
metric and refractive index is possible [36,58,59], then it could be possible to
use Fermat’s principle, with (3.1) taking the role of an optical Lagrangian. This
implies the solution to the variational problem which states that given a refractive
index \( n(x^0, r) \) the path followed by light is given by the extrema of:

\[
\delta \tau = \delta \int_{x_1}^{x_2} ds = 0,
\]

(3.3)

where the integration is done between the arbitrary points \( x_1 \) to \( x_2 \), with \( j = 0, \ldots, 3 \), and \( \delta \) indicates the functional maximization. Recursively, the solution to
(3.3) is the Lagrange-Euler equation (3.1).

Observe that in the integral of (3.3) the term \( ds \) introduces the metric using
the covariant metric tensor \( g_{ij} \) of the curved space:

\[
ds = \sqrt{g_{ij} dx^i dx^j}.
\]

(3.4)

Yet, we are left still with determining the relation between the metric tensor,
\( g_{ij} \), and the refractive index \( \tilde{n} \). This can be achieved by virtue of conformal
mappings, where it is possible to build the relation between the geometry and the
electromagnetic properties of a [meta]material [36,59,60]. Specifically, if the line
element of spacetime takes the form

\[
ds^2 = g_{00} dx^0 dx^0 - g_{ij} dx^i dx^j,
\]

it is possible to map the curved spacetime to an isotropic, non-dispersive and non-absorbing
medium as [59,61]:

\[
\tilde{n} = \tilde{\eta}_c = \tilde{\eta}_b = \sqrt{-g g^{ij} / g_{00}}
\]

(3.5)

where \( g = \text{det}(g_{ij}) \). Furthermore if we consider Minkowski’s metric of special
relativity, the tensor \( g \) has entries:

\[
g = \text{diag}(g_{00}, g_{11}, g_{22}, g_{33}) = \text{diag}(1, -1, -1, -1),
\]

(3.6)

then \( \tilde{n} \) is diagonal, with entries \( n = n(x^0, r) \). Consequently, the length element,
\( ds \), in (3.3) can be written as:

\[
ds^2 = \frac{1}{n^2} dx^0 dx^0 - dx^i dx^i, \quad i = 1, 2, 3
\]

(3.7)
where we have assumed an isotropic medium.

### 3.1.1 Photon’s path equations

Accordingly, using \([3.1]\) we can derive the ODEs for the light-path, where in cartesian coordinates takes the form:

\[
\ddot{x}^i = \left(\dot{x}^0\right)^2 \frac{\partial_x n}{n^3}, \quad i \geq 1 \tag{3.8a}
\]

\[
\ddot{x}^0 = \frac{\dot{x}^0 \left(\dot{x}^0 \partial_x n + 2 \dot{x}^i \dot{x}^i \partial_x n\right)}{n} \tag{3.8b}
\]

where again we have used the shorthand provided by Einstein’s summation rule, and all derivatives marked by \(\dot{}\) and \(\ddot{}\) are taken with respect to the affine parameter \(\tau\), e.g. \(\dot{r} = \partial r / \partial \tau\). Equations \([3.8]\) describe the parametrized path of a light beam traveling in a spacetime with such geometry or equivalent refractive index.

For reasons that will become evident in the next section, it is convenient to write these equations in centro-symmetrical coordinates, particularly in cylindrical coordinates, \(\{r, \phi, z, t\}\), equation \([3.8]\) takes the form:

\[
\ddot{r} = r \dot{\phi}^2 + \frac{\dot{t}^2 \partial_r n}{n^3}, \tag{3.9a}
\]

\[
\ddot{\phi} = -2r \dot{r} \dot{\phi} + \frac{\dot{t}^2 \partial_{\phi} n}{r^2}, \tag{3.9b}
\]

\[
\ddot{z} = \frac{\dot{t}^2 \partial_z n}{n^3}, \tag{3.9c}
\]

\[
\ddot{t} = \frac{\dot{t} \left(\dot{t} \partial_t n + 2 \left(\dot{z} \partial_z n + \dot{\phi} \partial_{\phi} n + \dot{r} \partial_r n\right)\right)}{n}, \tag{3.9d}
\]

### 3.2 Inverse paraxial problem: confinement of light

The inverse problem begins by defining a set of \textit{a priori} conditions that describes an idealized scenario to what one wishes the path of light to be. And so the problem resides in finding the values of \(n\) that would yield the desired path. The general solution to this problem, however, is complex and a unique solution is not guaranteed \([30, 62, 63]\).
In this part of our work we set forth to find refractive index mappings where light can be confined or trapped. We will describe light being trapped, when the geodesics are perpetually bounded to some region of space, for as long as the material properties remain unchanged. In this sense a light trapping geodesic is one where any of the following conditions arise:

1. $\dot{r}, \dot{\phi} \to 0$,
2. $\dot{r} \to 0$ and $\phi_{\text{min}} \leq \phi \leq \phi_{\text{max}}$,
3. $\dot{\phi} \to 0$ and $r_{\text{min}} \leq r \leq r_{\text{max}}$,
4. $r_{\text{min}} \leq r \leq r_{\text{max}}$ and $\phi_{\text{min}} \leq \dot{\phi} \leq \dot{\phi}_{\text{max}}$,

for all $\tau \geq \tau^*$; where $\tau^*$ marks the moment at which the initial conditions for trapping are met. The first condition is only possible if the refractive index $n$ goes to infinity, or if the refractive index co-moves with the wave [20, 25]. The other three cases can be realized in stationary refractive index [61, 64]. Thus, they can be imposed as general conditions to solve the inverse problem to equations (3.9).

If we impose premises 1 to 4 described earlier, the path equations reduce to new set of equations where the affine parameter is time itself; whence we can rework equation (3.9) into polar coordinates:

$$\ddot{r} = \frac{n r \dot{\phi}^2 - 2 r \dot{r} \dot{\phi} \partial_\phi n - r^2 \partial_r n + r^2 \dot{\phi}^2 \partial_\phi n}{n}.$$  \hspace{1cm} (3.10a)

$$\ddot{\phi} = -\frac{2 nr \dot{r} \dot{\phi} - r^2 \partial_\phi n + r^2 \dot{\phi}^2 \partial_\phi n + 2 r^2 \dot{r} \dot{\phi} \partial_r n}{nr^2}.$$  \hspace{1cm} (3.10b)

Since we are interested in the general stationary case, we impose the fourth condition above, ensuing $0 \leq \dot{r} \leq \dot{r}_{\text{max}}$ and $\phi_{\text{min}} \leq \dot{\phi} \leq \dot{\phi}_{\text{max}}$, on equation (3.10a) and equation (3.10b), and find a non-singular refractive index distribution, $n(r, \phi)$, that satisfies them. Notice that we require the refractive index to be smoothly varying and $C^2$ continuous, i.e. $\nabla n \cdot e^i \leq M$, where $M$ is a real valued number, and $e^i$ a vector in a give direction in spacetime.
The latter being said, the problem can be simplified further if we recall that a trapping orbit occurs when the radius $r$ is bounded to a region of space, i.e. $r_{\text{min}} \leq r \leq r_{\text{max}}$, for all $\phi$; whence $\dot{r}(r_{\text{max}}) = \dot{r}(r_{\text{min}}) = 0$, and $r$ can be written in terms of the angle $\phi$ or the time $t$. Hence a natural solution to the inverse problem is an autonomous refractive index that varies with the radial variable, i.e. $n = n(r)$. This refractive index map resembles the centro-symmetric characteristics of gravitational fields, where, as pointed out independently by Genov and Ni [61,64], light would behave similarly to that traveling in curved spacetime. Such distribution can be constrained to the conditions listed previously.

This result is significant in terms of fabrication where novel photo-refractive [metal]materials could be used. The refractive index in these composites can be modulated by the intensity of the change-inducing beam; which can be controlled by shaping its transversal profile [17,30,65,66]. Accordingly several families of refractive index distributions can be achieved, e.g. Gaussian, Laguerre, or Bessel, which are all centro-symmetrical.

### 3.3 Confinement of light: dynamic equilibrium

Any second order ODE can be rewritten as the sum of two functions as:

$$\ddot{x} = -h(x, \dot{x}) - g(x).$$  \hspace{1cm} (3.11)

Since the refractive index is a function of the radius, equation (3.10) can be rewritten in the form:

$$\ddot{r} = \left( r^2 \dot{\phi}^2 - \dot{r}^2 \right) \partial_r \ln n + r \dot{\phi}^2, \hspace{1cm} (3.12a)$$

$$\ddot{\phi} = -2 r \dot{r} \frac{n + r \partial_r n}{nr}, \hspace{1cm} (3.12b)$$

the system’s symmetry now allows us to integrate (3.12b), hence:

$$\dot{\phi} = \frac{\ell}{\mu n^2}, \hspace{1cm} \mu = n^2.$$  \hspace{1cm} (3.13)
where \( \ell \) is a constant of integration. This equation is reminiscent of orbital mechanics, with the sole exception that \( \mu \), the mass in celestial mechanics, varies with the radius. Substituting the latter result into \((3.12a)\), and rearranging yields:

\[
\ddot{r} = \left( \frac{\ell^2}{n^4 \mu r^2} - \dot{r}^2 \right) \frac{\partial_r \ln n}{\partial r} + \frac{\ell^2}{n^4 \mu r^4}.
\]  

(3.14)

The arrangement in \((3.14)\) allows us to calculate the ratio of external energy supply, which is a measure of the equilibrium stability of the system \[67,68\]; simplifying we get:

\[
\mathcal{E}_t = \frac{d\mathcal{E}}{dt} = -\dot{r} \dot{h}(r, \dot{r}) = \dot{r} \left( \frac{\ell^2}{n^4 \mu r^2} - \dot{r}^2 \right) \frac{\partial_r \ln n}{\partial r}.
\]  

(3.15)

By virtue of Bertrand’s theorem \[61,69\], we know that \( \dot{r} \neq 0 \), for all time \( t \); then from premises \[3\] and \[4\] it follows that \( \dot{r}_{\min} \leq \dot{r} \leq \dot{r}_{\max} \), where \( \dot{r}_{\min} < 0 \); and from the definition of \( n(r) \) as a monotonous decreasing function it follows that \( \partial_r \ln n \leq 0 \). Therefore, as the radius decreases, the radial velocity goes to its minimum and \( \mathcal{E}_t \leq 0 \), therefore the system approaches the equilibrium point and the amplitude of the path decreases. On the other hand, as the radius increases, the velocity tends to a maximum, and \( \mathcal{E}_t \geq 0 \), thus the system is driven away from the equilibrium point and the amplitude of the path increases. In Figure 3.1 we show \( \mathcal{E}_t \) for a Gaussian like refractive index described in section 6.1. Observe that in the light confinement scenario we will see an oscillatory behavior in \( \mathcal{E}_t \).

### 3.3.1 Orbit stability

To conclude we study the stability of the orbits. by means of Lyapunov’s stability theory for the governing equation \((3.14)\), and derive the constraints applicable to the refractive index mapping to attain stable orbital paths \[61\]. First, let us rewrite equation \((3.14)\) as:

\[
\dot{r} = \chi,
\]

\[
\dot{\chi} = (r^2 \beta^2 - \chi^2) \chi(r) + r \beta^2,
\]  

(3.16)
Figure 3.1: Ratio of external energy supply, $E_t$, for a radial symmetric system, where $x = r$ and $y = \dot{r}$. Notice that there exists a $x_c$, critical radius, at which for all phase space pairs $\{x, y| x \geq x_c\} E_t = 0$, which implies that the light geodesics do not describe an orbital motion.

with $\beta = \dot{\phi}$ and $\chi(r) = \partial_r \ln n$. Then, if we introduce small perturbations $r = r_o + \delta$ and $\varpi = \varpi_o + \epsilon$, expand $\chi(r)$ in a Taylor series around $r_o$, and drop all higher order terms for $\delta$ and $\epsilon$; we can rewrite equation (3.16) as a linear system of equations for the perturbation terms:

$$
\begin{pmatrix}
\dot{\delta} \\
\dot{\epsilon}
\end{pmatrix} =
\begin{pmatrix}
0 & 1 \\
W & 2V
\end{pmatrix}
\begin{pmatrix}
\delta \\
\epsilon
\end{pmatrix},
$$

(3.17)

$$
V = -\varpi_o \chi_o, \quad W = 2\chi_o \beta^2 r_o + \chi'_o (r_o^2 \beta^2 - \chi_o^2),
$$

where $\chi_o$ and $\chi'_o$ are the linear terms of the Taylor expansion of $\chi(r)$ around $r_o$. Ensuing the eigenvalues of the matrix above are given by:

$$
\lambda_{1,2} = V \pm \sqrt{V^2 + W}.
$$

(3.18)

The geodesics will be stable if the real part of the eigenvalues of (3.17), $\Re\{\lambda_{1,2}\}$, are negative or equal to zero. Recall that $0 \leq \beta \leq \lim_{r \to \infty} n(r)^{-1}$, and $\chi(r) \leq 0$; and therefore the condition for Lyapunov stability is reached if:

$$
-\frac{\partial}{\partial r} \chi(r) \bigg|_{r=r_o} \leq 0, \quad V^2 + W \leq 0,
$$

(3.19)
This constrained is met for all points $r$ near the stability point $r_o = 0$, provided the radial velocity meets $\dot{r}_o \leq 0$. In general, since the refractive index is monotonous decrescent, the system will be Lyapunov stable at points where $\dot{r} \leq 0$, see, for example, the phase-space plots in Figures 6.4b and 6.6b. In addition, it is interesting to analyze whether the system will be Lyapunov stable under the conditions necessary to sustain a circular orbit. In this case $\kappa_o = 0$, and $r_o = a$, constant, for all time $t$; consequently $V = 0$, $W \leq 0$, and the second term in equality (3.19) is imaginary, provided that $\chi(r) \leq 0$; thus resulting in $\Re\{\lambda_{1,2}\} = V = 0$.

These conditions, however, result in a different family of refractive indexes. In our study we focus on Gaussian-like refractive index distributions, feasible through photo-refraction, where $\kappa \neq 0$, ergo the system will not describe closed circular orbits.

In summary, light confinement will occur as long as the conditions cited earlier apply. Under them the system will oscillate around the equilibrium point as depicted by the ratio of external energy supply. In the next section we will present the confinement geodesics resulting from these refractive index distributions. We will show that the geodesics in this system mimic those of a spinning black hole and other celestial objects, thus reproducing the paths of light traveling in curved space.
Chapter 4

Beam transformation and the inverse problem

Finally we study the second problem described in Section 1.2.2, the inverse problem to (1.4). In this case, the field $q$ is known at different points in time and space, and are the material properties that are left to be found. This is the starting point for the inverse electromagnetic problem which we discuss in this chapter in the context to refractive index mapping for beam transformation.

The inverse problem in heterogeneous media is ill-defined, and hence unique solutions, if any, are not guaranteed \[22,30,35,38\]. On the other hand, beam transformation is the idea that a refractive index mapping can change the transversal profile of a wave from its original shape into any other, similar to what happens when light is diffracted by an arrangement of slits for example. In practice a beam transformation device should consist of a planar refractive index map constrained to realistic material properties, which can smoothly modify the beam’s transversal profile into the desired shape \[62,70,72\] (see Figure 7.1).

4.1 Helmholtz equation for $q$

We begin by dividing space into two regions: the transformation region $\mathcal{A}$ and the space around it $\mathcal{B}$. The fields in either region can be thought of as made of
an infinite superposition of monochromatic harmonic waves of frequency $\omega$. Whence, in the subsequent discussion we choose one of this many harmonic fields and use it to derive our model, keeping in mind that it is possible to apply the same principle herein to every element of the field expansion.

Consequently, the input and output fields take the form,

$$q_l = \nu_l(k, r)e^{j\omega t}, \quad j = \sqrt{-1}$$

(4.1)

where $l = i, o$ identify the input or output field respectively, $\nu : \mathbb{R}^3 + 3 \rightarrow \mathbb{R}^3$ is the field amplitude or field transversal shape, $k \in \mathbb{R}^3$ is the wave vector, and $r \in \mathbb{R}^3$ is the position vector. We assume that the field amplitude $\nu$ satisfy Helmholtz equation,

$$\nabla^2 \nu + k^T \cdot \nu = 0$$

We can rearrange (1.4) to obtain the second order PDE wave equation for $q$,

$$\nabla^2 q_l - \omega^2 (\bar{\eta}_m \cdot \bar{\eta}_l) \cdot \partial_t^2 q_l = -\nabla \left( (\bar{\eta}_l^{-1} \cdot q_l) \cdot \nabla \bar{\eta}_l \right)$$

(4.2)

Where we have assumed that $\bar{\eta}_l$ is independent of time. Substituting (4.1) into (4.2) eliminating similar terms and simplifying yields,

$$\nabla^2 \nu_l - \omega^2 (\bar{\eta}_m \cdot \bar{\eta}_l) \cdot \nu_l = -\nabla \left( (\bar{\eta}_l^{-1} \cdot \nu_l) \cdot \nabla \bar{\eta}_l \right)$$

(4.3)

Thus the transversal shape of the field, $\nu$, is determined by the solution to Helmholtz equation. Therefore, the problem reduces to determining the mapping that transforms $\nu_i \rightarrow \nu_o$ after some finite propagation distance, $s$.

### 4.2 An inverse problem for $q$

We tackle now the derivation of the PDE for $\bar{\eta}_l$ departing from (4.3). Because all we know aside of this equation, are the incident and output fields, $\nu_{i,m}$ let us examine the general amplitude of the field in all spaces $\nu$. 
Denote by $S_i$ and $S_o$, the boundary surfaces between regions $\mathcal{A}$ and $\mathcal{B}$, respectively. Then $\nu$ can be split into the three regions:

$$
\nu(r) = \begin{cases} 
\nu_i(r) & \forall \ r \in S_i, \\
\nu_t(r) & \forall \ r \in \mathcal{A}, \\
\nu_o(r) & \forall \ r \in S_o,
\end{cases}
$$

(4.4)

where $\nu_t$ indicates the field in the transformation region. Since we have control over the transformation region, we can define at whim $\nu_t$. To this effect, let us introduce the real valued transformation-functions $f, g : \mathcal{A}^3 \to [0, 1]$ and $\gamma : \mathcal{A} \to \mathbb{R}^3$, $C^2$ continuous, and square integrable; i.e. smooth functions. Their purpose is to represent the transforming beam through a superposition of the input and output fields, plus an arbitrary field, $\gamma$, that describes the residual beam. Thus, the transformation field takes the form:

$$
\nu_t(r) = f(r)\nu_i(r) + g(r)\nu_o(r) + \gamma(r).
$$

(4.5)

Where the boundary conditions dictate that:

$$
f(S_i) = g(S_o) = 1,
$$

$$
f(S_o) = g(S_i) = 0, \quad (4.6)
$$

$$
\gamma(S_i) = 0.
$$

Now, substituting (4.5) into (4.3) and simplifying yields,

$$
\omega^2 \bar{\eta}_m \nu \bar{\eta}_h(r) + (\nu \cdot \nabla) \nabla \ln \bar{\eta}_h(r) + \nabla \psi (\nabla \ln \bar{\eta}_h(r)) \cdot \nu = \Theta. \quad (4.7)
$$

where,

$$
\Theta = \nabla^2 \nu
$$

(4.8)

and $\nu$ is completely defined by (4.5) in all the domains. That is, equation (4.7) is the inverse problem to $q$, with boundary conditions $\bar{\eta}_h(\delta \Omega) = \bar{\eta}_h(\delta \mathcal{B})$, where $\delta \Omega$ is the boundary of the transformation region.
The boundary conditions for (4.7) should be tailored specifically to secure that the transformation region complies with fabrication limits.

The computation of an inverse problem as the one hitherto described by (4.7) is not trivial, and analytical solutions are rarely found. Moreover, the problem is ill-defined, i.e. its solution is not unique and is dependent continuously on the data \[63,74\]. Over the years different methods have been elucidated to solve this problem, e.g. adjoint solution \[74,75\], linear sampling \[76,78\], variational methods \[79\], and lately transformation optics \[36,72\]. Accounting for the advantages and drawbacks of each we built a hybrid numerical scheme based on the adjoint and variational methods \[30\].

It is important to note that both, the variational and adjoint problem methods, while widely tested may render inexact solutions due to numerical approximations which can lead to instability and are in general related to the limited resolution of any numerical method. To counterweight this difficulties the general approach is to use smaller grid sizes even at the expense of computational time increasing exponentially.
Part II

Results & Analysis
Chapter 5

Fullwave solution:

spacetime-varying media

Here we use the scheme developed in Chapter 2 to model the interaction of the electromagnetic field, $q$, with spacetime-varying media. Specifically, we calculate the solution to (1.4) when transient smooth-perturbations modify the background material properties.

Two general problems ensue from the the definition of the material properties, $\bar{\kappa}$ (see equation (1.8) and subsequent),

$$\bar{\kappa}(q,r,t) = \bar{\eta}^0 \cdot (\bar{\eta}^r + k \bar{\chi}^{(k)} \cdot q_{k-1}^l), \quad k \geq 2.$$

1. Linear materials, no explicit dependence on $q$, i.e. $\bar{\chi}^{(n)} = \bar{0}$

2. Nonlinear materials, explicit dependence on $q$, incorporated by setting any or all of $\bar{\chi}^{(n)} \neq \bar{0}$

Hereafter, mention of linear and nonlinear materials will refer to either of these definitions.

We assume all the materials in this section to be isotropic, hence $\bar{\eta}_l$ is diagonal with entries $\eta_{ii} = \eta(q,x,t)$; and have unitary impedance, i.e. $\bar{\eta}_e = \bar{\eta}_h = \bar{\eta}_{\text{par}}$

Similarly, the initial condition for all problems is the Gaussian-like pulse

$$q_{o}(r,t = 0) = \exp \left( -\frac{x^i - x_{oq}^i}{\sigma^i} \right)^2,$$  \hspace{1cm} (5.1)
centered in \( x_{oq} = \{x_1^o, x_2^o, x_3^o\} \) and \textbf{full-width-half-maximum (FWHM)} \( \sigma = \{\sigma^1, \sigma^2, \sigma^3\} \).

Unless otherwise stated, based on their spatial dimension the initial and boundary conditions for any the problems in this chapter are as follows,

1. One-dimensional problem (1D)
   - purely right-moving pulse \( (5.1) \) centered in \( x_o = 10.0 \), and \textbf{FWHM} \( \sigma^1 = 2.0 \)
   - Reflecting boundary conditions (left, right)

2. Two-dimensional problem (2D)
   - purely outward-moving pulse \( (5.1) \), centered at the middle of the domain, and \textbf{FWHM} \( \sigma^1 = \sigma^2 = 2.0 \).
   - Reflecting boundary conditions (left, right, top, bottom)

\section*{5.1 Derived quantities}

Typically in any experimental setup measuring the individual components of \( q \) might be impractical; thus let \( I \) denote the 2-norm of \( q \), the intensity of the field,

\[
I(r, t) = \sqrt{\sum_{i=1}^{m} q_i^2(r, t)}. \tag{5.2}
\]

In other problems is convenient to look at the directional energy flux,

\[
S = q_e \times q_h \tag{5.3}
\]

called the Poynting vector, whose magnitude \(|S|\) is again the 2-norm of \( S \).

Similarly, let \( n \) denote the magnitude of the material profile, the refractive index

\[
\bar{n} = \sqrt{\bar{n}_e \cdot \bar{n}_h}. \tag{5.4}
\]

*This is achieved by setting \( q^2 = q_o(x, t) \), while \( q^0 = q^1 = 0 \)
Finally let $F = I, n, |S|$, then we can define the maximum $F_{\text{max}}(t) = \max_r F(r, t)$, and the path described by it $r_F(t) = \{r : F(r, t) = F_{\text{max}}\}$.

From this point forward we will employ these quantities when describing the numerical results.

## 5.2 EMClaw

To obtain the results in this Chapter and as part of this thesis we developed EMClaw [80], it is a multi-dimensional numerical solver for Maxwell’s electromagnetics in spacetime-varying and nonlinear media, based on the scheme described in Chapter 2. EMClaw was designed as an extension of the Clawpack software [55]. Additional examples, videos, and description are available on [80].

The examples in this section are aimed to demonstrate some of types the problems that can be modeled using EMClaw and its capabilities.

## 5.3 One-dimensional electromagnetics

In this section we study wave propagation in homogeneous and heterogeneous time-varying materials. First we consider a spatially homogeneous material where the background properties oscillate in time; later we consider the case of trapping in a spacetime-varying material.

For all examples in this section we set the number of grid cells $mx = 8192$.

### 5.3.1 Time-dependent material

Let $\eta$ be the time-varying smooth function

$$\eta = \eta_0 + \delta \eta \sin(\omega t),$$

(5.5)
where \( \eta_0 \in \mathbb{R} \) is the background material parameter, and

\[
\omega = \frac{n_\omega \pi}{L},
\]

where \( n_\omega \in \mathbb{R} \) is the oscillation rate of the material, and \( L \) the propagation length.

From the characteristic curves \( \text{ODE (1.19b)} \) we expect the velocity of the right-moving pulse to follow the inverse of \( \eta \); that is, as the pulse evolves in time its velocity should also oscillate. Figure 5.1 shows \( I \) for the numerical results for the case \( n_\omega = \{4, 24\} \).

![Figure 5.1: Time-staggered plots of \( I \) for a medium with vibrating \( n \).](image)

(a) \( n_\omega = 4 \)  
(b) \( n_\omega = 24 \)

In Figure 5.2 we have plotted \( x_I(t) \), together with its time rate of change. Notice that the velocity and position oscillate as we had expected from the characteristic curves.

### 5.3.2 Flowing media

Here we recall the material profile used in the convergence study of Section 2.3 where \( \eta \) is described by a Gaussian-like profile,

\[
\eta = \eta_0 + \delta \eta \exp \left( - \left( \frac{x^i - v^i t - x^i_o}{\sigma^i} \right)^2 \right), \tag{5.6}
\]

where \( \eta_0 \in \mathbb{R} \) is the background material parameter, \( \delta \eta \in \mathbb{R} \) is the perturbation amplitude, \( v^i \in \mathbb{R} \) is the velocity, \( x^i_o \in \mathbb{R} \) is the offset, and \( \sigma^i \in \mathbb{R} \) is the width.
The solution to this problem in the approximation of ray optics is well known, when the velocity of the moving medium is in the range \( \frac{1}{\eta_0 + \delta \eta} < v^i \leq \frac{1}{\eta_0} \), rays will asymptotically converge to a point co-moving with the Gaussian-like perturbation \([24, 26, 81, 82]\). This is inline with what we expected from studying the characteristic curves in Section 1.3, where we asserted that it is possible to trap light if similar conditions for the material perturbation were met.

To illustrate, let \( \bar{\eta}_o = 1.5 \), \( \delta \bar{\eta} = 0.15 \), \( \sigma^i = 5.0 \) and \( v = \{0.55, 0.61\} \); and consider the initial condition (5.1) to be a Gaussian pulse traveling to the right.

Figure 5.3 shows the evolution of the field’s intensity, \( I \), as it interacts with
Figure 5.3: Time-staggered plots of $I$ (black) and $n$ (green); where $n$ is a Gaussian-like moving medium with velocity $v$.

As it can be observed, trapping occurs when the velocity of the perturbation is within the prescribed range. This behavior becomes clearer when looking at Figure 5.4, where we have plotted $x_I(t)$ and $x_n(t)$ for comparison. Observe that for $v = 0.61 \leq \frac{1}{\eta_0 + \delta\eta}$ the position and velocity of the pulse asymptotically converge to a line parallel to the trace of the perturbation.

Alternatively, consider the perspective from the co-moving frame plotted in Figure 5.5 (see Section 1.3.2). From this perspective we observe that when the velocity of the medium is $v = 0.61$ the pulse velocity asymptotically converges to 0, as one would expected if trapping occurs.

As a summary, position and velocity as measured from the co-moving frame for different material displacement velocities, $v$, are plotted in Figure 5.6.

### 5.4 Nonlinearities and spacetime-varying media

In this section we study a hybrid material that incorporates the spacetime-varying medium of the previous section together with a background nonlinear material, $\chi^{(3)} \neq 0$. This problem is difficult to study in the paraxial approximation, and
Figure 5.4: Position and velocity of $I_{\text{max}}$ (blue) and of $n_{\text{max}}$ (red) as measured from the laboratory frame; $n$ is a Gaussian-like moving medium with velocity $v$.

usually a numerical scheme is required.

For comparison Figure 5.7 shows the effect of this nonlinearity in the absence of the moving perturbation (5.6). Note that as the pulse evolves the nonlinearity in the medium compresses the pulse where $q_x \geq 0$ and expands it where $q_x \leq 0$, that is we observe the formation of a shock and rarefaction, respectively.

Allow us now to introduce the flowing material of equation 5.6 and observe the evolution of the right-moving pulse (5.1). In particular, we choose $\bar{\chi}^{(3)} = 0.1$ and the perturbation velocity $v = \{0.55, 0.61\}$.

Figure 5.8 shows the evolution of $I$ as it interacts with the nonlinear material and the moving perturbation. A quick observation of this figure, suggests that
trapping still occurs under these conditions. See $x_I(t)$ and $x_n(t)$ in Figures 5.9 and 5.9 when the velocity of the medium is $v = 0.61$ the plots tell us that the velocity of the pulse still asymptotically converges to 0, and it follows a path which co-moves with the perturbation. However, the dynamics of trapping are different due to the nonlinear term.

The results in Figure 5.8 suggest that the moving perturbation balances the dispersion introduced by the nonlinearity; or in other words, the former causes the front of the pulse to expand, while the moving perturbation compresses it. To better appreciate this dynamic let us look at the time rate of change of $I_{max}$ plotted in Figure 5.11 in particular when trapping occurs and $\chi^{(3)} = 0.1$, notice that as the pulse interacts with the perturbation it begins to compress and increase in
amplitude, while at the same time the nonlinearity causes rarefaction; ultimately this leads to an equilibrium, as exemplified by the fact that $\frac{dI_{\text{max}}}{dt} \approx 0$.

It is important to note that the time-rate change of the intensity is not strictly increasing in the linear material. In the linear case, by using the ray equation Cacciatori et al. showed that the intensity was ever-increasing when considering trapping \[25\]. The discrepancy is due to the finite grid size, for example see Figure 5.12.
An extension on the initial time-independent problem is to study a problem with a fixed space variation with an added vibration, \( v.gr. \)

\[
\eta = \eta_0 + \delta \eta \cos (\omega^0 t) \sin (\omega^1 x) \sin (\omega^2 y),
\]

where \( \omega^i \in \mathbb{R} \) defines the spatial and time frequencies.

Let \( \{x, y\} \in [0, L_1] \times [0, L_2], \omega^i = \frac{2\pi}{L_i}, \) and \( \omega^0 = \frac{4\pi\omega_\chi}{\sqrt{L_1^2 + L_2^2}}. \) Then we can
Figure 5.9: Position and velocity of $I_{\text{max}}$ (blue) and of $n_{\text{max}}$ (red) as measured from the laboratory frame; $n$ is a Gaussian-like moving medium with velocity $v$ and $\bar{\chi}^{(3)} = 0.1$. Observe the magnitude of the energy flux $S$ in time at different $n_\omega$. For comparison purposes Figure 5.13 shows the result for the case when the material is time-independent.

In this case the initial condition is a Gaussian pulse located at the center of the domain, with $q^0 = q^1 = 0$ and $q^2 = q_\omega(x, t = 0)$, where $q_\omega$ is the Gaussian profile (5.1).

Figure 5.14 shows $|S|$ for $n_\omega = 16$. As it can be appreciated from the figure such media can be used to reconfigure a pulse and be used in light coupling devices or directional illumination. However, more exploration into possible applications of these kinds of mappings is still ongoing.
Figure 5.10: Position and velocity of $I_{max}$ (blue) and of $n_{max}$ (red) as measured from the co-moving frame; $n$ is a Gaussian-like moving medium with velocity $v$ and $\bar{\chi}^{(3)} = 0.1$. 
Figure 5.11: Time rate of change of \( I_{\text{max}} \) as measured from the laboratory frame; where \( n \) is a Gaussian-like moving medium with velocity \( v \) and \( \tilde{\chi}^{(3)} = \{0, 0.1\} \).
Figure 5.12: Time rate of change of $I_{\text{max}}$ for two different grid sizes, $m\times$, as measured from the laboratory frame; where $n$ is a Gaussian-like moving medium with velocity $v$ and $\bar{\chi}^{(3)} = 0$.

(a) $v = 0.61$, $\chi^{(3)} = 0$, $m\times = 8192$  
(b) $v = 0.61$, $\chi^{(3)} = 0$, $m\times = 16384$

Figure 5.13: Magnitude of energy flux, $|S|$, for vibrating media with $n_\omega = 0$

(a) $t = 3.75$  
(b) $t = 18.75$

(c) $t = 41.25$  
(d) $t = 60.0$
Figure 5.14: Magnitude of energy flux, $|S|$, for vibrating media with $n_\omega = 16.0$
Chapter 6

Paraxial solution, light attractors

Figure 6.1: Life path for trapped light in Gaussian like refractive index mappings as a function of parameters $n_a$ and $n_c$, with $n_{\text{max}} = 3.8$ and $\sigma = 50$. Observe the increment in $r_{\text{min}}$ with $n_c$, while $\Delta r = r_{\text{max}} - r_{\text{min}}$ diminishes.
6.1 Single attractor

A Gaussian refractive index distribution has the form:

\[ n = n_a e^{-r^2/\sigma^2} + n_c. \] (6.1)

Then making it possible to constrain the maximum and minimum of the refractive index distribution to feasible values, e.g. \(0.8n \leq 3.8\). Hence, given a range of values for the background and maximum refractive index, \(n_c\) and \(n_a\), respectively, we can evaluate different light confinement scenarios, see Figure 6.1.

As discussed in the previous section the orbital paths are open, while their shape and stability depend significantly on the initial conditions, \(n(r)\) and \(\{r_o, \dot{r}_o, \phi_o, \dot{\phi}_o\}\). As portrayed by Figure 6.1 different initial conditions will result in new orbit manifolds with distinct characteristics, albeit maintaining a common morphology. As it can be seen from these figures the orbital paths are highly sensitive to the modifications in the refractive index and the initial conditions; a change in \(\sim 0.5\%\) in \(n_c\) alters the orbit, as seen from the plot of radii extrema in Figure 6.2.

![Figure 6.2: Inner and outer radius as a function of the background refractive index \(n_c\).](image)

As it increases we observe that the outer radius diminishes, while the inner increases.

In Figure 6.3 we show the 2D open orbit for a refractive index map where \(n_c = 0.8\) and \(n_a = 3.0\). As detailed in Figure 6.4a, the radial velocity describes an oscillatory form, which indicates that the radius follows a similar motion, swinging between two extrema, as expected in a confine and open orbital motion. The latter
Figure 6.3: Confinement orbit for light traveling in a Gaussian attractor where \( n_a = 3.0 \) and \( n_c = 0.8 \). (a) Shows a schematic representation of the planar trapping device where the refractive index increases towards the center, where red indicates maximum refractive index \( n = 3.8 \), and light blue \( n = 0.8 \); (b) polar-2D path as calculated by the simulation routine.

can be observed in greater detail by analyzing the phase-space, plotted in Figure 6.4b; notice that when the velocity \( \dot{r} \) reaches zero the orbit radius \( r \) reaches an extrema; for a closed single loop the amplitude of the velocity oscillation would be zero, and the phase space would become a horizontal line at \( \dot{r} = 0 \). The behavior of the angle versus the radial velocity, and consequently to the radius movement, is described by Figure 6.4c where the absolute value of the radial velocity is plotted against the angular position, which results in a periodic motion. Observe that in the limit at every angle there would be a time at which the radial velocity would be zero, which is typical of open orbits.

### 6.2 Mexican hat

We study a variation on the Gaussian trap to understand the potential modifications on the trapping orbits when large modifications \( \sim 20\% \) of the refractive index take place. The mathematical description of the *mexican hat* is:

\[
n = \left( n_a - \frac{n_a \sigma^2}{\sigma^2} \right) e^{-r^2/\sigma^2} + n_c
\]  

(6.2)
Figure 6.4: Phase space for Gaussian-like refractive index map with $n_a = 3.0$, $n_c = 0.8$.

The plots show: (a) radial $\dot{r}$ and angular $\dot{\phi}$ velocities, (b) radial phase space, and (c) radial velocity as a function of the angle (c).

Using the same conditions as in the previous analysis we set $n_c = 0.8$, $n_a = 3.0$, and set $n_d = 0.2$. The results, shown in Figures 6.5 and 6.6, display an orbit whose appearance resembles that of the regular Gaussian trap studied earlier. However, a closer look reveals that the trap confinement area is $\sim 2\%$ slimmer, and the oscillatory frequency of the radial and angular velocities, Figure 6.6a, increases by $\sim 30\%$. Whereas the radial phase-space, Figure 6.6b, shows a smaller eccentricity compared to its Gaussian counterpart, and the absolute value of the radial velocity versus the angle, Figure 6.6c, describes the typical behavior of an open orbit.

These variations in the trapping conditions could potentially be used to differentiate trapping in transient optical memories to allocated binary data.

6.3 Binary systems

Interested in observing phenomenologically trapping in a binary system we evinced a planar refractive index map resulting from the superposition of two Gaussian functions,

$$n = n_a(e^{-(r-r_{off1})^2/\sigma^2} + e^{-(r-r_{off2})^2/\sigma^2}) + n_c. \quad (6.3)$$
Figure 6.5: (a) Schematic of mexican hat like refractive index map where \( n_a = 3.0 \) and \( n_c = 0.8 \) and depression is \( n_d = 0.2 \); (b) depicts the resulting trapped orbit in polar coordinates as calculated by the simulation routine.

The resulting orbits are shown in Figure 6.7. A binary system, however, presents a relatively higher sensitivity to modifications in the refractive index, where a distortion of \( \Delta n > 0.03 \) modifies the trapping orbits, in some cases releasing the light beam. Yet, it is possible to confine the light beam to an orbit which mimics the behavior of Newton’s three body problem, where, as expected, small perturbations result in sundry possible solutions to the path equation, *i.e.* chaos.
Figure 6.6: Phase-space for a *mexican hat* refractive index map with $n_a = 3.0$, $n_c = 0.8$.

The plots show: (a) radial $\dot{r}$ and angular $\dot{\phi}$ velocities, (b) radial phase space, and (c) radial velocity as a function of the angle (c).

Figure 6.7: Geodesics for light in a binary system. Observe that trapping also occurs for certain initial conditions at specific background and maximum refractive index.
Chapter 7

Beam Transformation: Gauss to Bessel-Gauss beams

We use the technique derived in section 4 to create a Bessel to Gauss-Bessel beam conversion device. We chose Bessel-Gauss beams due to its peculiar intensity distribution, which is focused on the propagation axis, and non-diffracting propagation [30, 83, 84].

Introduced in 1987 by Durnin, non-diffracting $J_p$ Bessel beams are members of a family of solutions to the homogeneous Helmholtz equation, with distinctive properties, e.g. their transverse profile does not change as the beam propagates in free space, and exhibit self-regeneration when disturbed by non-transparent obstacles [83].

Whilst mathematically viable, pure Bessel beams are not square integrable, i.e. the beam contains infinite energy, thus, rendering the ideal solution infeasible [85, 86]. Yet good approximation exists, namely Bessel-Gauss beams. Introduced by Gorin et al. [86] these solutions to Helmholtz homogeneous equation resemble the ideal $J_p$ Bessel beam with the sole difference that they bear finite power; and, therefore, can be realized experimentally, while retaining the primordial characteristics of self-reconstruction and diffraction-free propagation for lengths of interest to many optical applications, e.g. optical tweezers and mi-
Experimentally, Durnin et al. \cite{89} were the first to show that it is possible to generate Bessel-Gauss beams by means of a circular slit and a lens placed one focal length away. Hakola et al. \cite{90} proposed a Nd:YAG cavity with a diffractive mirror to transform the Gauss beam from a pump laser into a Bessel-Gauss beam of arbitrary order; Arrizón et al. \cite{91} and Otero \cite{92}, independently, used holograms to alter Gauss beams and produce zero and first order Bessel-Gauss beams; lately, Zhan \cite{93} has shown that it is possible to generate them by using a radially polarized beam and surface plasmon resonance. Alternatively Cong \cite{94} used phase elements to generate zero order Bessel-Gauss beams. Recently novel designs have used waveguides to produced diffraction-free beams, \textit{v.gr.} Canning \cite{95} presented a Fresnel waveguide as a diffraction-free mode generator, and Ilchenko et al. \cite{96} experimentally showed that cylindrical waveguides can produce truncated Bessel-Gauss beams; and Tsai et al. \cite{97} showed that is possible to use an acoustic tunable lens to generate this family of beams.

The afore mentioned methods produces high quality beams. Nonetheless their design and fabrication on photonic integrated circuits (PIC) or planar lightwave circuits (PLC) would involve complex processing steps, rendering the integration into most PICs platforms impractical. It is a matter of debate whether resonator/waveguide designs (see for example \cite{95,96}) could be used for this purpose. In our experience on such devices, the quality of the beam, and conversion efficiency critically depend on the coupling efficiency. Moreover the converted beam free space propagation is limited to $\sim 1\text{mm} \cite{96}$. Hence the motivation to attain a fully integrated Gauss to Bessel-Gauss micro-convertor based on current Silicon foundry technologies is justified. If viable, it could be readily integrated into semiconductor-chip-based optical elements of great importance to a manifold of optical applications. For instance they have been shown to increase the scanning resolution and tissue penetration depth of optical coherence tomography (OCT)
systems by $\sim 50\%$ \cite{98}.

## 7.1 Methodology approach

We begin by noting that if the input and output beams are symmetrical around the propagation axis $z$. Because the transforming field $\nu_i$ is defined based on these known fields it follows that it is also symmetrical along the $z$ axis. Therefore, we can scale down the problem to two-dimensions: $z$ and $y$, the longitudinal and transversal direction, respectively.

![Figure 7.1: Schematic representation of a Gauss to $J_0$-Bessel-Gauss transformation via a heterogeneous medium, the transformation device in region $A$ has a refractive index map that needs to be calculated in order to achieve the desired beam reshaping. The device is embedded in a homogeneous medium $B$, where the input and output beams are known solutions to the Helmholtz equation.](image)

Accordingly, the simulation space is discretized on a grid size $d^2$ by $d^y$. The solver is given an initial guess of the permittivity map $\hat{\eta}(z_i, y_j)$ across the region $A$ at every point $\{z_i, y_j\}$. The solution to (4.7) can then be computed via a variational approach as described in \cite{79}: at every point $z_i$ the transversal function of $\hat{\eta}(z_i, y_j)$ is determined by solving equation (4.7) where the functions $f$ and $g$ chosen to create a smooth variation in the fields, this determines $\nu(z_i-1, y)$ and $\nu(z_i+1, y)$; and the field at that point $\nu(z_i, y)$. This iterative approach is carried for every point $z_i$. Thus the transversal shape of $\hat{\eta}(z_i, y_j)$, and consequently that of $n_{ij}$, is determined to match the resulting field to the ideal transformation given
This method solely does not guarantee that the solution will be exempt of extreme or singular values, withal the variational method is especially sensitive numerical approximations [79]. To account for the latter and work out the extrema in the refractive index, we implement a solution coming from the adjoint problem [74]. The extreme and singular values are approximated to the closest value in the defined range. We then propagate the initial Gauss beam through the device and determine how much the field at every point diverges from the ideal transformation of equation (4.5), including as well the near and far fields. An iterative refinement on this grid regions follows, as described in [74,75], to match the numerical computation output to the ideal Bessel-Bessel-Gauss beam. The beam propagation method is used to propagate the initial Gauss beam through the heterogeneous region $\mathcal{A}$.

Figure 7.2: Illustration of (a) superposition of transition stages in the transformation of Gauss to Bessel-Bessel-Gauss beams; and (b) the transformation functions $f$ and $g$.

The transformation functions $f$ and $g$ are plotted in Figure 7.2b. The initial guess for the permittivity map is a Gaussian profile in the transversal direction $y$ for all points along $z$, width $\sigma = 5$ and a maximum peak of $\bar{\eta}_{\text{max}} = 9$ or $n_{\text{max}} = 3$. The initial beam in region $\mathcal{B}$, follows a Gaussian function, with width $10\mu m$ and
normalized energy to unity.

7.2 Beam transformation

The outcome of the calculation and optimization process described earlier is depicted in the schematized Figure 7.3 and the fine resolution \((d = 1 \text{nm})\) plot of the refractive index in Figure 7.4. The refractive index map is symmetric around the propagation axis \(z\), and is comprised of a smooth variation of the refractive index between 1 and \(\sim 2.57\). The minimum feature size, \(d = d^z = d^y\), is 1 nm, and has the final dimensions 200\(\mu\text{m}\) length by 20\(\mu\text{m}\) wide. Notice that the minimum feature size defines the smoothness of the refractive index map.

![Figure 7.3: Sketch of proposed refractive index map for the conventor. Device length 200\(\mu\text{m}\) and width 25\(\mu\text{m}\). Albeit depicted in 11 steps, the refractive index varies smoothly between 1 to 2.57. The device is rotationally symmetric around the propagation axis \(z\).](image)

The initial impinging Gauss beam in region \(B_i\) propagates through the device in region \(A\), and it is transformed into a Bessel-Bessel-Gauss beam with a 95\% efficiency. Figure 7.5a shows the results for the field at 5\(\mu\text{m}\) from the exit of the device, with the corresponding far field depicted in Figure 7.5b. As described earlier, this is the optimized value considering the current state-of-the-art nano-
fabrication techniques and facilities available to realize the device.

In Figure 7.5, it is observed that both near and far fields follow a Bessel-Bessel-Gauss profile with 98% accuracy. The converted beam divergence is less than 1% after propagating 50µm and less than 5% after traveling 1mm. The energy density at the principal peak is 95% of the converted beam’s total energy, which makes it ideal for OCT applications and free space light-based communication. Losses due to material absorption, scattering and back reflections are 10% of the incident field, or −0.457dB, which can be significantly reduced by using antireflection coatings at the input and output surfaces.

Within the known limitations in fabrication processes, it is noted that not all values of the index of refraction can be achieved. A theoretical study is required to define the tolerance to minimum feature size and its repercussions in the beam profile. We study this case by further modifying the grid size, i.e. the minimum feature size, \( d = d^x = d^y \) from 1nm to 10nm. The results are shown in Figure 7.6.

As it is evident from Figure 7.6a, modifying the refractive index grid size results in a beam that also resembles a Bessel-Bessel-Gauss beam with a 95% accuracy, with the sole difference that this beam as it propagates will evolve into a non-Bessel-Gauss beam. This can be drawn from the far field, plotted in Figure 7.6b. Observe that at infinity the field no longer corresponds to the far field of a Bessel-Bessel-Gauss beam. Nevertheless, a coarse mapping will produce a highly focused beam, where 95% of the energy is localized at the first peak, and the beam diffraction over 1mm propagation is less than 5%.

Bessel-Gauss beams, alike Bessel beams, exhibit self regeneration when their path is perturbed by a non-transparent scatterers. To examine this self-healing property of the outbound Bessel-Bessel-Gauss beam, we insert a random index medium on its propagation path. The results are shown in Figure 7.7.

The generated Bessel-Bessel-Gauss beam is made to impinge on a random index media, which consists of a circle-like region of 4µm, set at 50µm from the output
of the device, and refractive index of \( n = 2.0 \). The scatterer partially obstructs
the propagation of the beam. The scattered beam profile is computed at 50\( \mu m \)
from the alien obstruction (see Figure 7.7a and its magnified version in Figure
7.7c), as well as the far field (see Figure 7.7b). As can be seen from the results in
Figure 7.7, the beam described earlier (see Figure 7.5) exhibits self-regeneration.
The divergence, computed by comparing the width of the principal peak, from the
scattered field to the original transformed beam is 0.3\%. Since the beam is not a
full Bessel beam, some light is scattered by the object, as expected, giving rise to
a loss of 19\% or \(-0.915dB\).

The 2D mapping for beam conversion heretofore described while challenging
to fabricate, could be built using current nano-manufacturing techniques. A pro-
totype, \textit{verbi gratia}, could be obtain by controlling the degree of oxidation in
\( Si/Si_{1-y}O_y/Si_{1-x-y}Ge_xC_y \) \textsuperscript{99,100} systems, or by horizontally stacking nano-
layers of photo-refractive materials such as chalcogenide glasses which have been
shown to have a wide range of refractive index \textsuperscript{31,65}. The advantages of these
materials are that they are relatively well-developed, and the material systems are
compatible with PICs and PLCs.
Figure 7.4: High resolution refractive index map for the beam transformation. Minimum feature size $d = 1\text{nm}$. Device length $200\mu\text{m}$ and width $25\mu\text{m}$. The refractive index varies smoothly between 1 to 2.57 in 50 steps. Practical implementation could be achieved on a $Si/Si_{1-y}O_y/\text{Si}_{1-x-y}Ge_xC_y$ together with controlled oxidation or inclusion of photorefractive materials. The device is rotationally symmetric around the propagation axis $z$. 
Figure 7.5: Magnitude of transverse electric field for the transformed beam: (a) near field at 5 \( \mu m \) from the output of the device (green), and comparison to \( J_0 \)-Bessel-Gauss (red); and (c) detail of principal peak.
Figure 7.6: Magnitude of transverse electric field for the transformed beam with varying grid size: (a) grid size 1nm (green); and (b) grid size of 10nm (blue). Near fields calculated at 5µm from the output of the device. The far fields for both output beams (b), for optimal grid size (green) and modified grid (blue); and (c) detail of principal peak.
Figure 7.7: Magnitude of transverse electric field for scattered field, (a) transformed beam (green), fit (red), and scattered field profile (blue), computed at 50µm from the scattering region. The far field for the undisturbed and perturbed beams is plotted in (b); and (c) detail of principal peak.
Part III

Material Proposal
Chapter 8

Material proposal

Whilst the main goal of our project is to produce new theoretical methods and designs to manipulate light, we acknowledge the necessity to study a material base, through which, achieve the practical realization of light manipulation. This, naturally, encompasses the understanding the dynamics of the electromagnetic properties of the material base and how they can be manipulated; these are key to enabling and extending many of the devices proposed so far and achieve light control.

A material base to serve this purpose requires to satisfy certain characteristics to be compatible with planar photonic circuits and photonic integrated circuits, namely:

- Fabrication process adaptable to Si-foundry technologies, e.g. PLD, e-beam evaporator, sputtering, . . .
- Wide dynamic range of electromagnetic properties, $\varepsilon$ and $\mu$, in the visible spectrum feasible of manipulation by photon or electron injection,
- Variable and controllable dispersion characteristics,
- Low absorption in the visible range of spectrum,
- Anisotropic and dichroic,
Arguably there is a wide miscellany of [meta]materials that comply with the aforementioned features, however one stands due to is unique properties, availability, and research opportunity: chalcogenide glass.

8.1 Understanding chalcogenide glasses

Over the last decades, chalcogenide glasses have been subject of great interest due to the myriad photon-induced phenomena they exhibit, captivating the imagination of scientists and engineers to prompt countless photonic applications ranging from biology [16,101] and telecommunications [102,103], all-optical chips [16,103], single photon sources [104,105] to holography [106]. Furthermore, they have been worthy of great attention from fundamental science, owing to the seemingly oxymoron nature of the physical effects observed when the material is illuminated by photons within its band-gap energy range ($E_g \sim 2.4eV$), e.g. giant photo-expansion [107] versus photo-contraction [108], photo-liquidity [109,110] versus photo-crystallization [111,112], photo-darkening [113,114] versus photo-bleaching [113], and, more frequently, photo-refraction [114,117], to cite a few. Studies from fundamental physics and material science have led to various models attempting to explain the mechanisms behind the exciting structural reconfiguration capabilities and phenomena observed in chalcogenide glasses upon energy absorption. That being said, the physical processes, in addition to many of the phenomena reported, remain both a matter of debate and a hot topic in fundamental and applied research [16,31].

The principal experiments, observations and models in chalcogenide glass deal with phenomena triggered by light irradiation, and to a lesser degree with electrons.
Photon induced phenomena in chalcogenide glass comprises: \textit{photon-induced} refractive index modification, -liquidity, -dichroism, -anisotropy, -crystallization, -darkening, -bleaching, and -vitrification \cite{107,118}, in addition to other innate effects present in highly non-linear materials, v.gr. second harmonic generation \cite{119,120} for example. To understand the nature of these effects, and the electronic and atomic processes involved, it is essential to investigate the charge carrier transfer, energy spectrum, and the mechanisms by which radiation (electron or photon) interacts with the material modifying its chemical and atomic structure \cite{108,110,112,121,125}.

Electron irradiation induced refractive index modification has also been reported. Suhara \textit{et al.} \cite{126}, found a maximum change of $\Delta n/n = +3.6\%$, with no significant modification in the thickness of the film. On the other hand, Normand \textit{et al.} \cite{127,129} and Tanaka \textit{et al.} \cite{130}, independently observed a $\sim 3\%$ increase in the refractive index of chalcogenide glass; simultaneously the formation of trenches and mounds, 180 nm and 110 nm respectively, in chalcogenide films of $5 - 11 \mu m$ thick, were observed. They posited that the morphological and optical alteration derives from the structural reorganization and re-bonding of the homopolar and heteropolar bonds, in addition to the electrostatic effects arising from the charge density variation \cite{127,130}.

Whilst many of these effects appeal to our research interest, we are particularly intrigued by the alteration in the optical properties of chalcogenide glass thin films, and its possible applications. However, in most of the previous studies only the refractive index has been characterized\footnote{It is worth to discern the difference, and connection, between the refractive index and the electromagnetic properties of materials. The former is the ratio between the propagation speed of waves inside a material to that of vacuum; whereas the latter, permittivity ($\varepsilon$) and permeability ($\mu$), are the physical representation of a material’s intrinsic electric and magnetic properties; which arise from the atomic, electronic and molecular configuration and interactions with the electric and magnetic fields, ultimately shaping their propagation dynamics. Accordingly, the} and understanding how can
they be modified, with little information available on how the electromagnetic components, *i.e.* permittivity and permeability, reshape under energy absorption, vital to achieve the control of light.

In this section we present the results of our investigation on the permittivity dynamics of chalcogenide glass As$_2$S$_3$ thin film under energy absorption by means of EELS [31].

### 8.2 Electron Energy Loss Spectroscopy

As discussed earlier, As$_2$S$_3$ chalcogenide glass, exhibits electron- and photon- irradiation induced modification of its optical properties. In our study we use low-loss EELS [131,132] to characterize the real and imaginary parts of the permittivity of As$_2$S$_3$.

When high energy electrons, 300keV impinge on a sufficiently thin material, thickness $\leq 300$nm, a vast majority of the electrons will pass through the sample without being perturbed, and a small fraction of them will undergo inelastic scattering loosing energy to the sample, typically in the order of $10^1 - 10^2$ eV. It is important to note, however, that some of the electrons will also be elastically scattered and will transfer some energy to the system; yet, this energy is not enough to perturb the overall atomic arrangement of the material, even on a head-on collision with the atom the elastic scattered electron energy loss will be in the range of 1 eV, which is not sufficient to displace the atoms and therefore change the molecular arrangement. The inelastic scattering, nevertheless, yields enough energy to the system to sustain bond-breaking and alterations in the electron density of the material. The latter electron loss can be experimentally measured via an electron

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refractive index and the electromagnetic properties of materials are entwined by the widespread relation: $n = \sqrt{\varepsilon_r \mu_r}$, where the subscript $r$ refers to the relative permittivity or permeability, *i.e.* $\varepsilon_r = \varepsilon / \varepsilon_0$ and $\mu_r = \mu / \mu_0$. 
The inelastic scattering process is characterized by the electron scattering angle, $\theta$, or momenta, $q$, and the electron energy loss, $E_s$, due to their interactions with the material, which includes phonon excitation, inter- and intra-band transition, plasmons excitation, inner shell ionization, and Cherenkov radiation. These interactions can be summarized by the dielectric response function, $\varepsilon(q, \omega)$; which describes the interaction of photons and electrons with the material [132].

Admittedly, the interaction of photons and electrons with those in the solid is different; photons displace the electrons in the material in a direction perpendicular to their direction of propagation, with the electron density remaining unchanged. Therefore, we define the optical permittivity as a transverse property of a medium; whereas electrons interacting with the material produce a longitudinal displacement of the electrons, and change the electron density. Moreover, the energy transfer mechanisms for photons differs from that of electrons; in the former the energy transfer is mostly mediated by inter- and intra-band transitions (valence-to-conduction band), e.g. (i) bandgap absorption, (ii) defects, (iii) free carriers, among other transitions. In the scenario of electron irradiation, energy transfer takes place by means of inelastic scattering, and to a lesser degree by elastic scattering. Despite the fundamental differences, however, it is possible to establish a correlation between the permittivity measured by electrons or photons if we constrain to small energy losses, which translates small scattering angles for electrons. Under this condition $\varepsilon(q, \omega)$ varies insignificantly with $q$, and hence $\varepsilon(q, \omega) \approx \varepsilon(q = 0, \omega = E/h)$, the latter being the optical permittivity [132][134].

Whence stems the versatility of low-loss EELS over other methods to measure the permittivity of thin film samples constraint to small probing areas. Specifically, if scanning transmission microscopy (STEM) is used, the volume of study can be reduced to nano-metric scale, allowing us to study the material and its response locally. As discussed in the preceding paragraph in a typical EELS experiment low
angles of collections are used, and thus most inelastic collisions result in energy losses to the incoming electrons of less than 100 eV. This energy loss range in turn deciphers information about the permittivity within an energy range of interest to optics and photonics, \( i.e. \leq 10 \text{ eV} \). The latter is achieved by post-processing the energy loss spectra by means of Kramers-Kronig relations to evince the real and imaginary parts of the optical permittivity [132,135–140].

8.3 Experimental arrangement

In our experiment, high energy electrons (300 keV) impinge on an As\textsubscript{2}S\textsubscript{3} thin film, 300 nm \( \pm 5 \) nm thick, grown on a 2 \( \mu \)m holey-Cu TEM grid by means of electron-beam evaporation, and the roughness, film thickness and stoichiometry are characterized by atomic force microscopy (AFM), ellipsometry, energy dispersive X-ray (EDX), and X-ray photo emission spectroscopy (XPS), respectively.

To ensure the validity of the low energy loss limit approximation, we use a scanning transmission electron microscope (STEM), coupled to a low-loss EELS, and perform the experiment in the low momentum transfer relativistic approximation. We set the electron source to 300 keV, with a collection angle of 6 mrad, and incident semi-angle of 4.575 mrad. Under these conditions the energy resolving power of the electron loss spectrometer is better than 0.1 eV in the range 0.8 eV – 50 eV; electrons are accelerated to 77.561% the speed of light, corresponding to a de Broglie wavelength of \( 1.9687 \times 10^{-3} \) nm, which results in a minimum spatial resolution of \( 1.2048 \times 10^{-1} \) nm. The scanning area for the STEM is 50 \( \times \) 50 nm\textsuperscript{2} on the holey region of the film support to avoid any contamination from the carbon support of the grid. The density of electrons per second incident on the sample is 175 \( e^-/\text{nm}^2\text{s} \). To achieve different electron dosages we control the irradiation time in steps of 100 ms \( \pm .05 \) ms (see table 8.1). These steps are divided into two irradiation sequences, sequence A and sequence B; which are separated by a
**relaxation** time defined as the period of time where zero electrons are incident on the film. This arrangement allows us to determine if after a given time of repose the material returns to its initial state, *i.e.* if it exhibits memory or a hysteretic behavior.

<table>
<thead>
<tr>
<th>Irradiation steps (step)</th>
<th>Sequence A</th>
<th>Relaxation</th>
<th>Sequence B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Irradiation exposure time ( t^* ) (s)</td>
<td>0.1</td>
<td>0.2</td>
<td>0.3</td>
</tr>
<tr>
<td>Accumulated irradiation time ( t ) (s)</td>
<td>0.1</td>
<td>0.3</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 8.1: Irradiation sequence summary, including steps, exposure, and accumulated time. The symbol “+” is used to demark the fact that the material was exposed to irradiation sequence A and relaxation before the new measurement.

### 8.4 Electron-induced permittivity variation

In order to obtain the optical and electronic characteristics of the material, the loss spectra needs to be de-convoluted, and the zero loss subtracted: this is attained by the Fourier-Log Two Gaussian method \[132\] (see Figure 8.1).

Figure 8.1: Low-loss Electron Energy Loss spectra, raw measurement results at different dosages as specified in table \[8.1\]. The causal variable marks the energy lost by the electrons to the material through inelastic scattering, \( q\nu \).
A meticulous inspection of Figure 8.1 reveals that the peak of the loss spectra decreases as a function of electron dosage, as depicted in Figure 8.2a, after irradiation sequence A, and before relaxation, the peak value changes 8%. It is also evident that the process has some degree of elasticity, where after relaxation some recovery occurs such that the electron intensity before and after relaxation suffers a 2% return (see Figure 8.2a). However, this return goes hand in hand with a blue-shift of the peak dispersion of \(\sim 3\) eV (see Figure 8.2b). Yet there is a striking effect, subsequent irradiation for long periods of time has a reverse effect, increasing the total electron intensity rather than decreasing it as was the case before relaxation in sequence A. As we will elucidate later this effect can be explained by the breaking of the homopolar bonds, and the continuous reconfiguration of the heteropolar bonds within the material. It is capital to recall that our experiment is carried in a vacuum environment (10\(^{-8}\) Torr), therefore eliminating any chance of oxidation and contamination on the material surface.

![Graphs of peak loss](image)

**Figure 8.2:** Analysis of peak loss for steps 1 through 6, the behaviour of the peak in reference to the irradiation step is shown.

As discussed earlier, the electron energy loss is linked to the real and imaginary permittivity (see equation (8.1)), and hence we can expect them to follow a somewhat similar pattern to that of the energy loss. 

[132]
\[ \sigma_{\text{EELS}} = \Im(-1/\varepsilon) = \frac{\varepsilon_2}{\sqrt{\varepsilon_1^2 + \varepsilon_2^2}}. \] (8.1)

By virtue of the above equation and the Kramers-Kronig relations we obtain the imaginary part of the permittivity function, \( \varepsilon_2 = \Im(\varepsilon) \), and the real part, \( \varepsilon_1 = \Re(\varepsilon) \), here shown in Figure 8.3.

Figure 8.3: (a) Real (\( \varepsilon_1 \)) and (b) imaginary (\( \varepsilon_2 \)) parts of the transversal permittivity function derived via Kramers-Kronig relations from the electron energy loss spectra. The peak trace, \( i.e. \) dispersion relations, for (c) \( \varepsilon_1 \), and (d) \( \varepsilon_2 \), clearly show the semi hysteretic behaviour of the permittivity.

It is essential for the ongoing discussion to remark that in the curves of Figure 8.3 and subsequent, the causal variable, \( h\nu \), refers to the photon energy, for recall that these result from the Kramer-Kronig analysis of the electron energy loss spectra at the low momentum approximation. Therefore, they can be regarded as
dispersion relations for the permittivity at different electron irradiation dosages.

As predicted at analyzing the electron energy loss spectra, the real and imaginary parts of the permittivity decrease as the electron dosage augments. Moreover, Figures 8.3c and 8.3d confirm the semi hysteretic comportment of the permittivity. Particularly, observe that the maxima of $\varepsilon_1$ reduces, and shifts following a semi hysteresis loop, as the total dosage rises; while its minima shifts to higher energies, although seldom changing its dispersion energy $h\nu$. On the other hand, the maxima of $\varepsilon_2$ exhibits a similar decrement, as that portrayed by $\varepsilon_1$ as a function of dosage, with the difference that there is no evidence of a hysteretic behavior, rather the maximum shifts to higher energies together with electron dosage.

To acquire a deeper insight on the permittivity of the material and its dynamics we sampled it by splitting the dispersion energy range in two, range $A$ comprises energy values around the bandgap of the material, i.e. $2.0\text{eV} \leq h\nu \leq 3.6\text{eV}$; and range $B$ includes higher energies $4\text{eV} \leq h\nu \leq 10\text{eV}$. At either set we compare the results to the global maximum and minimum, denoted by max and min, receptively. Within range $A$ the sampling results, Figures 8.4a and 8.4c, clearly evince the hysteretic behavior of the electron-induced permittivity change. At comparing the curves given by the maximum peaks of $\varepsilon_1$ and $\varepsilon_2$, before and after relaxation, it is patent that some degree of restoration occurs in the system which allows a recovery of up to 75% of the initial values. Furthermore, the dynamics of the extreme values of either the real or imaginary permittivity echo an almost identical pattern, with an initial fast rate of change during the first irradiation steps $0 \leq t^* \leq 0.2\text{ ms}$, closely followed by a sustained decrement on its absolute value, i.e. the pace at which the permittivity changes tends to zero for a sufficiently large irradiation time (see Figures 8.5). As we will explain in section 8.4.1 this effect can be understood through the variation in the density and rearrangement of the homopolar and heteropolar bonds, which significantly modifies the response
of the material to energy absorption.

Figure 8.4: Selected samples of the permittivity function $\varepsilon$ (real and imaginary) in reference to the dispersion energy, range A (a) and (c), and range B (b) and (d), at different irradiation dosages.

As it can be appreciated at comparing the results between the two energy ranges, either for real or imaginary parts of the permittivity, shows significantly different comportments. The test values for the real permittivity in range A closely follow the pattern and magnitude modification of the global maximum, while the global minimum remains virtually unperturbed. In range B, however, the selected values present different bearing to that observed previously. Specifically, before relaxation, samples at $h\nu \geq 6\text{eV}$ initially increase in magnitude as much as 10%, in contrast to the marked decrease of the global maximum. Yet, with the exception of the sample at 10eV subsequent electron exposures regain the decreasing pattern.
of the maximum, albeit to a lesser magnitude, and rate of change (see Figure 8.5b). After relaxation, however, some degree of elasticity is observed, with most of the test samples recovering to the initial state, although exposing the relaxed material anew to electron irradiation results in an increment of the permittivity value in clear contrast to the global maximum bearing.

Concerning the imaginary part of the permittivity, the previous description gets somewhat inverted when compared to the measurements of $\varepsilon_1$ in both ranges. In range $A$ the initial behaviour is mixed, with some of the samples increasing in magnitude, while others decrease. Notably, test samples below the band-gap energy of the material show a similar behavior to that of the imaginary permittivity in range $A$, an initial increment followed by a steady decrease with new dosages. Range $B$ on the other hand shows a behaviour close to the comportment of the global maximum, with the anomaly of test sample at 10 eV. After relaxation the degree of recovery is mixed, in range $B$ the hysteretic behavior is conspicuous. But in range $A$ the results are to some extent extraordinary, all the samples beyond the band-gap of the material show some degree of recovery, in some cases surpassing the initial value by as much as 15% for example at 3.6 eV; below the band-gap energy test samples show an eerie result not only there is no recovery to the initial state, but a considerable increment instead. After relaxation all samples show the same decreasing pattern as observed in their real counterpart. In range $B$ all the samples follow a similar pattern to that of the maximum; an initial fast decrease, followed by a sustained decrease in magnitude, although steadily reducing the rate of change. The physical explanation to this peculiar reaction of the material, reflected by the permittivity, in response to electron bombardment can be reasoned in term of the modification to the physical bonding between the Arsenic and Sulphide atoms, and the electron traps within the material, assuming that there is no increment in the initial number of electrons in the material, which to this effect is grounded.
To fathom the physical process behind this phenomenon it is necessary to gain some understanding about the atomic configuration of \( \text{As}_2\text{S}_3 \) chalcogenide glass. Either amorphous or crystalline, the structure of chalcogenide material based on As and S is composed of pyramidal arrangement in threads that form layers linked by homopolar (As–As and S–S) and heteropolar (As–S) bonds (Figure 8.6). The bonding energies in the homopolar case are 1.88 eV and 2.39 eV for As–As and S–S bonds, respectively; whilst for the heteropolar (As–S) the bonding energy is 2.29 eV [141]. Our film has similar proportions of As and S atoms, 51% and 49% respectively and by weight, as measured by XPS in the surface of the material. To evaluate the overall bulk composition of the film we use EDX finding atomic proportions closer to that of \( \text{As}_2\text{S}_3 \) chalcogenide glass (As 58% and S 42%). The atomic composition measured before and after the experiment by EDX did not show any net flux of atom concentration. It is important to note that our TEM instrument has the ability to do STEM, TEM and EDX within the same chamber, thus avoiding the possibility of contamination or oxidation of the sample by keeping it under high vacuum. Under irradiation exposure the incoming electrons (300 keV) can break the homopolar and heteropolar bonds with ease by mean of inelastic collisions; whence a structural rearrangement follows, with the broken homopolar bonds switching to heteropolar bonds [142,143]. This structural rearrangement will continue for as long as the material keeps being bombarded with electrons. However, since the concentration of As atoms is higher, the re-bonding of the S and As atoms, mostly coming from the broken homopolar bonds, will lead to dangling uncoordinated As atoms. Under relaxation, the dangling As atoms, in vacuum, re-bond in homopolar As–As pairs. Consequently, the density of homopolar bonded As increases, resulting in a diminished response to electron irradiation as observed in the decrement in the rates of change before and after
the first irradiation and relaxation period \[8.5\]

Concomitant to the re-bonding process is the nano-crystallization of the material, which causes a reduction in the number of the trapped carriers, either by promoting a large fraction of the electrons to the conduction band, or by reducing the number of carrier traps in the material. The overall modification of the electronic density states originates the prominent reduction in the permittivity. Recall that in amorphous and semi-crystalline materials the permittivity heavily depends on the density of trapped carriers. This comes from the fact that carrier transport in these materials, like chalcogenide glass, is controlled by traps; at any given point in time a fraction of the carriers is confined, and since the dipole moment of the filled and empty traps may vary broadly it changes the permittivity of the material \[124,144\]. A working model for the dielectric constant based on the electron trapping was given by Arkhipov et al. \[145\],

\[
\varepsilon(r, t) = \varepsilon_0 + 4\pi\kappa_0 \int_0^\infty \rho(r, t; E) dE,
\]  

(8.2)

where \(\rho dE\) is the carrier density trapped in the energy interval \(E\) to \(E + dE\), \(r\) is the position vector, \(t\) the time, \(E\) is the trap energy, \(\varepsilon_0\) is the vacuum permittivity, and \(\kappa_0\) is a coefficient that depicts the change in the dipole moment of the traps due to the capturing of electrons in them. Observe that in order to reduce the permittivity at \(t > t_0\) a reduction in the density of trapped electrons is inexorable, \(i.e.\ \rho(r, t_0; E) < \rho(r, t_0; E)\).

Evidence of such electronic rearrangement under energy absorption by \(\text{As}_2\text{S}_3\) chalcogenide thin film has been reported separately by Tanaka et al. and Lee et al.. Tanaka et al. \[146\], observed chemical and medium range re-ordering in \(\text{As}_2\text{S}_3\) film under photon energy absorption. Meanwhile, using X-rays, Lee et al. observed modification in the structure order of chalcogenide films \[147\]. Albeit focusing on the dynamics of photo-darkening and anisotropy, respectively, both studies show
that upon energy absorption the material suffers an alteration in both the electron energy density and the bond structure; in agreement with our observations, where the alteration of the permittivity springs from the changes in the structural and electronic states of the film.

8.4.2 Prospective deduction, the refractive index

Earlier we discussed the inextricable relation between the refractive index, \( n \), and absorption, \( k \), with the electromagnetic properties of the material, \( \varepsilon_r \) and \( \mu_r \). Often, in the deduction of the refractive index, the permeability, \( \mu_r \), is set to a constant value, generally 1, resulting in a set of relations widely available in the basic literature. Here we present the calculated optical parameters, \( n \) and \( k \), based on these relations (see Figures 8.7a and 8.7b respectively).

Under the former assumption, the computed results show similar behaviour for \( n \) and \( k \) to that observed for \( \varepsilon_1 \) and \( \varepsilon_2 \), with the peak of the refractive index, \( n \), reducing by \( \sim 23\% \) after an irradiation time of \( t = 1 \) s. The minimum change takes place at 6.5eV where the reduction is \( \sim 8\% \). For energies close to the band-gap the reduction is on average \( \sim 20\% \). The absorption, \( k \), also shows a striking decay, down to 40\% from its peak value, and a minimum of \( \sim 10\% \), with an average reduction of \( \sim 35\% \) for dispersion energies close to the band-gap. Calculation of the extrema of the refractive index and absorption coefficient are shown in Figures 8.8a and 8.8b.

The observed measurements, and the calculated optical properties therein, are extraordinary, in the sense that all previously published experiments, with high energy electrons (40 keV), reported an increase in the refractive index between 3\% to 8\% \[126 130 148\]. In contrast to the vast literature reporting photon-induced refractive index change, which has yielded as much as an 8\% increase in the refractive index of As\(_2\)S\(_3\) film under illumination \[112 114\], in our experiment the
refractive index decreases as much as 23%. Bearing in mind that the conditions in the cited experiments are significantly different from those reported here, we believe the discrepancy could be explained by two different mechanisms. The first would state that, as described in the previous section, the permeability remains unchanged, while the number of electrons and the number of homopolar and broken heteropolar bonds increases; leading to the recombination mechanism described earlier. These structural alterations, in turn, induce nano-crystallization, ultimately leading to the generalized reduction in the number of energy traps, especially within energies in range $A$; all these simultaneous changes will cause reduction in the permittivity, and therefore reduce the refractive index.

On the other hand, to reconcile previous published results with ours, it would be necessary to acknowledge a dynamic change of the permeability with respect to electron irradiation. This would require the electrons to alter the atoms intrinsically by means of elastic collisions, and/or induce current loops, causing the magnetic dipoles in the material to reorganize, so inducing paramagnetic states, and hence increasing the permeability. However plausible the latter explanation, an experimental confirmation is required, together with further studies on the permeability of chalcogenide glass under high energy electron- and photon- irradiation.
Figure 8.5: Derivatives of the permittivity function with respect to the causal variable dosage, $t^*$.

![Derivatives of the permittivity function](image)

Figure 8.6: Homopolar and heteropolar bond breaking process under electron irradiation in $\text{As}_2\text{S}_3$.

![Bond breaking process](image)
Figure 8.7: (a) Refractive index $n$, and (b) absorption constant $k$, derived from the real and imaginary permittivity.

![Graphs showing refractive index and absorption constant](image)

Figure 8.8: Peak trace sampling of (a) refractive index, $n$, and (b) absorption constant, $k$, derived from the real and imaginary permittivity.

![Graphs showing peak trace sampling](image)
Part IV

Epilogue
Chapter 9

Closing Remarks

Through this work a new characterization procedure and analysis of the permittivity of Chalcogenide glass has been presented. Based on low-loss Electron Energy Loss Spectroscopy (EELS), the results are extendable to the optical regime by means of the small angle scattering approximation. Furthermore, they allow us to calculate an approximate form of the refractive index, assuming constant permeability, and suggest the possibility of magnetic alterations induced by electron irradiation. The calculated results and observations found that high energy electrons induced a reduction in the permittivity, real and imaginary, of the material. The real permittivity underwent a maximum reduction of $\sim 40\%$, while the imaginary permittivity decreased by $\sim 50\%$. The results can be explained in terms of the atomic bond reconfiguration; in this model the incident electrons break the homopolar and heteropolar bonds, leading to a reduction of the former, correcting the wrong bonds.

The results are significant to the development of manifold photonic applications, with applications to numerous areas of research and engineering. Namely, the observed reduction in the permittivity could enable a new range of transformation optic devices, which have been so far limited to the realm of far-IR range of the electromagnetic field. Furthermore, these results could be significant to future implementation of reconfigurable photonic circuits, infrared telecommunications,
photonic crystals, and all optical conversion and computing.

Based on this material properties we have demonstrated that, under the paraxial description of light in heterogeneous media, it is possible to use centro-symmetrical refractive index distributions as attractors for light, which are able to perform light trapping or confinement in open orbits. These mappings are bound within fabrication constrains, and due to the paraxial approximation they are several times larger than the mean beam width and wavelength, $\sim 50$ times larger. The proposed mappings have potential applications to transient optical memories, delays, concentrators, random cavities, and beam stirrers, to cite a few; which could enable the next generation of photonic integrated circuits, PICs, processors and computation systems. Due to their sensitivity to the change in the refractive index these devices could be employed as a sensor platform. Furthermore, since they are drawn in close analogy to celestial phenomena they could be used as laboratory setups to test a large variety of effects in celestial mechanics.

Furthermore, we have, to the best of our knowledge, theoretically demonstrated the viability of the first PIC and PLC compatible device utilizing a heterogeneous refractive index map, to achieve the transformation of a Gauss beam into a Bessel-Gauss-$J_0$ beam. The computed device has a loss of $0.457\, dB$, and high energy focus, where $95\%$ of the output beam energy is concentrated at the principal peak of the Bessel-Gauss-$J_0$ beam profile. The beam has a divergence of $\leq 5\%$ over a propagation distance of $1\, mm$, and exhibits self-healing when partially obstructed by an opaque object. The resulting beam has a Bessel-Gauss-$J_0$ beam profile for both near- and far-fields. It is note that our design is based on current manufacturing techniques, such as controlled oxidation of $Si/Si_{1y}O_y/Si_{1xy}Ge_xC_y$ or by stacking different layers of chalcogenide glasses. An integrated Gauss to Bessel-Gauss-$J_0$ beam convertor could enable on-chip applications which take advantage of the beam’s self-healing and non-diffractive properties, such as micro optical tweezers, traps and couplers, photonic integrated circuits for telecommunications.
and computerized micro tomography and microscopy.

Finally, we have developed a numerical scheme to model light propagation in spacetime-varying and nonlinear materials. The results suggest that our scheme is second order accurate. Some examples of light trapping and nonlinearity compensation were numerically demonstrated, together with two spatial dimensions examples of light propagation in an oscillatory medium. While our discussion revolves around Maxwell’s electromagnetic equations, the methods can be applied to other physical wave phenomena in time-varying media.

This numerical scheme resulted in the development of EMClaw an extension to the Clawpack Software.

An abridge summary of this thesis could be condensed in the following points:

- Developed a novel fabrication and characterization techniques for time-varying materials, and structures for light confinement,

- Presented a novel characterization of the electric properties of $As_2S_3$ chalcogenide glass and

- Demonstrated an electron-induced refractive index increase in $As_2S_3$ chalcogenide glass

- Developed a numerical scheme to model wave phenomena in spacetime-varying media, and

- Created EMClaw, an extension to the Clawpack software, to model spacetime-varying and nonlinear media. EMClaw could be used in other problems beyond the scope of photonics, for example interest to use this package has been raised by communities in plasma and solar physics.

- Devised [PICss] to trap and transform light that could potentially be used as time delays and power portable tomography scanners.
What is next?

Through the course of this thesis ideas were drawn and later abandoned due to many reasons, some depended on external collaborators and other went beyond the scope of this thesis. However, the elements set forth by this work could be apply to the development of some ideas like

• Ultra fast coupling in time-varying waveguide couplers

• Incorporation of dispersion and absorption in the numerical scheme for spacetime-varying materials

• Analysis of chaos in light trapping orbits

• Light in random-time ordered media

• Moving and sudden cloaking in real-like materials, i.e. spacetime-varying cloaks.

• ...
Part V

References and Appendices
REFERENCES


APPENDICES
Riemann Solver

A.1 2D Riemann solver

In this case equation (1.4) takes the form:

$$\bar{\kappa} \partial_t q(x, y, t) + \partial_x f^1(q; x, y, t) + \partial_y f^2(q; x, y, t) = \psi,$$  \hspace{1cm} (A.1)

Because electromagnetic waves are transversal, in two dimensions we can decompose any wave into a polarization basis, habitually called transverse electric, $E$, and magnetic, $M$ modes [4],

$$q_M \equiv \begin{pmatrix} E^1 \\ E^2 \\ H^3 \end{pmatrix}, \quad q_E \equiv \begin{pmatrix} H^1 \\ H^2 \end{pmatrix}. \hspace{1cm} (A.2)$$

If the medium is isotropic and linear, only the diagonal entries of $\bar{\kappa}$ are non-zero, with values $\kappa^{ii} = \eta^i$. Then, expanding the $E$ mode yields:

$$\eta^0 q^0_t + \eta^0 q^0 - q^2_y / \varepsilon_o = 0 \hspace{1cm} (A.3a)$$
$$\eta^1 q^1_t + \eta^1 q^1 + q^2_x \varepsilon_o = 0 \hspace{1cm} (A.3b)$$
$$\eta^2 q^2_t + \eta^2 q^2 + q^1_x \mu_o - q^0_y \mu_o = 0 \hspace{1cm} (A.3c)$$

A similar set of equations can be calculated for $M$ mode. In this particular case the flux functions take the form:

$$f^1 = \begin{pmatrix} 0 \\ q^2 / \varepsilon_o \\ q^1 / \mu_o \end{pmatrix} \quad \text{and} \quad f^2 = \begin{pmatrix} -q^2 / \varepsilon_o \\ 0 \\ -q^0 / \mu_o \end{pmatrix}. \hspace{1cm} (A.4)$$
Then we can calculate the flux Jacobian for each $f^i$ and obtain:

$$A \equiv f_q^1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1/\varepsilon_o \\ 0 & 1/\mu_o & 0 \end{pmatrix} \quad \text{and} \quad B \equiv f_q^2 = \begin{pmatrix} 0 & 0 & -1/\varepsilon_o \\ 0 & 0 & 0 \\ -1/\mu_o & 0 & 0 \end{pmatrix}.$$ \hspace{1cm} (A.5)

Because $AB \neq BA$, there is no single transformation that will simultaneously diagonalize $A$ and $B$. Hence we diagonalize each matrix separately,

$$A = R^x \Lambda^x (R^x)^{-1}, \quad B = R^y \Lambda^y (R^y)^{-1}$$ \hspace{1cm} (A.6)

where $R^i$ is the matrix whose columns are the eigenvectors, $r^{i,p}$, of either $A$ or $B$, and $\Lambda^i$ the diagonal matrix of the corresponding eigenvalues $\lambda^{i,p}$ set in increasing order. The matrix $A$ yield the right eigen-vectors:

$$r^{x,1} = \begin{pmatrix} 0 \\ -z \\ 1 \end{pmatrix}, \quad r^{x,2} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad r^{x,3} = \begin{pmatrix} 0 \\ -z \\ 1 \end{pmatrix}.$$ \hspace{1cm} (A.7)

And matrix $B$ has the right eigen-vectors:

$$r^{x,1} = \begin{pmatrix} -z \\ 0 \\ 1 \end{pmatrix}, \quad r^{x,2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad r^{x,3} = \begin{pmatrix} -z \\ 0 \\ 1 \end{pmatrix}.$$ \hspace{1cm} (A.8)

Either one with eigenvalues:

$$\lambda^{i,1} = -c, \quad \lambda^{i,2} = 0, \quad \lambda^{i,3} = c$$ \hspace{1cm} (A.9)

Where the values $z$ and $c$ are defined as:

$$c = 1/\sqrt{\varepsilon_o \mu_o},$$ \hspace{1cm} (A.10a)

$$z = \frac{\mu_o}{\varepsilon_o}.$$ \hspace{1cm} (A.10b)

Note that the inverse of $z$ is commonly known as the impedance in electromagnetic theory, while $c$ defines the speed of the waves.
From (A.7) and (A.8) we obtain $R^{x,y}$:

$$R^x = \begin{pmatrix} 0 & 1 & 0 \\ -z & 0 & z \\ 1 & 0 & 1 \end{pmatrix} \quad \text{and} \quad R^y = \begin{pmatrix} z & 0 & -z \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad \text{(A.11)}$$

With inverse $(R^{x,y})^{-1}$,

$$(R^x)^{-1} = \begin{pmatrix} 0 & -\frac{1}{2z} & \frac{1}{2} \\ 1 & 0 & 0 \\ 0 & \frac{1}{2z} & \frac{1}{2} \end{pmatrix} \quad \text{and} \quad (R^y)^{-1} = \begin{pmatrix} \frac{1}{2z} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2z} & 0 & \frac{1}{2} \end{pmatrix} \quad \text{(A.12)}$$

Now we can solve for $\beta^{x,y}$ in (??) with $\Delta f^1 = (0, \Delta q^2, \Delta q^1)$ and $\Delta f^1 = (-\Delta q^2, 0, -\Delta q^0)$, to obtain:

$$\beta^{x,1} = \frac{-\Delta f^{1,2} + \Delta f^{1,3}z}{2z} \quad \text{(A.13a)}$$

$$\beta^{x,2} = 0 \quad \text{(A.13b)}$$

$$\beta^{x,3} = \frac{\Delta f^{1,2} + \Delta f^{1,3}z}{2z} \quad \text{(A.13c)}$$

$$\beta^{y,1} = \frac{-\Delta f^{2,1} + \Delta f^{2,3}z}{2z} \quad \text{(A.14a)}$$

$$\beta^{y,2} = 0 \quad \text{(A.14b)}$$

$$\beta^{y,3} = \frac{\Delta f^{2,1} - \Delta f^{2,3}z}{2z} \quad \text{(A.14c)}$$
Simulation Parameters

B.1 Clawpack Simulation parameters

Summary of convergence tests for *maxwell variable coefficients in 1D* \( \text{(emclaw:maxwell_vc_1d)} \),
calculation settings:

Material shape is given by,

\[
n + \delta n \exp \left( -\frac{(x - (v_0 t - x_{\text{offset}}))^2}{\sigma^2} \right)
\]  
(B.1)

Excitation, source, shape is defined by,

\[
q^{0,1} = A_{0,1} \exp \left( -\frac{(x - (-2.0 + v_0 t))^2}{\lambda^2} \right)
\]  
(B.2)
Publications and Conferences

C.1 Journal publications


C.2 Conference articles

*(invited talk)* D. I. Ketcheson and D. P. San-Roman-Alerigi, *High order parallel WENO-wave propagation algorithms for hyperbolic PDEs in three dimensions*, World Congress on Computational Mechanics (WCCM), 2014.


D. P. San-Roman-Alerigi, A. B. Slimane, T. K. Ng, M. Alsunaidi, and B. S. Ooi, *On a pragmatic approach to optical analogues of gravitational attractors*, Photonics Global Conference (PGC), Singapore, December 2012


C.3 Book contributions


C.4 Talks, seminars and presentations


D. P. San-Roman-Alerigi, *Similarities between spacetime geometries and refractive index mappings*, Seminar Series on Quantum and Classical Optics, College of Sciences, National Autonomous University of Mexico (UNAM), Mexico 2012.


C.5 News features

Laser Focus World: 2D refractive-index mapping models cosmological systems. July 2013.

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<td>Wavelength, $\lambda$. It defines the pulse width, i.e. $\sigma$</td>
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<td>$1/bkg_n$</td>
<td>Relative velocity of wave in the medium</td>
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<td>$zo$</td>
<td>Amplitude of electric field, $E \equiv q^0$</td>
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<td>$Hz$</td>
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<td>Amplitude of magnetic field, $H \equiv q^1$</td>
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**Excitation (Source2D)**

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