What microcavities can do in photonics: coupling resonances and optical gain

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Abstract

The present master’s thesis deals with numerical modeling of solid-state micrometrical-sized polymeric dye lasers, commonly denoted as microcavities. It is part of a large research initiative carried out in the optics group, at the MAP (Microelectronics and Applied Physics) department in KTH (Kungliga Tekniska Högskolan - Royal Technical School) and targeted towards the design and manufacturing of micro- and nano-scaled polymeric components for nano-photonics, primarily lasers.

The finite element method (FEM) in frequency domain is used as a primary modeling tool through the simulation software COMSOL Multiphysics©. Models for spontaneous emission, optical losses and gain are developed and demonstrated.

A specific layout is studied: the double hexagonal microcavity. While it was expected to be a good candidate for a laser, the design shows unexpected properties making it useful for sensing applications.

Finally, the transposition of models to time domain is initiated: a replacement solution for the lacking perfectly matched layer (PML) in Comsol is developed and demonstrated. Methods for modeling materials parameters in time domain are investigated, together with the possible use of a more suitable algorithm: finite differences in time domain (FDTD) or Yee’s scheme.
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Introduction

Micrometrical sized optical cavities of various shapes \[1 \ 2\] are increasingly attracting interest for their properties and potential applications as couplers or lasers.

Nowadays fast growing interest for lab-on-chip (LOC) \[3\] and photonic integrated circuits reveals the need for small-sized, cost effective and reliable on-chips light sources. Microcavity lasers being good candidates, the study of their properties is one of the research fields the optics groups takes actively part in \[4\].

Solid-state lasers made of poly(methyl methacrylate) (PMMA) doped with dyes, like, for example, Rhodamine 6G \[5\], are expected to provide nearly monochromatic, highly coherent, and easily tunable lasers at low costs.

The goal of this project is to — starting from previous work accomplished in the group — improve current numerical models and study a particular design, candidate for laser applications, the double hexagonal cavity (Figure 1).

![Figure 1: Sample cavity design studied in this project.](image-url)
Outline

The present work is part of the research done in the optics group. It is nor
a starting point, nor an end. Through those pages, we base ourselves on former
work accomplished in the group, bring some improvements, and introduce new
ideas to be investigated and improved further.

An introduction to physics of microcavity lasers is given in chapter 1 in
order to make reader familiar with the topic. An overview of the tools available
to us follows in chapter 2, where we introduce or re-introduce basic notions of
the finite element method (FEM), and present the software used in the group,
COMSOL Multiphysics©, our main modeling tool.

In chapter 3, we discuss fundamental differences between an optical cavity
and a laser cavity together with their consequences on models. Methods to
calculate cavity modes in general — and in particular for laser cavities — are
developed. Finally, a model for spontaneous emission is introduced.

Chapter 4 introduces a systematic method to represent accurately materi-
als parameters available as experimental data. Optical absorption and gain
are studied in details. An innovative model for optical gain is introduced. A
complete laser model is built and demonstrated on a simple case in order to
highlight its strengths and limitations.

Properties of hexagonal cavities are discussed in chapter 5 and compared to
the more classical circular and rectangular shapes. The double hexagonal cav-
ity, expected to be candidate for a laser, is studied and unexpected properties
are observed.

All simulations so far being carried on in the frequency domain on 2D ge-
ometries, chapter 6 mentions briefly notions of 3D models. Extension to time
domain and consequent problems are discussed in details : a replacement for
the perfectly matched layer (PML) is developed and demonstrated. Notions of
material parameters in time domain are introduced : an overview of auxiliary
differential equations (ADE) and recursive convolution is presented. Finally, a
new algorithm — finite differences in time domain (FDTD) or Yee’s scheme —,
more suitable for time domain than FEM, is introduced.

All the way through this work, we take a very pragmatic point of view :
the ideas behind present formulations, their mathematical expressions and the
approximations done are heavily influenced by the software used, COMSOL
Multiphysics©, by its strengths and limitations as well as by the hardware used
— its amount of memory and computing power. Purely technical details are
kept well hidden when unnecessary, however reader needs to keep in mind that
when talking about a model, what is actually meant is a model solvable with
COMSOL Multiphysics© on the hardware available in the group.
Chapter 1
Physics of Microcavity Lasers

As it is well known from basic optics classes [6], a laser is a device able to generate intense beams of coherent monochromatic light. It is made up of four essential parts: an optical cavity, a gain medium, a pump and an output coupler.

1.1 The right theory of light

Along years, many theories of light were developed, each corresponding to a different level of approximation: ray optics is valid at scales of several meters, beam propagation methods bring satisfactory corrections for scales of a few centimeters, etc... For optics at micro-metric scale, the electromagnetic nature of light needs to be considered.

Both near-field and far-field phenomena, reflection, refraction, diffraction, interference, etc... are taken into account through Maxwell’s equations, provided that we achieve to construct an accurate model corresponding to each material properties.

On the other hand, lasing is a purely quantum phenomenon, which, in order to be described accurately, requires to consider light as a beam of particles: photons. However, a photon-based theory at a the scale of a microcavity would require to consider billions of atoms one by one, a far too complex task.

In this work, we will analyze light propagation in cavities by solving Maxwell’s equations. Quantum nature of light is not modeled directly but considered when required, and consequent effects are translated into larger scale, electromagnetic, phenomena.

1.2 Cavity and Output Coupler

A cavity is any system able to produce reflections of an optical beam, in a way causing interferences within itself. For a given cavity, those interferences
are constructive or destructive depending on the wavelength. Configurations corresponding to constructive interferences are called resonance modes or cavity modes.

Cavity modes are often conveniently represented under the form of a plot, the cavity modes diagram, as on Figure 1.1: a value representative of the resonance — typically the output intensity or the optical energy accumulated within the cavity — is plotted against the free-space wavelength or, equivalently, the frequency.

![Figure 1.1: Representation of cavity modes.](Image)

Often, a measure of the quality of those modes is introduced: the $Q$-factor, defined for oscillatory phenomena as the ratio of energy stored in the cavity over energy dissipated per cycle. Practically, a high $Q$-factor corresponds in the cavity mode diagram (Fig. 1.1) to a peak with high height to width ratio.

**Fresnel’s coefficients**

A cavity is often an empty area surrounded by mirrors, but mirrors are not the only method available to create reflections. Any interface between two media with different refractive indexes causes reflections governed by the Fresnel’s coefficients:

\[
R_s = \frac{\left(n_1 \cos \theta_i - n_2 \sqrt{1 - \left(\frac{n_2}{n_1} \sin \theta_i\right)^2}\right)^2}{n_1 \cos \theta_i + n_2 \sqrt{1 - \left(\frac{n_2}{n_1} \sin \theta_i\right)^2}}, \quad T_s = 1 - R_s, \\
R_p = \frac{\left(n_1 \sqrt{1 - \left(\frac{n_2}{n_1} \sin \theta_i\right)^2} - n_2 \cos \theta_i\right)^2}{n_1 \sqrt{1 - \left(\frac{n_2}{n_1} \sin \theta_i\right)^2} + n_2 \cos \theta_i}, \quad T_p = 1 - R_p,
\]

(1.1)

where $R$ and $T$ are the reflection and transmission coefficients for the interface on Figure 1.2(a). The subscripts $s$ and $p$ denote respectively a perpendicular and an in-plane polarization.

In the case of a semiconductor or polymeric cavity, those coefficients lead to two conceptually very different regimes, yet they result from the same phenomenon (Figure 1.2(b)):

- **Partial reflection**: light reaching the interface with small angles of incidence is partially reflected and partially transmitted. The transmitted part represents a loss for the cavity.
• Total internal reflection (TIR): when the angle of incidence is high, light is reflected without any losses.

Figure 1.2: (a) Optical beam incident on an interface (b) Reflection coefficients for an inner reflection. [7]

Output coupler

The output coupler is a component of the laser — part of the cavity or external to it — which allows us to retrieve light out of the device. It can be a partially reflective mirror, a piece of dielectric material close enough to the cavity to induce optical tunneling, or even just a partially transmissive facet.

The output coupler is not necessary for the laser to operate, but essential to make anything useful out of it.

1.3 Gain medium and Pump

A gain medium is any material able to provide optical amplification.

According to Albert Einstein, light and matter may interact in three ways: absorption, spontaneous emission and stimulated emission (Figure 1.3).

Figure 1.3: Three interactions between light and matter: (a) absorption (b) spontaneous emission (c) stimulated emission. [8]
1.3. **GAIN MEDIUM AND PUMP**

As illustrated, stimulated emission is the phenomenon responsible for optical amplification, but happens notably only if a majority of electrons are on high energy levels: this is an unnatural state of matter called population inversion.

It is now well-known that two levels systems as on Figure 1.3 cannot achieve population inversion. Three and four-levels systems (Figure 1.4) are commonly used in lasers.

![Figure 1.4: Three and four-levels systems suitable for gain media in lasers](image)

The role of the pump is to excite electrons from ground to upper-most level. A fast decay follows and brings electrons to the meta-stable level 2. Stimulated emission occurs between level 2 and ground level in three-levels systems, and between level 2 and 4, followed by a fast decay to ground state, in four-levels systems.

The value of optical gain at each place and moment depends ultimately on the number of electrons on both levels involved in lasing. Population of each level is in return governed by the rate equations:

\[
\frac{\partial N_j}{\partial t} = \sum_i (B_{ij}(N_i - N_j) - A_{ij}N_j),
\]

where \(N_i\) is the number of electrons on levels \(i\), \(B_{ij}\) represents the stimulated transition probability — absorption or stimulated emission — from state \(i\) to \(j\), \(A_{ij}\) the spontaneous transition probability, and \(I\) an optical intensity, pump or incoming beam depending on the transition considered.

Solving the rate equations leads to the value of gain, but requires knowledge of all the \(A\) and \(B\) coefficients.

For dye-based lasers, the ground and upper levels become manifold (Figure 1.5(a)) and solving rate equations becomes illusory. Instead, the medium will often be characterized through experimental measurements of absorption and gain (Figure 1.5(b)).
1.4 Laser operation

Finally, it is interesting to consider how a laser operates, how lasing phenomena arises when all parts of the laser are put together:

1. The first step for lasing is to create a population inversion in the gain medium, initially at rest (Figure 1.6(a)). This is done by turning on the pump.

2. As soon as the pump is activated, some electrons reach high energy levels. Shortly after, photons start to be emitted with random wavelengths, phases and directions through spontaneous emission (Figure 1.6(b)).

3. Those photons initiate stimulated emissions within the material: this is the stage of amplified spontaneous emission (Figure 1.6(c)). Simultaneously, some photons reach cavity borders and are reflected.

4. Due to those reflections, interferences appear within the cavity (Figure 1.6(d)): wavelengths corresponding to cavity modes interfere constructively, others are filtered out.

5. If and only if gain is high enough to compensate losses, cavity modes are amplified further and become laser modes (Figure 1.7). Output intensity increases and gain decreases due to depletion in population inversion until an equilibrium is reached. The laser is fully operational (Figure 1.6(e)).

At each step as well as at steady state, pump permanently re-populates upper levels and spontaneous emission continuously acts (not illustrated on Figure 1.6).

This work focuses mainly on steady state: further, we consider almost exclusively the full operation mode, but the initial steps described here will play an important role.

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1 Reproduced from IO2651, Optics, Sergei Popov.
2 Based on experimental data from [5].
1.4. LASER OPERATION

1 PHYSICS OF MICROCAVITY LASERS

Figure 1.6: Three main steps in laser operation.\(^1\)

Figure 1.7: Schematic representation of major parameters for lasing: cavity modes, gain and losses level \(^8\).

Chapter 2

Modeling methods and Software tools

This chapter introduces or reintroduces basics of the finite element method (FEM), the algorithm extensively used in this work. We focus on fundamental building blocks of the method and do not go deep into its technical details nor practical implementation, extensively covered in [9] and unnecessary for this work. Good knowledge of fundamental ideas and underlying principles is, on the contrary, a sine qua non prerequisite for clear understanding of methods and results presented in following chapters.

We then present the software used in the group: COMSOL Multiphysics©. An overview of its features, formalisms, strengths and limitations is provided since those clearly influenced the turn of this work.

Finally, we cover in details modeling assumptions taken further.

2.1 Galerkin’s method

Boris Galerkin, 1871-1945

Let’s consider the following partial differential equation together with a set of boundary conditions:

$$\begin{align*}
\mathcal{L} u &= f \quad \text{on } \Omega \\
f(u) &= 0 \quad \text{on } \partial \Omega \\
u, f &\in \mathcal{V},
\end{align*}$$

(2.1)

where $\mathcal{L}$ denotes a linear differential operator and $\partial \Omega$ is the boundary of domain $\Omega$. The ensemble $\mathcal{V}$ is the vectorial space of functions defined on $\Omega$ and $f(u) = 0$ represents a set of boundary conditions (BCs) suitable for the problem.

Multiplying equation (2.1) by a function $v \in \mathcal{V}$ and integrating over domain $\Omega$, we get

$$\int (v \mathcal{L} u - v f) d\Omega = 0 \quad \forall v \in \mathcal{V}.$$  

(2.2)
Let \( V_0 \) be a particular subspace of \( V \) such that the ensemble
\[
\{ \phi_i : \phi_i \in V_0 \}
\]
constitutes a complete - but not necessarily orthogonal - basis of \( V_0 \).

Let’s define \( u_0 \in V_0 \) as
\[
u_0 = \sum_j \rho_j \phi_j, \tag{2.3}\]
such that
\[
\int (v \mathcal{L} u_0 - v f) \, d\Omega = 0 \quad \forall v \in V_0. \tag{2.4}\]

Moreover, since this is valid in general for any \( v \in V_0 \), it is valid in particular for \( v \) equal to each of the basis functions \( \phi_i \). Thus
\[
\int \left( \phi_i \mathcal{L} \sum_j \rho_j \phi_j - \phi_i f \right) \, d\Omega = 0 \quad \forall \phi_i \tag{2.5}
\]
or, using linear properties of the operator [10],
\[
\sum_j \rho_j \int \phi_i \mathcal{L} \phi_j \, d\Omega = \int \phi_i f \, d\Omega. \tag{2.6}
\]

Equation (2.6) is the Galerkin’s formula for generation of linear equations: for a subspace \( V_0 \) of finite dimension \( n \) and a given set of \( n \) basis functions \( \phi_i \), this formula provides a systematic scheme to generate the system
\[
A \rho = b, \tag{2.7}
\]
with
\[
A_{i,j} = \int \phi_i \mathcal{L} \phi_j \, d\Omega \quad \text{and} \quad b_i = \int \phi_i f \, d\Omega,
\]
where \( A \) is commonly called the mass matrix and \( b \) the load vector. Solving system (2.7) gives us the coefficients \( \rho_j \) and allows to calculate \( u_0 \).

A meaning needs to be attached to our – so far arbitrary – function \( u_0 \). From equation (2.2), we restrict \( v \) to the subspace \( V_0 \) and (2.4) - (2.2) gives
\[
\int (v \mathcal{R}) \, d\Omega = 0 \quad , \quad \mathcal{R} = \mathcal{L} e \quad , \quad e = u - u_0 \quad \forall v \in V_0, \tag{2.8}
\]
where we just defined the error \( e \) and the residual \( R \).
Equation (2.8) is called the *Galerkin’s orthogonality relation* and should be read as follows: for any function \( v \in V_0 \), the \( v \)-weighted integral of \( R \) in (2.8) vanishes. In terms of vectorial spaces, this means that \( e \) is orthogonal to all functions \( v \) and thus that the error is the minimum possible for the given choice of subspace \( V_0 \).

Galerkin’s method constitutes a powerful tool to approximate a given function by a linear combination of other, known and simpler, functions. It provides at the same time a systematic way of generating a linear system of equations and the certainty that the approximation based on its solution is the best possible in the sense of Galerkin’s orthogonality (2.8) for the given set of functions.

### 2.2 The choice of Basis Functions

We already introduced the word *finite* when derivating the linear system (2.7), this section introduces the notion of *elements* and *mesh*.

We now consider the simplistic case of a scalar equation in 1D on the domain \([0, 1]\) with our linear differential operator \( L \) being the identity operator:

\[
    u = f(x). \tag{2.9}
\]

Let’s apply Galerkin’s method with basis functions defined as

\[
    \phi_k(x) = e^{-2ik\pi x} \quad k = 0, \pm 1, \cdots, \pm n. \tag{2.10}
\]

The Galerkin’s approximated solution resulting from (2.4) and (2.7) is

\[
    u_0(x) = \sum_{k=-n}^{n} \rho_k e^{-2ik\pi x}, \tag{2.11}
\]

which is a truncated discrete Fourier transform of \( f \).

Choosing our basis functions to be the polynomials

\[
    \phi_k(x) = x^k \quad k = 0, 1, \cdots, n \tag{2.12}
\]

gives

\[
    u_0(x) = \sum_{k=0}^{n} \rho_k x^k, \tag{2.13}
\]

the well known Taylor serie around 0 limited to \( n \) terms.

---

Footnote 1: This requires to show that the expression of the \( A_{i,j} \) terms in equation (2.7) is a scalar product. The proof [9] is equation dependent and puts restrictions on problems solvable by FEM.
Two choices of basis functions lead to totally different but fundamental tools of modern mathematics. Those examples illustrate how important is this choice. The whole FEM is nothing else than Galerkin’s method applied with a particular set of basis functions.

A canonical choice is to consider $P_1^h$ defined as the subspace of piece-wise linear functions associated to the computational grid $h$, and to take for basis the so called *hat functions*. A visual definition of those is given on Fig. 2.1(a): the $k^{th}$ hat functions is associated to the node $x_k$ and differs from zero only on the segments $[x_{k-1}, x_k]$ and $[x_k, x_{k+1}]$. Such functions are said to have a compact support.

Compact support is the key of the algorithm: back to the system of equations (2.7), the matrix elements $A_{ij}$ become

$$A_{ij} = \begin{cases} \int_{x_{i-1}}^{x_{i+1}} \phi_i \mathcal{L} \phi_j \, dx & \text{if } i = j, j + 1, j - 1 \\ 0 & \text{otherwise} \end{cases}.$$  

(2.14)

This leads to a sparse system of equations: a numerically remarkable property, saving a lot of storage space and computational efforts.

Applying the method to the simplistic equation (2.9) gives us a linear approximation to $f$, as illustrated on figure 2.1(b).

![Figure 2.1](image)

Figure 2.1: (a) Hat functions (blue), typical basis of $P_1^h$ in 1D and a linear combination of them (red). (b) The same linear combination is a linear approximation to the function in blue.

Those notions can be easily generalized to problems in 2 or 3 dimensions. There, one introduces the notion of mesh, which is a convenient visual representation of the basis functions set. Nodes of a mesh represent centers of basis functions and elements represent overlapping areas subject to integration in terms of (2.14). A plot of a hat function on a mesh for a 2D case is given on Figure 2.2.
In practice, hat-functions are seldom used in favor of more complex shapes and piece-wise polynomials of higher orders. Many types of basis functions exist. The optimal choice of a particular form is a science in itself, it is both problem and implementation dependent. Often, this choice is made at programmer side rather than by the final user.

What is left to the user is the choice of mesh. Choosing the mesh means choosing a set of basis functions. Since, on a given mesh, Galerkin’s orthogonality relation ensures that the computed solution is the most accurate possible, improving the solution can only be done by a better choice of mesh.

2.3 Meshing

Meshing is the process of choosing basis functions, often done by drawing a set of elements on top of a geometry. How exactly the mesh affects a solution is very difficult to analyze in general. More and smaller elements are very likely to produce a more accurate solution, but will also increase memory consumption and solution time. Fortunately, reasonably good results can be obtained applying a few simple rules of thumb:

(a) *Mesh should be fine enough to fairly represent the geometry:* obviously, trying to represent a circle with six triangles will produce bad results! In particular, sharp corners often need particular attention.

(b) *Put more elements where solutions varies a lot.* This can be intuitively understood by considering the approximation in Figure 2.1(b) and might be a serious problem when user has a priori absolutely no idea of how the solution looks like. Intelligent meshing algorithms exist for such cases: those have the ability to interactively refine the mesh where needed, at the cost of lower performances.

However, for problems in electromagnetic propagation, one has an a priori estimate of a typical solution’s variation length: the wavelength. The

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1Illustration by Werner Scholz, Vienna University of Technology, reproduced from http://magnet.atp.tuwien.ac.at/scholz/
rule of thumb for the elements size $h$ is:

$$h \leq \frac{\lambda_0}{6 \times n},$$

with $\lambda_0$ the free-space wavelength and $n$ the local refractive index.

Underlying ideas in this rule are the same as for Shannon’s sampling theorem: just like there is an upper limit on the frequency of a signal representable by a set of temporal samples, there is a lower limit on the wavelength representable on a given mesh.

Note that relation (2.15) is a hard limit on $h$ which will produce rough results. When some accuracy is required, one will probably choose

$$h \simeq \frac{\lambda_0}{8 \times n} \quad \text{or} \quad h \simeq \frac{\lambda_0}{10 \times n}.$$ (2.16)

(c) *Avoid deformed elements as much as possible*: this comes from numerical problems arising during integrations of (2.14): the integration is usually performed on a reference element by mapping of the coordinate system. For highly deformed elements, the Jacobian brought into play by this mapping might amplify dramatically tiniest numerical errors.

The amount of deformation of each element is commonly measured by the element quality. There exist many ways of defining this quantity, details on how this is done in [Comsol](https://www.comsol.com) can be found in the documentation together with corresponding lower limits.

In practice, dealing with elements quality in [Comsol](https://www.comsol.com) is a fake problem. The meshing algorithm, one of the strengths of this software, takes care of elements shapes entirely and — unless an especially designed pathological case is used — always manages to achieve high quality results transparently, reducing the mesh quality step to a simple and quick check.

### 2.4 Overview of COMSOL Multiphysics©

COMSOL Multiphysics© (formely FEMLab) is a general purpose finite element solver initially based on the work of Germund Dahlquist (January 16, 1925 Uppsala - February 8, 2005 Stockholm), formely student and later professor at [KTH](https://www.kth.se). [Comsol](https://www.comsol.com)’s core is built upon a set of high performance solvers together with modules implementing main equations of physics and providing a convenient way of defining problems through physically meaningful parameters. Each parameter may be a constant or a function of any variables available in the model.

The software comes with a graphical user interface (GUI) providing a convenient way to define geometry, physics and mesh, as well as with powerful [Comsol](https://www.comsol.com) documentation unreasonably relaxes this limit to $\lambda/5$, probably in order to boost performances.
post-processing tools. A text-based interface makes it possible to run simple
scripts for automation of tasks.

Finally, the software features the ability to interface itself with the popular
technical computing software Matlab®. The interfacing works both ways: Matlab® receives a toolbox making it possible to use Comsol’s solvers and post-
processing tools within a Matlab script file (M-file), and reversely — probably
the most interesting — problem parameters may be defined using any available
Matlab function or script.

Practically, every time the solver comes across a parameter defined as a
script or function, the corresponding M-file is executed in Matlab® and the
result is sent back to the solver. This ability to interact with the solver through
scripts of virtually unlimited complexity makes Comsol extremely handy and
powerful.

Note on non-linear solvers

In our introduction to FEM, we talked only about cases with linear differen-
tial operators and we silently used their properties to establish the algorithm.
This does not come from a simplification: FEM works only for linear differential
equations.

This may seem to be a severe limitation since non-linearities are common in
many problems. For such cases, a pretty straightforward solution exists, based
on the following: a non-linear differential equation is nothing else than a linear
differential equation whose differential operator is solution-dependent:

\[ \mathcal{D}(u) = f \iff \mathcal{L}u = f. \]

Non-linear problems are then handled by numerical schemes solving iter-
atively linearized equations: first the scheme chooses an initial guess \( u_0 \), evaluates
\( \mathcal{L}u_0 \) and solves the problem for this operator to obtain a solution \( u_1 \). Information
from \( u_1 \) is used to build a new guess \( u'_1 \) and so on. The process is stopped
when \( u_i \) and \( u_{i+1} \) are sufficiently close, and the problem is considered as solved.

Nothing however guarantees that this solution is unique nor that the itera-
tion will at all converge.

Note on time-dependent solvers

Similarly to non-linear problems, initial-value time dependent problems are
solved by transforming them into an iterative scheme called time stepping.

An equation of the type

\[ \partial_t u + \mathcal{L}u = f \]

is transformed into

\[ (\mathcal{L} + 1)u(t + \Delta t) = \Delta t f + u(t). \]  

Starting from an initial state \( u(0) \), the solution can be calculated at any \( t \)
by iteratively solving equation (2.19). Here, we restricted ourselves to a linear
differential operator, but non-linear time dependent problems can be solved as
well, simply by calling a non-linear solver at each time step.
2.5 The RF module

The RF module is the tool in Comsol which deals with electromagnetic propagation: all our models will be based on it. Within this module, several modes are available for various types of problems. The relevant ones for this work are:

- **In-Plane transverse electric (TE) Waves**: Analyzes propagations in a plane with the assumption that the electric field is perpendicular to the considered surface (Figure 2.3(a)).

- **In-Plane transverse magnetic (TM) Waves**: Similar, but here magnetic field is assumed to be perpendicular to the plane (Figure 2.3(b)).

- **In-Plane Hybrid Waves**: In-plane propagation with no assumption on the polarization of fields (Figure 2.3(c)).

- **Electromagnetic Waves**: Volume propagation of electromagnetic field with no assumptions on polarization.

Additionally, for each mode, four different formalism are available:

- **Harmonic propagation**: Performs calculations in frequency domain, fields components are phasors.

- **Eigenfrequency analysis**: Aimed towards quick analysis of resonance modes.

- **Transient analysis**: Performs calculations in time domain.

- **Scattered harmonic propagation**: Separates fields into two unphysical parts: the incident and scattered fields. Calculations are performed in frequency domain for scattered fields only. Aimed towards specific types of problems.

Beside this, the module supplies an interface to define problem directly through physical parameters like refractive index, free space wavelength, conductivity, etc., as well as a set of pre-defined and easy accessible quantities like power flow, energy density, electric potential, etc...
Post-processing tools

Comsol comes with a set of powerful post-processing tools which let user easily measure any pre-defined physical quantities as well as any combination of them.

Different types of probes are available:

- **Point probes**: Those allow to get the value of any physical quantities anywhere in the system. This concept is mainly used in the form of a plot of the spatial distribution of that quantity, which gives us a qualitative idea of the physical situation in the model.

- **Boundary integration**: Integrates any quantity over one or several segments of the model. In particular, boundary integration of the energy flow corresponds to an intensity detector, with the addition that this numerical detector can take any shapes and sizes and does not disturb the field in its surrounding.

- **Domain integration**: Integrates any quantity over one or several domains. An important quantity of this type is the energy density integral which gives the amount of energy stored in a cavity. Note that quantities of this type of can seldom be measured directly in practice.

Moreover, when those tools are not sufficient, the entire solution can be conveniently exported to Matlab for more advanced or automated post-processing.

### 2.6 Modeling assumptions in this work

The present work is aimed towards analysis of micro-cavities properties in frequency domain. Most of the modeling is done using the in-Plane TE waves harmonic propagation. An overview of its formalism, assumptions and their consequences is thus required.

**Harmonic formalism**

In harmonic formalism, fields are represented in terms of phasors. The phasor $\hat{A}$ representing the quantity

$$A(t) = A_0 \cos(\omega t + \phi)$$

(2.20)

is

$$\hat{A} = A_0 e^{i\phi}$$

(2.21)

and is related to $A(t)$ through

$$A(t) = \text{Re}\left\{A_0 e^{i(\omega t + \phi)}\right\} = \text{Re}\left\{\hat{A} e^{i\omega t}\right\}.$$  

(2.22)
Note that this is equivalent to the Fourier transform $A(t) \rightarrow \hat{A}(\omega)$. Consequently, the associated derivation and integration theorems hold:

if 

$$f(t) \rightarrow F(\omega),$$

then 

$$\partial_t f(t) \rightarrow i\omega F(\omega),$$

(2.23)

$$\int f(t) \, dt \rightarrow \frac{-i}{\omega} F(\omega).$$

(2.24)

The biggest benefit is the subsequent simplification of equations: partial differential equations in space and time become partial in space only. This removes the necessity of time stepping in the solving process.

The restrictions introduced by harmonic formalism are:

• Only quantities of the type of equation (2.20) can be represented.

• The simulation is narrow-band: only a single frequency — or equivalently, a single wavelength — can be simulated at a time.

As a result, only steady-state behaviors can be obtained this way and the solution to our problems will often be presented under the form of a frequency response.

All this is however true only for linear oscillators — a fundamental assumption silently taken when introducing phasors formalism as a Fourier transform. Harmonic mode cannot model interactions between phenomena occurring at different frequencies. In particular, it cannot model directly an optical pump in a laser.

2D assumptions

In 2D, we consider a geometry defined in the $xy$-plane only, with an assumption of translation symmetry along the third axis. According to this statement, what is really simulated depends on the reference system.

In most cases, the reference system is cartesian and the considered 2D plane represents a slice of an infinitely long geometry along $z$-axis (Figure 2.4(a)). Choosing a reference system with cylindrical coordinates leads to simulate a volume as on Figure 2.4(b) which may or may not be what is expected.
In this work, we will use only cartesian systems. Our calculations are thus carried on under the assumption of no variations along the $z$-axis, meaning that effects of top and bottom interfaces of the cavity are totally omitted. The solutions calculated that way are valid if and only if those surface effects are negligible.

In reality, this last assumption is probably wrong when accuracy counts. However, one may reasonably expect that surface effects will not change radically the qualitative behavior. Obviously, this assumption — like any modeling assumption — needs to be checked against experimental results.

Finally, every quantity calculated this way is expressed \textit{per unit of thickness}. Thus, for example, the unit of an electric field in 2D is $V/m^2$, unit of an energy is $J/m$, unit of volume becomes $m^3/m$, etc...

Equation system

In the present mode, the equation system presented in the GUI is

$$
\nabla \times \left( \frac{1}{\mu_r} \nabla \times \mathbf{E} \right) - \left( \varepsilon_r - \frac{i\sigma}{\omega \varepsilon_0} k_0^2 \mathbf{E} \right) = 0,
$$

$$
\mathbf{E} = E_z \mathbf{e}_z,
$$

$$
\varepsilon = n^2,
$$

with the ability to define $\varepsilon_r$, $\mu_r$ and $\sigma$ independently, or to specify only $n$, taking automatically $\sigma = 0$ and $\mu_r = 1$.

However, this is just a user interface. The equation which is actually solved is

$$
\nabla \cdot \left( -c \nabla E_z - \alpha E_z + \gamma \right) + aE_z + \beta \cdot \nabla E_z = f,
$$

called the coefficient form.

Coefficients in equation (2.26) are by default automatically calculated from the problem definition and equation (2.25). It is also possible to specify manually one or several of those, the automatic calculation being then overridden.
2.7 Modeling tools in the 2D TE harmonic mode.

A broad set of tools to define the physics of the problem is available within the RF module. Some of those tools are common to all modes, some are more specific. We detail here only the most important one available under 2D TE.

Similarly to post-processing, those tools come in three families:

- **Point properties**: Each point in the geometry can be associated to a current, turning it into a source of cylindrical waves. Defining such a source of electric field through a current may seems surprising at first.

  A pseudo-physical interpretation may be given as follows: due to hypothesis taken for 2D representation, a point represent in real space a line perpendicular to the plane - thus a infinitely thin wire. Such a wire sustaining an oscillating current generates an oscillating magnetic field, which in return generates an oscillating electric field. A more rigorous interpretation of this notion will be given in section 3.4.2.

- **Boundary properties**: Several types of boundaries may be defined

  - *Electric field and Perfect electric conductor*: Those correspond respectively to a non-homogeneous and homogeneous Dirichlet’s BC - i.e. the electric field is constrained at the boundary to a certain value or to zero. From a physical point of view, those BCs are 100% reflective.

    *Magnetic field and Perfect magnetic conductor* are similar but constrains the magnetic field. Their behavior is also reflective, but with a different phase shift.

  - *Surface current*: This is similar to the notion of point sources, the current in the wire now becomes a current density in a plane. It may be used as a source similarly to the *Electric field condition* except that it is transparent for an incoming field while used on an interior boundary (it is also reflective while specified on a domain boundary).

  - *Scattering boundary condition, Matched boundary, Impedance boundary condition*: those are semi-transparent BCs - i.e. transparent in some cases, reflective in others.

    For example, the *Scattering boundary condition* is defined as follows

    “The Scattering boundary condition is transparent for the scattered electric field. It is also transparent for a plane wave.”

    The distinction between a scattered field and a total field is well-defined only for a scattered harmonic solution. In other modes, a
non-plane wave — or even a plane wave with non-normal incident — hitting this boundary results, in some cases, in a reflection of up to 50% in terms of electric field.

While those boundaries are useful in specific cases, they should not be used as general purpose absorbing boundary conditions.

- Port and Periodicity: Designed for very specific uses. Port is used for analysis of coupling between several inputs and outputs in a system. Periodicity models infinitely periodic structures like crystals.

- Domain properties: Different domains represent different materials, thus each domain is associated to a set of material parameters: relative electric permittivity $\varepsilon_r$, relative magnetic permeability $\mu_r$ and electric conductivity $\sigma$, directly or through refractive index $n$.

A special type of domains is the perfectly matched layer (PML). A PML is an artificial material which shows the ability to damp any incoming wave without causing any reflection. PMLs are often placed around a domain like on Figure 2.5 and used as an absorbing pseudo boundary condition in order to truncate and simulate a part of an infinitely large area. Note that a boundary around the surrounding layer is still needed since PMLs are domains and not boundaries, but its role is not significant.

Figure 2.5: perfectly matched layers used as absorbing boundaries around the domain of interest (red).

An optimal PML should be made of 6 to 12 elements along the absorbing direction, the physical thickness is not important in itself. A good practice is to draw this layer with a thickness more or less equal to the wavelength of the problem. Consecutive meshing using the rule of thumb from equation 2.15, just like for any other areas in the model, gives back this optimality.

---

2 This is only true with some restrictions: like any material, a PML has material parameters and a refractive index. At a material-PML interface, a mismatch of those does produce partial reflection in agreement with Fresnel’s coefficients.
2.7. MODELING TOOLS IN 2D TE HARMONIC 2 MODELING METHODS & TOOLS
Chapter 3

Cavity Modes Calculation

When modeling a complete optical circuit or a part of it, one can usually determine pretty easily inputs and outputs in the system, sources which generate light and places where this light leaves the system.

Similarly, when modeling a cavity as part of a circuit, one considers this circuit as a whole and identifies sources, paths and outputs. Boundary conditions and excitations can then be set up to mimic the effect of the non-modelled optical circuit.

In order to illustrate this, we consider on Figure 3.1 a ring resonator used as a coupler between two optical fibers. The optical source and detectors lie outside of the domain considered here, but we know where they are and how they work. With this information, it is then easy to choose a set of BCs and optical excitations which will mimic the effect of the omitted areas.

![Figure 3.1: Ring resonator used as coupler in an optical circuit. The dashed lines represent part of the circuit which are not modeled, but whose information is used to build relevant boundary conditions and excitations.](image-url)
Once the problem is defined this way, one can solve it for a set of wavelengths, obtain the field distribution everywhere in the area of interest and calculate any subsequent electromagnetic quantities. The relevant quantity in this problem is the throughput as a function of wavelength (Figure 3.2). In the present case, it is widely known the last is mainly dependent on the geometry of the ring: we thus conclude that it is an intrinsic property of this element.

Figure 3.2: Throughput for the coupler on Figure 3.1

3.1 Cavity Modes

As mentioned previously (chapter 1), the cavity is one of the building blocks of a laser, as well as the central component of previous example. Knowledge of cavity modes is thus essential in many cases, just like knowledge of the throughput is essential in the example above.

3.1.1 Direct calculations

*Comsol* eigen frequency analysis tool is precisely designed for calculation of those resonance modes. This tool provides very efficiently resonance frequencies of the cavity as well as all possible field distributions corresponding to each of those frequencies.

However, this tool is mainly oriented towards analysis of wave-guides cross-sections [11], and consequently shows severe limitations. The most notable one is a total incompatibility with PMLs. Other semi-transparent BCs happen to be by far insufficient to produce any reliable results.

In practice, it turns out that our only option to model a cavity is to use a perfect electric conductor (PEC) for cavity boundaries. A typical result obtained using this method is shown on Figure 3.3: the solver provides a discrete set of wavelengths corresponding to resonance modes (Fig. 3.3(a)) and, for each of those wavelengths, one or several field distributions in the cavity (Fig. 3.3(b) and 3.3(c))

---

1. Throughput is defined as the ratio of power flows at locations of the domain *arbitrarily* chosen as input and output.
2. For a classical laser cavity, a resonance frequency corresponds to a longitudinal mode and associated field distributions correspond to transversal modes.
3. A typical result is that the modes obtained this way are dependent on the size of the free-space area considered in the model, an obviously non physical result.
3 CAVITY MODES

3.2 MEASUREMENT TOOLS

Figure 3.3: (a) Resonance modes of a rectangular cavity made of perfectly reflective mirrors, calculated using the *eigen frequency analysis* tool. (b)-(c) Example of electric field distributions in the cavity as obtained using the *eigen frequency analysis* solver.

If this approximation may hold for a cavity made of mirrors, its physical meaningfulness vanishes for an air-glass or air-[PMMA] interface. Due to these limitations, the tool happens to be simple unusable for the present problem and we need to take a radically different approach.

3.1.2 Calculation by spectral sweeping

Let’s consider the experimental process of finding cavity modes: the experimenter would send a monochromatic beam towards the cavity and measure the intensity at one or several outputs. Tuning the wavelength of the source, the operation is repeated until the whole spectrum is scanned.

We will thus simple transpose this experiment into the numerical model. We actually already did this silently in the introductory example of this chapter.

This leaves us with the problem of choosing what type of source to use, where to put it and what to measure. Unlike in a laboratory, numerical probes do not suffer from practical limitations and the range of what can be done is much wider, making this choice even more important.

3.2 Choice of a measurement tools

Among the available numerical probes, two are useful in the present case:

- Integral of energy flow over a boundary: this corresponds to intensity detection. It is the method used in the ring resonator example. This technique is particularly helpful when one can clearly define an output in the model — i.e. a location in the system where intensity is what we are interested in. This output may be the output coupler for a laser, but is undefined when considering a cavity independently of its surrounding.
• Integral of energy density over the cavity: this is a measure of the amount of energy stored inside the cavity, a notion introduced with the $Q$-factor in section 1.2. This quantity cannot be measured directly experimentally. However, it is maybe a more accurate indicator than intensity since it considers the cavity itself and only the cavity: we do not define an arbitrary output.

   This does not mean that this quantity is independent of the output. Changing an output physically affects field distributions and thus total energy. It is independent of the choice of output - i.e. independent of which segment in the geometry is arbitrarily labeled as output. This is particularly helpful when such an output is not clearly defined.

   Yet different, both notions are closely related: the internal resonance of the cavity directly affects the output.

Integration of energy density over the whole cavity provides a direct insight through a single scalar quantity on what is happening inside a cavity - a really valuable tool which we will use extensively. However, energy stored in a cavity is seldom the quantity we are eventually interested in: what we see and measure is always an intensity. It is a convenient first indicator for cases where one does not know yet how and where exactly to define an output in the numerical problem. A fortiori, it is a good indicator when considering a cavity independently.

3.3 Intrinsic and Calculated properties

Let’s consider a simplistic rectangular cavity of size $L \times l$ made of a material with uniform refractive index, $n = 2$. The cavity is placed in free-space. We now consider the problem of calculating its resonance modes.

We choose as measurement tool the energy density integral as described in previous section. We excite the system using different methods: a plane wave incoming along $x$-axis, $y$-axis and with an incidence angle of $45^\circ$, as well as 4 excitation points placed as on Figure 3.3. For a set of wavelengths $\lambda$, we integrate the energy density over the cavity volume and plot the result as a function of $\lambda$ on Figure 3.5. Electric field distributions at a sample resonance frequency for different excitations are shown on Figure 3.6.

![Figure 3.4: Rectangular cavity with PML and the 4 excitation points.](image)
A direct result is that the calculated modes diagrams and electric field distributions do depend on our choice of excitation. What we compute here are not the intrinsic modes, property of the cavity, but a set of them weighted by how efficiently the chosen excitation can activate a given mode.

More intuitively: a plane wave traveling along \( x \)-axis can hardly put the cavity in a resonance mode like on Figure 3.6(b) or 3.6(e) without serious violation of symmetry.

Figure 3.6(g) shows a field distribution similar to what we obtained in Figure 3.3(c) using the eigen frequency analysis tool, which also corresponds to the highest energy in Figure 3.5 and the closest to what one intuitively expects. Unfortunately, nothing allows us to tell that this is the right mode nor to know in advance which excitation will produce this result.

Consequently, we cannot really calculate cavity modes as a intrinsic property of the cavity. The best result one can get is that for that particular excitation, the cavity resonates this way at this particular set of wavelengths. We need to put aside the idea of calculating modes of a cavity independently and always consider it as part of a broader system.

Note that this may only be a practical impossibility: it is unknown if there exists solvers able to do the type of calculation from section 3.1.1 for any kinds of cavities together with PMLs. The present implementation cannot.
3.4 Excitation in a Laser cavity

The case of a laser cavity is particular: it constitutes a whole optical system in itself. The outputs are optical losses — output intensity can be regarded as a loss for the cavity. The source of optical excitation is spontaneous emission: a source of completely incoherent light coming from within the material of the cavity. A realistic model for a laser needs to take this into account.

3.4.1 Random excitation points

A first natural attempt to model this spontaneous emission is to randomly distribute a certain number of points inside the cavity and use them as point-sources. Physically, those points represent atoms or molecules involved in the spontaneous emission.

One may reasonably expect that for an important number of point-sources the solution will be stable with regard to points distribution. We also hope that this excitation will be able to excite if not all modes, at least all of those involved in lasing. Nothing can however guarantee this.

In principle, the method described above works but requires in a realistic case several hundreds to a few thousands points.
While applying the FEM, comes a technical problem: each point-source in the model becomes a node of the mesh. This is illustrated on Figure 3.7. As a result, hundreds or thousands additional points in the model will generate an unreasonable number of additional mesh elements, leading to huge increase of memory consumption and blowup of computing time.

Figure 3.7: Illustrates how additional points constrain the mesh.

3.4.2 Excitation as a continuous source term

We now propose a new formulation for our point-sources which does not suffer from this meshing problem. The tool developed here happens to be much more general, giving us the ability to describe any arbitrary source.

The method is shown for the 2D TE harmonic mode in Comsol. It can be transposed to any other modes of the software, but requires specific analytic treatment for each case.

As described in section 2.6, Comsol is solving the following equation

$$\nabla \cdot \left( -c \nabla E_z - \alpha E_z + \gamma \right) + a E_z + \beta \cdot \nabla E_z = f.$$  \hspace{1cm} (3.1)

A more careful analysis of the right hand side (RHS) shows that

$$f = j \omega \mu_\epsilon \mu_0 J^f_z, \quad \omega = \frac{2\pi c_0}{\lambda_0},$$

where $\lambda_0$ is the free-space wavelength and $J^f_z$ has the dimensions of a density of current.

Taking $J^f_z$ as a function of coordinates, one can describe a coordinate dependent source in the domain. In particular, taking

$$J^f_z(x, y) = I_0 \delta(x - x_0, y - y_0),$$  \hspace{1cm} (3.2)

\textsuperscript{1}The reason behind this is the way the numerical integrations are performed on elements during matrices assembly: only the nodes are guaranteed to be evaluated, and are thus the only points where it make sense to use discrete source terms.

\textsuperscript{2}The proof is based on rewriting Maxwell’s equations in the form of Equation (3.1). The mathematical derivation is given in appendix A and the result is confirmed to comply with implementation [12].
3.4. EXCITATION IN A LASER CAVITY

where $\delta(x,y)$ is the two dimensional Dirac’s delta function, $J_z^f$ corresponds to a point-source at the point $(x_0, y_0)$.

It is important to note that the source term $f$ corresponds to a source of electric field. The fact that we express it through an auxiliary current density is a consequence of the form of equation (3.1). One should not try to give any kind of physical meaning to $J_z^f$ : it is not necessarily a physical density of current, it is an auxiliary quantity with the dimensions of a density of current used to conveniently - i.e. independently of the wavelength - describe a source of electric field.

Similarly, equation (3.2) allows us to give a more rigorous interpretation to the point-source described in section 2.7 : the current associated to a point does not need to correspond to a physical current crossing the plane. It is an auxiliary variable which describes a point source of electric field independently of other quantities, like $\lambda_0$.

$J_z^f$ has been introduced as a function of coordinates, but it can be extended, like any other variable in Comsol, to a function of wavelength, electric field, etc... as well as to a script. The last allows us to model any source we want and makes this auxiliary current density a valuable tool.

Following the ideas introduced in section 3.4.1, we can now represent a virtually unlimited number of points without affecting the mesh, and without subsequent performance and memory issues. A set of point-sources located at coordinates $(x_k, y_k)$ with intensity $I_k$ may be simply represented by

$$J_z^f(x, y) = \sum_k I_k \delta(x - x_k, y - y_k).$$

(3.3)

While such a function is mathematically correct, it is undesirable in Comsol. Going through the FEM algorithm, equation (3.1) is integrated numerically – i.e. using a finite number of discrete points. Nothing guarantees that the integration points chosen by the algorithm will corresponds to the points $(x_k, y_k)$, unless those are nodes of the mesh, which brings us back to the initial problem.

The workaround is to replace $\delta$-peaks from equation (3.3) by some other, spatially wider, functions. Gaussian functions are good candidates tough many other functions would suit as well.

Our source term becomes

$$J_z^f(x, y) = \sum_k \frac{I_k}{w\sqrt{\pi}} e^{\frac{(x-x_k)^2 + (y-y_k)^2}{w^2}}.$$  

(3.4)

The limit for $w \rightarrow 0$ gives equation (3.3) back. In practice, $w$ must be taken big enough to make sure each gaussian will be integrated with sufficient accuracy, and small enough not to loose completely the meaning of a point-sources.

The optimal value for $w$ can be determined by a simple test : since our aim is to mimic points using gaussian functions, we build the very simple problem shown on Figure 3.8(a) where we consider a single point source in free-space.
We calculate the solution once using a geometrical point-source and keep it as a reference. We then change the source to be a gaussian with variable width. The problem is solved again, and the solution is compared to the reference. Error is measured by \( \frac{||E_{\text{ref}} - E_{\text{Gauss}}||}{||E_{\text{ref}}||} \) and the resulting plot is shown on Figure 3.8(b).

Figure 3.8: (a) Test problem used to find optimal width \( w \): single point source in free-space. (b) Relative error on norm of electric field with respect to gaussian width \( w \) for three different wavelengths. All lengths in units of mesh size.

In order to mimic a point-source with a gaussian, its optimal width \( w \) should be taken approximately equal to 4% of the mesh size. Any value between 3 and 10% of mesh size will produce acceptable result (less than 1% relative error on norm of solution). Note that the error is only weakly dependent on the wavelength considered, the key parameter here being mesh size.

### 3.5 A model for Spontaneous emission

Back to section 3.4.1, we tried to describe spontaneous emission by a set of point-sources randomly distributed. We now have an efficient tool able to represent many point-like sources without affecting much memory and solution time. Spontaneous emission being completely random, not only in positions of sources, one may want more randomness in the model.

Formalism of harmonic calculations doesn’t allow to represent randomness over time: sources may be described only as steady-state sinusoidal oscillators with an identical frequency. We can however randomize intensity and phase of each point-like source.

Random intensities tend to cause normalization problems in practice. The random phase term showed little influence: we include it here in order to be more coherent with physics and keep in mind that it can safely be omitted for simplicity and performances.
3.5. A MODEL FOR SPONTANEOUS EMISSION

The proposed model for spontaneous emission is:

\[ J_z (x, y) = \sum_{k=0}^{N} \frac{I_0}{N w \sqrt{\pi}} e^{\frac{(x-x_k)^2+(y-y_k)^2}{w^2}} e^{i \phi_k}, \]  

(3.5)

with

- \( I_0 \) : an arbitrary current density.
- \( w \) : chosen to be around 4% of the mesh size.
- \((x_k, y_k)\) : randomly chosen coordinates of points within the cavity.
- \( \phi_k \) : represents the phase for the corresponding point-like sources, chosen randomly in \([0, 2\pi]\).
- \( N \) : number of point-like sources used. This is a critical and problem dependent parameter.

A visual representation of such a source term is provided on Figure 3.9.

![Figure 3.9](image)

Figure 3.9: (a) Representation of the source term \( J_z \) used to model spontaneous emission. (b) Zoom on a small area of (a).

The parameter \( N \) needs to be adjusted such that the solution — i.e. the set of resonance frequencies and field distributions at resonance — is sufficiently stable with regard to random parameters. Increasing the parameter \( N \) improves the solutions to a certain point only. This can be seen on Figure 3.10: from 50 to 500 point-like sources, the solutions improves, however, the leap from 500 to 5000 does not bring significative improvements, and even worsen the solution.

A plot of the electric field at resonance for two different distributions of 500 point-like sources is shown on Figure 3.11.
Conclusions

Our discussion about calculations of cavity modes lead to one important and unfortunate conclusion: based on the tools available to us, we cannot really calculate modes as an intrinsic property of the cavity and what can be calculated shows a high dependence on user’s choice of initial excitation.

For the case of a laser cavity, physical considerations lead us to the excitation built on the idea of random points. Performance considerations lead us to the continuous source term formalism based on the auxiliary current density.

The consequent model for spontaneous emission is able to provide approximate values for resonance frequencies as well as approximate field distributions. This may be enough for a first qualitative approach, but it definitely fails to gives reliable quantitative results.

Representing atoms randomly emitting photons by a set of sinusoidal oscillators generating cylindrical waves is probably not a very accurate description. So far, excitation sources were limited to points and segments. The continuous source term allows to represent virtually any source – within the limit of the underlying mathematical formalism. Radically new ideas may now be tried.
Chapter 4

Modeling of materials properties

In this chapter, implementation of materials properties into Comsol models is discussed. It is a continuation of previous work done in the group, in particular in [13], where quantitative models for dispersion and losses were developed and demonstrated.

We do not redevelop those models but rather build a more general method for implementing those. We demonstrate a systematic way to integrate efficiently any frequency dependent parameter in a model. We then develop a new model for optical gain and demonstrate its strengths and weaknesses.

4.1 Three fundamental parameters

Light being an electromagnetic radiation, its behavior is governed by Maxwell’s equations. Those are, in frequency domain and with no free charges,

\begin{align}
\nabla \cdot D &= 0, \\
\nabla \cdot B &= 0, \\
\nabla \times E &= -j\omega B, \\
\nabla \times H &= J + j\omega D. 
\end{align}

Maxwell’s equations are valid anywhere, anytime, but do not constitute a well-defined system. In order to extract any meaning from them, three more equations are needed:

\begin{align}
D &= \varepsilon E, \\
B &= \mu H, \\
J &= \sigma E. 
\end{align}

Those are the constitutive equations, are specific to a material, and characterize completely its electromagnetic behavior. In the most general case, \( \varepsilon \), \( \mu \) and \( \sigma \) are complex tensors. Restricting ourselves to isotropic materials, those become scalars.
4.2 REFRACTIVE INDEX

It is common to describe permittivity and permeability through their relatives values: one defines \( \varepsilon = \varepsilon_r \varepsilon_0 \) and \( \mu = \mu_r \mu_0 \) where \( \varepsilon_0 \) and \( \mu_0 \) are permittivity and permeability of the vacuum, and only mentions \( \varepsilon_r \) and \( \mu_r \). In this work, we do not consider any magnetic material, thus we’ll always take \( \mu_r = 1 \) in every subsequent case.

We will also assume that \( \varepsilon_r \) and \( \sigma \) are real. This assumption is not restrictive in any ways: last equation from system (4.1) becomes

\[
\nabla \times H = (\sigma + j\omega \varepsilon_r \varepsilon_0) E, \tag{4.3}
\]

which shows that a complex part of \( \varepsilon_r \) is of the same nature as the real part of \( \sigma \) and vice-versa.

As a result, one can model any electromagnetic, and a fortiori any optical, behavior using only the three parameters \( \varepsilon_r, \mu_r \) and \( \sigma \) from equations (4.2). In most of cases — non-magnetic materials, \( \mu_r = 1 \) — two of those are sufficient.

4.2 Secondary parameter : the refractive index

In optics, it is common to describe materials by their refractive index \( n \) defined as

\[
n = \frac{c_0}{c}, \tag{4.4}
\]

where \( c \) is the speed of light in the material, and \( c_0 \) the speed of light in the vacuum.

It is also common to describe a dissipative material by adding a complex part to its refractive index. We’ll now relate the notion of complex refractive index to the parameters introduced in previous section.

From (4.1) and (4.2), we can write

\[
\nabla \times E = -j\omega \mu H. \tag{4.5}
\]

Using the identity

\[
\nabla \times \nabla \times E = \nabla (\nabla \cdot E) - \nabla \cdot \nabla E
\]

and recombining equations from previous section, we get

\[
\nabla^2 E = -\omega^2 \mu_r \mu_0 \left( \varepsilon_r \varepsilon_0 - j\frac{\sigma}{\omega} \right) E. \tag{4.6}
\]

This is the mathematically well-known wave equation. The corresponding generalized propagation speed \( \tilde{c} \) is given by

\[
\frac{1}{\tilde{c}^2} = \mu_r \mu_0 \left( \varepsilon_r \varepsilon_0 - j\frac{\sigma}{\omega} \right). \tag{4.7}
\]

Since speed of light in vacuum is by definition

\[
c_0 = \frac{1}{\sqrt{\varepsilon_0 \mu_0}},
\]

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we get
\[ \tilde{n}^2 = \mu_r \left( \varepsilon_r - j \frac{\sigma}{\omega \varepsilon_0} \right). \] (4.8)

In general, the RHS of equation (4.8) has three times more degrees of freedom than its LHS, justifying the secondary appellation chosen here. However, under the assumptions of section 4.1 — \( \mu_r = 1 \), real \( \varepsilon_r \) and \( \sigma \) — both descriptions become mathematically strictly equivalent.

In further sections, both notions are used indifferently. However, at implementation, we will always favor the \( \varepsilon_r/\mu \) formalism for two reasons:

- Two real parameters are often easier to handle and more meaningful than a single but complex one.
- Implementing equation (4.8) requires a complex square root, a mathematically non-uniquely defined operation. Which of the two conjugated roots is actually selected on a given implementation is a matter of convention: using the fundamental parameters is thus safer.

### 4.3 Frequency dependence from experimental data

Previous work within the optics group [13] showed that phenomena like dispersion or losses can be represented by simply introducing a frequency — or equivalently a wavelength — dependence into the refractive index. Often, this frequency dependence is provided as set of measurements. In order to implement those, one needs to express them through an analytical expression, usually obtained by fitting. How precise is the fitted model depends on the chosen fitting function, and the whole technique is limited by how complex an implementable fitting function can be.

This section introduces a systematic method to fit accurately any experimental data. It deals with software specific details and may be skipped by readers not interested in purely technical details.

First, we introduce a general purpose family of fitting functions called splines: a spline of degree \( k \) is continuous function such that it’s \( k^{th} \) derivative is constant by part. An example of such a function is illustrated on Figure 4.1.
A handful property of splines is their ability to fit any realistic shape with good precision, together with — for the smoothing splines variant — a built-in ability to filter out potential noise in the data. Their main drawback is an unreasonable complexity in their analytical expressions.

Figure 4.2(a) shows how splines can be used to fit a realistic set of data: the gain curve of rhodamine 6G. Figure 4.2(b) shows the same fit after addition of noise to initial data.

This type of fit can be done extremely easily using Matlab® but, due to the particular complexity of those functions, the result of the operation is not the usual set of parameters but a non-humanly readable structure which behaves just like a function.

Transferring this structure and using it inside a Comsol model requires the bridging ability between Comsol and Matlab®, and is based on the — undocumented — property that, while bridged, both softwares use the same memory address space. It is thus possible to access within the Comsol solver not only Matlab functions, but also Matlab global workspace.

In practice, before launching the solver, the fit is performed in Matlab® and sent to the global workspace. Then, in Comsol, the corresponding parameter is

\footnote{The method is reported to work using COMSOL Multiphysics® 3.4 and Matlab® 2007b under Windows XP 64bits and MacOS X 10.5. It is known to fail with Matlab® 2008a on the same systems.}
defined as a Matlab function of the type \( f(\lambda) \). Finally, the corresponding \( M \)-file is written in order to pull the fitted structure out of the global workspace and return the value corresponding to \( \lambda \).

This type of in-memory transfer being undocumented, we provide a complete sample code below.

- In Matlab, before solving:

  ```matlab
  % User choice
  Smoothing = .999; % Smoothing factor, in ]0,1[, 1 = no smoothing. Very sensitive!!!
  Norma = 1e7; % Normalization factor for lambda
  % Do the fit and show the result
  gcurve = fit(lambda_data'*Norma,gain_data,'smoothingspline','smoothingparam',Smoothing);
  figure;plot(lambda_data,gain_data,'xb',lambda_data,gcurve(lambda_data*Norma),'-r')
  % Sends data to global memory
  global gain;
  gain.curve = gcurve;
  gain.min = min(lambda_data*Norma);
  gain.max = max(lambda_data*Norma);
  gain.norma = Norma;
  ```

- In Comsol GUI simply do

  \[
  parameter = \text{gainrhod6G}(\lambda)
  \]

- Create `gainrhod6G.m` as follows:

  ```matlab
  function y = gainrhod6G(lambda)
  % Retrieve structure from Global memory
  global gain;
  lambda = lambda*gain.norma; % Normalize lambda
  y = gain.curve(lambda); % Calculate gain at corresponding wavelength
  % Optionally, prevent extrapolation
  y((lambda<gain.min) | (lambda>gain.max))=0;
  ```

### 4.4 Losses as positive conductivity

An optical beam propagating in a lossy medium sees its intensity decreasing exponentially with the distance. For a plane wave the intensities at two points distant by \( d \) are related by

\[
I_2 = I_1 e^{-\alpha d},
\]

where \( \alpha \) is the extinction coefficient expressed in \( m^{-1} \) (\( dB/m \) or \( dB/cm \) being also commonly used). It is a material and wavelength dependent parameter which describes how strongly a given material damps a given wavelength.

We’ll now relate the extinction coefficient \( \alpha \) to the fundamental parameters introduced in section 4.1. Knowing that the wavelength dependence can be implemented afterwards, through the method of section 4.3 for example, we will
omit it for simplicity.

We know from basic optics \[6\] that intensity of a beam is proportional to the square of the electric field. Thus equation (4.9) can be translated in terms of electric field as follows:

\[
\left( E_2 e^{j(k \cdot r_2 - \omega t)} \right)^2 = \left( E_1 e^{j(k \cdot r_1 - \omega t)} \right)^2 e^{-\alpha d},
\]

(4.10)

with \( d = (r_2 - r_1) \cdot \hat{k}, \hat{k} = k/|k| \).

Or, in terms of phasors

\[
\hat{E}_2 = \hat{E}_1 e^{-j(k \cdot r_1 - \alpha d + jk \cdot r_2)},
\]

(4.11)

which can be rewritten as

\[
\hat{E}_2 = \hat{E}_1 e^{jk'd},
\]

(4.12)

where \( k' = k + \frac{\alpha}{2} \).

Since \( k = \frac{2\pi}{\lambda} = \frac{2\pi}{\lambda_0 n} \), we can relate \( k' \) and \( \alpha \) to the complex refractive index from section 4.2:

\[
\tilde{n} = \frac{\lambda_0}{2\pi} k' = \frac{\lambda_0}{2\pi} (k + j\frac{\alpha}{2}) = n + \frac{n\lambda_0\alpha}{2\pi},
\]

(4.13)

where \( n \) is the refractive index in the sense of 4.4. Finally, using relation 4.8 with \( \mu_r = 1 \), we get

\[
\tilde{n}^2 = \varepsilon_r - j\frac{\sigma}{\omega \varepsilon_0} = n^2 - \frac{\lambda_0^2\alpha^2}{16\pi^2} - j\frac{n\lambda_0\alpha}{2\pi}.
\]

(4.14)

Thus

\[
\varepsilon_r = n^2 - \frac{\lambda_0^2\alpha^2}{16\pi^2} \approx n^2.
\]

(4.15)

The second term can often be neglected: in the optical range, \( \frac{\lambda_0^2\alpha^2}{16\pi^2} \sim 10^{-15} \) m, and the extinction coefficients for materials used in our cases are at most of the order of 1 dB/cm \( \sim 10^4 \) m\(^{-1}\).

\[
\sigma = n\varepsilon_0 \frac{\lambda_0\omega}{2\pi} = n\varepsilon_0\mu_0 = n\sqrt{\frac{\varepsilon_0}{\mu_0}} \alpha = \frac{n\alpha}{Z_0},
\]

(4.16)

where \( Z_0 \) is the wave impedance of vacuum.

Except for extreme cases, it is thus sufficient to introduce a positive conductivity as given by equation 4.16 in order to model absorption.

### 4.5 Gain as negative conductivity

When introducing gain, one canonically considers a plane wave traveling in a gain medium and writes

\[
E_2 e^{j(k \cdot r_2 - \omega t)} = E_1 e^{j(k \cdot r_1 - \omega t)} e^\gamma(r_2 - r_1).
\]

(4.17)
The quantity $\gamma$ is then labelled as the gain. Its units are $m^{-1}$ or $dB/cm$, $dB/cm^...$

Equation (4.17) is similar in every aspects to equation (4.10): gain and extinction coefficient can be identified by

$$\gamma = -\frac{\alpha}{2}$$  \hspace{1cm} (4.18)

And results from section 4.4 apply:

$$\varepsilon_r = n^2 + \frac{\lambda_0^2 \gamma^2}{4\pi^2} \simeq n^2,$$  \hspace{1cm} (4.19)

$$\sigma = -2 \frac{n \gamma}{\lambda_0}.$$  \hspace{1cm} (4.20)

Thus gain can be seen as negative losses, and represented by introducing a negative conductivity in the model. However, while for losses, throwing whatever constant value for $\alpha$ will result in a meaningful solution (Figure 4.3(a)), doing the same with gain will very likely lead to a numerical catastrophe as on Figure 4.3(b).

Figure 4.3: Distribution and cross-section of calculated electric field for (a) Constant losses (b) Constant gain.

A constant extinction coefficient means that the material damps the incoming optical wave regardless of beam intensity: while this may be only an approximation of reality, this assumption is still physically meaningful. On the contrary, a constant gain means that the medium is able to amplify the same way a beam regardless of its intensity - i.e. the medium is able to throw an

---

1 *Constant* here means intensity independent. Frequency dependence is still allowed since the simulation is narrow-band.
arbitrary amount of energy into the amplification process - which is obviously unphysical.

Numerically, however, a medium can supply an unlimited amount of energy to amplification, but this is very likely to generate numerical problems in the scheme, leading directly to the meaningless result of Figure 4.3(b).

What is the final value of gain in the form of $\gamma$ depends ultimately on the number of electrons available for stimulated emission, which means that it depends on material, wavelength, pump power but also on current and past beam intensity. The correct value for $\gamma$ comes ultimately from rate equations (section 1.3), where pump effect is taken into account.

In the case of a steady state problem with constant pump power — which is the only case representable under harmonic formalism — a simple relation for gain exists [14]:

$$\gamma = \frac{\gamma_0}{1 + \frac{P}{P_0}}$$

(4.21)

where $\gamma_0$ is the small signal gain, $P$ is the density of optical power and $P_0$ a reference density of power. This relation describes the saturation phenomenon of gain when optical intensity increases.

Based on this formula, we derive and implement in our models

$$\sigma = \frac{\sigma_0}{1 + \frac{|E_0|^2}{|E_0|^2}}$$

(4.22)

where

• $\sigma_0$ is the conductivity associated to the small signal gain. It has a frequency dependence given by the fluorescence curve of the material and a certain pump-dependence. This last one will be only taken into account qualitatively: it seems reasonable - up to some extends - that when pump power increases, small signal gain increases and vice versa.

• $E_0$ is a saturation electric field. It characterizes the depletion of population inversion resulting from strong optical amplification. Like the small signal gain, this value is frequency dependent and probably pump dependent.

It is important to note the limitations of the harmonic formalism here. Equation (4.22) considers in the saturation phenomenon the electric field correspond-
ing to one single wavelength only. By nature, harmonic formalism forbids inter-frequency phenomena: each frequency saturates independently of others.

Finally, equation (4.22) introduces a non-linearity into the equation system. A first practical consequence is that it requires to use non-linear solvers, which are iterative - thus slow - and not guaranteed to converge.

Secondly, the non-linearity breaks the superposition principle required to associate phasors notation to a Fourier transform. Computing a solution for a sinusoidal wave keeps its physical meaning, but the notion of frequency response cannot be used anymore.

Implementing this saturating gain into the problem of Figure 4.3(b), one obtains a much more physical solution (Figure 4.5).

Figure 4.5: Solution to problem on Fig. 4.3(b) with saturating gain.

### 4.6 A(n almost) complete laser model

Putting together all the building blocks developed so far, an almost complete model in frequency domain can be constructed.

The resulting model for laser achieves to provide results qualitatively in agreement with experiment. However, the model is non-linear and numerically pretty unstable, requiring a lot of tuning before a solution can actually be obtained.

#### 4.6.1 Weak dependence on initial excitation

Back in chapter 3, we showed cavity modes as calculated then - without including gain - did depend strongly on the choice of excitation.

Once again, we analyze, on our simple rectangular laser cavity, the effect of the initial excitation on electric field distribution corresponding to a resonance frequency. Figure 4.6 shows a comparison between results obtained with and without gain.

Calculated field distributions at resonance, with gain included in the model, become fairly similar and only weakly dependent on the initial excitation. A fortiori, using the model for spontaneous emission introduced in section 3.5, which already reduces this dependence in a no-gain model, improves the method further and gives stable patterns.
Figure 4.6: Solutions with (right) and without (left) gain for various point or plane wave excitations. Right color scale $\sim 100 \times$ left one.
4.6.2 Numerical limits to gain

A major drawback from the present model comes from its non-linearity: such a problem needs to be solved iteratively, and the whole process is not guaranteed to lead to a solution in any ways. In practice, models become sometimes numerically unstable and solutions can be obtained only in some range of values of $\sigma_0$ for which the solver converges. For other values — especially high values — of gain, the solver simply fails.

In terms of finite elements (section 2.1), Comsol solves iteratively the system

$$A_{Ez} Ez = f.$$ \hspace{1cm} (4.23)

Physically, a high gain means that for a weak excitation, the system response is high, thus electric field is high. This translates numerically into

$$\|E_z\| >> \|f\|,$$ \hspace{1cm} (4.24)

which in turn means a high condition number for the matrix $A_{Ez}$. Each linear system (4.23) becomes more and more numerically unstable when gain increases, until iterative solver fails to converge.

A rule of thumb for building a model is to first set the values of small signal gain through $\sigma_0$ and determine a saturation field $E_0$ according to physics.

Then, the model for spontaneous emission is introduced and calibrated such that the resulting average electric field amplitude in the no-gain model is around 5% and not lower than 1% of the saturation field. Lower values will seriously slow down or break convergence. Higher values do work and simply represents systems dominated by spontaneous emission rather than lasers.

If the model fails to converge, further tuning of excitation and saturation field are required. In some situations, convergence may simply be impossible to achieve.

4.6.3 Results

An experimental result for a trapezoidal cavity made of PMMA doped with Rhodamine6G is available in [15]. Paper reports successful measurements on a cavity with a side-length of 50 $\mu$m — reproduced on Figure 4.7 — as well as inconclusive measurements for a 10$\mu$m cavity.

Unfortunately, the 50$\mu$m cavity is far too large to make any simulation possible. Instead we will scale down the geometry by a factor 10 and build a model including spontaneous emission and the saturating gain curve for rhodamine 6G. Variation of pump power are taken into account by simply arbitrarily varying small signal gain.

\footnote{What is high gain depends on the problem, but sometimes even on the parameters given to the solver.}
Calculated cavity modes for several values of small signal gain are shown on Figure 4.8(a). Our model exhibits a higher spectral separation of modes, expectable due to the scaling. Output intensity as a function of small signal gain is shown on Figure 4.8(b): the plot shows an increase of output intensity up to a critical value where the iterative solver fails. For higher values of gain, convergence is recovered, but validity of the solution is more than questionable.

The proposed model achieves results qualitatively comparable to the experiment. This is encouraging but not enough to fully validate the model: exact relation between pump power and small-signal gain value is so far unknown and saturation field was taken here to an arbitrary value. Further comparison, with a fully known and controllable experimental setup are needed.
4.6.4 Conclusions

The model for gain developed here, based on gain saturation at steady-state, a simple approximation to rate equations, shows promising possibilities.

While it is a simple to understand and implement model, its numerical instability makes it difficult to apply on practical models: it will work only in some range of values and may requires some time consuming tuning of parameters for each model.

Further improvements to the model go surely through a more accurate expression for gain derived from rate equations, including directly the effect of pump power. Maybe numerically more stable relations can be derived as well.

Lots of space is left for improvements.
Chapter 5

The hexagonal shape

One of the simplest types of optical cavity is a parallelepiped — or rectangle in 2D — made of a dielectric material. Partial reflection and transmission at the interfaces play the role of mirror and output couplers. Resonance in such a cavity is well known and commonly described in terms of longitudinal and transversal modes: a longitudinal mode corresponds to a resonance frequency and transversal modes are associated to multiple field distributions allowed at this precise frequency (Figure 5.1).

![Figure 5.1: Representation of two transversal modes for a rectangular cavity.](a) ![Figure 5.1: Representation of two transversal modes for a rectangular cavity.](b)

Circularly symmetric structures — spheres, cylinders and rings — are known to support a very different type of resonance modes: the so-called whispering gallery modes (WGM) [16]. Unlike in volumes modes above — modes where the electric field occupies the whole cavity — in a WGM, light is trapped close to the surface of the cavity and travels guided by total internal reflection (Figure 5.2(a)).

Note that volume modes also exist for circular shapes (Figure 5.2(b)), but WGMs are dominant.

WGMs exhibit sharp resonance leading to very high Q-factor. A well-known application of those is the ring resonator (see example in chapter 3).

However, for lasers, this type of resonance is not efficient since only material close to the surface takes part in the optical gain, leaving the central area unused. Moreover, rounded edges are not suitable for good coupling.
5.1 Geometrical Optics approach

Yet geometrical optics at this scale is not a valid representation, simple considerations based on it may help us to understand such behaviors. Two phenomena act jointly: partial reflection and total internal reflection (TIR).

Partial reflection

Each partial reflections weaken the optical beam. Thus, in order to avoid high losses and produce notably constructive interferences, optical round paths with few reflections must be available.

In the rectangle, many such paths exist between opposite facets. Moreover, slight divergences are corrected by TIR on the second set of facets: modes based...
on partial reflections can build easily. In the hexagon, many two-reflections paths are available between opposite facets, but slightly divergent rays enter many-reflection paths.

Finally, in the circle, only rays traveling exactly through the center may perform a round trip in the cavity with only two reflections. Many-reflections paths are infinitely more probable: rays after a round trip are weakened too strongly to produce any notable interferences, modes based on partial reflection in a circle are thus difficult to obtain.

![Figure 5.4: Possible paths based on partial reflection.](image)

**Total Internal Reflection**

Let’s consider the round path based on TIR with the greatest incident angle possible: in a rectangle, it is a rhombus (Fig. 5.5(c)), in a hexagon, it is another hexagon (Fig. 5.5(b)). For the circle (Fig. 5.5(a)), any regular polygon is a candidate. The result is direct: interferences based on TIR in the rectangle can be obtained only for high refractive indexes because of the small incidence angles in the rhombus. In the circle, light can be trapped very easily in one of the multiple round paths along the surface.

For the hexagon, the situation is intermediate: TIR round-trips can be obtained at relatively low refractive index because of high incidence angles, but not as easily as in the circle. Moreover, the hexagonal round path lies deeper in the cavity than those corresponding to higher order polygons.

![Figure 5.5: Possible round paths based on TIR.](image)

Because of this situation in the middle where modes can arise from both TIR and partial reflection, hexagonal cavities are expected to show interesting properties.
5.2 The single hexagonal cavity

Potential laser cavity modes for the hexagonal cavity are calculated and compared to the ones for a circle and a square on Figure 5.6. Resonance modes of the hexagonal cavity are intermediate between the rectangular - here square - shape and the circle. Yet the hexagon improves $Q$-factor and resonance amplitude compared to the square, this improvement is only slight and surely not comparable to the one brought by the circular shape.

Figure 5.6: Calculated cavity modes for cavities of hexagonal, circular and square shapes. Inset shows geometric relation between cavities used in the simulation.

Behaviors of the hexagonal cavity in many other situations have been studied and an interesting phenomenon was noticed: when exposed to a plane wave, modes show a very particular sensitivity to incidence angle can be seen. In order to exploit this property, a potential sensor design is introduced on Figure 5.7(a).

Figure 5.7: (a) Proposed sensor design: a plane wave incoming with an angle $\alpha$ is directed by the cavity onto an intensity detector. Radius of hexagon — the distance from its center to one of the corners — is 1.5 $\mu$m (b) Example of electric field distribution in our sensor.
The intensity at the detector for several angles is shown on Figure 5.8. While most of the time resonance modes are pretty insensitive to the angle, boxed area shows two neighboring modes with radically different behaviors: when $\alpha$ varies, resonance amplitude on the right peak is stable while the one of the left peak is very sensitive. However, in this form, the effect weak.

![Figure 5.8: Intensity at the detector with regard to wavelength for several angles between 0 and 10° for sensor design from Figure 5.7(a). Boxed area shows unusual angular sensitivity.](image)

### 5.3 The double hexagonal cavity

Following results from previous section, a new design based on two hexagonal cavities coupled by facets is introduced (Figure 5.9). The target here being mainly to increase the newly observed angular sensitivity.

![Figure 5.9: Sensor design based on the double hexagonal cavity. Each cavity has radius 1.5 μm.](image)

#### 5.3.1 Optimal gap

A necessary step in the design of our double cavity sensor is to determine the optimal size for the gap. To do so, cavity modes are calculated varying gap
length (Figure 5.10). The optimality — the length corresponding to highest resonance amplitude — is found in this case to lie between 0.7 and 0.8 µm. It can be shown that, in general, optimal gap length lies around half the radius of hexagons.

Figure 5.10: Energy stored in the cavity with respect to wavelength. Each curve corresponds to a particular gap length expressed in µm.

5.3.2 Angular properties

Once again, a plot of calculated intensity at the sensor with respect to wavelengths for several angles is shown on Figure 5.11. Boxed areas show angular sensitivity similar to the one observed in previous section. The amplitude of the variation is notably increased in the new design (Figure 5.12). Various angular dependences are present: at 658 nm, the intensity is minimal for $\alpha = 5^\circ$, at 463 nm, a quasi linear behavior in the range 3.5 to 6.5° is observed.

Figure 5.11: Intensity at the detector with regard to wavelength for several angles between 0 and 10° for sensor design from Figure 5.9. Boxed areas show unusual angular sensitivity.
Finally, one may get pretty good physical understanding of the phenomenon by plotting calculated electric field distributions (Figure 5.13). In every cases, the first cavity resonates and directs light into the gap, but in two different manners: in Figure 5.13(a)-(c), the resonance is mainly a volume mode while in Fig. 5.13(b)-(d) the resonance is more similar to WGM.

Figure 5.13: Calculated field distributions for two incident angles for (a) (c) stable peak in left most box on Fig. 5.11 (b) (d) angular sensitive peak.

At $\alpha = 0^\circ$, in both cases, the second cavity collects lights from the gap and directs it onto the intensity detector through a ray-like path. For $\alpha = 6.5^\circ$, on Fig. 5.13(c), the second cavity is only weakly affected: light continues to be
directed towards the sensor through a similar ray-like path. On Fig. 5.13(d) the situation is however totally different: a WGM is excited in the second cavity, lights travels mostly along the surface and is partially backscattered, causing the observed variations of intensity at the detector.

5.3.3 Applications

Under the scope of those results, detectors based on double hexagonal cavities might be useful in beam steering application. A single sensor can cover an angular range of $3 \sim 4^\circ$.

Compared to classical techniques \cite{17} or nowadays state-of-the-art sensors \cite{18} performing angular measurements of incident optical beams in this range, the proposed design is far simpler and several order of magnitude smaller.

Moreover, due to their small size, many of such detectors might be packed into a small area and their various behaviors (Fig. 5.12) can be combined in order to increase precision or angular range.

5.3.4 External Field Enhancement

Another remarkable property of the double hexagonal cavity can be observed on Figure 5.13: a high-intensity spot appears in the gap.

Many optical cavities exhibit focusing-like effects, but those high-intensity regions are often located within cavity core, inside the material. For a single hexagonal cavity, this high field is located just across the facet (Figure 5.7(b)). Coupling two cavities increases this effect, broaden this region and enhances its intensity, regardless of the wavelength in the whole optical range. The cross section on Figure 5.14 shows this high field region in the gap.

Good use of this property can be made in lab-on-chip applications when high field is required, for example, while probing fluids, chemicals or biological samples.

![Figure 5.14](image)

Figure 5.14: (a) Cross section showing optical intensity enhancement in the gap. (b) Electric field distribution. Red line indicates location of the cross section in (a).
5.3.5 Stability

Stability with regard to waveshape

Many times we assumed an incident plane wave on our device: this is an idealization of reality only, it is thus important to verify that our result are reproducible for other types of beam shape.

We setup in a numerical model a source emitting curved wavefront (Figure 5.15). Calculated modes for various radii of curvature of the wavefront are shown on Figure 5.16.

The overall behavior of the device appears to be stable. The only effect of an increasing wavefront curvature is uniform scaling of the diagram, indicating a drop of the coupling efficiency between the incident beam and the device rather than a sensitivity to curvature itself.

Figure 5.15: Setup for checking stability with respect to wavefront shape: Upper plot shows calculated field distribution in the cavity. Lower plot shows the incident unperturbed wavefront. Wavefront curvature is tunable.

Figure 5.16: Cavity modes calculated varying wavefront curvature. Arrow shows evolution for increasing curvature: the pattern is uniformly scaled down.
5.3. THE DOUBLE HEXAGONAL CAVITY

Dependence on gap refractive index

Behavior resulting from variations of the refractive index in the gap is analyzed on Figure 5.17. An increase of this refractive index shifts modes towards longer wavelengths, increases coupling between both cavities but also destroys resonance properties.

Such a behavior is undesirable for a laser but might be turned into a useful property in sensing applications.

Figure 5.17: Cavities energy for several values of refractive index in the gap, increasing from 1 to 1.5. Arrows show the effect of this increase.
Chapter 6

Further analysis and Other types of models

So far, we performed all our computations in 2D [TE] harmonic mode. Extending our models to other modes and types of calculations is a natural continuation.

Extension to 2D [TM] harmonic mode requires only to adapt the model into a new formalism. This step requires good understanding of those new tools and some experience with them, but does not face any technical limitations. 2D hybrid mode is then just a summary of both cases.

Both TM and hybrid modes keep the assumptions of translation symmetry along z-axis and harmonic formalism, but remove the one about the z-polarized electric field.

Extension to 3D and/or to time domain are technically more interesting and relax other, maybe more significant, assumptions previously made in models.

6.1 Extension to 3D

Extending our models into the third dimension removes the assumption of infinite translation symmetry present in 2D. This means that we may now take into account all the interfaces of the microcavities, i.e. the air-cavity interface at the top and the substrate-cavity one at the bottom. Also, no polarization is assumed.

Unfortunately, 3D calculations happen to be computationally much more heavy for three reasons:

• The number of elements increases dramatically: in 2D, we need to apply a mesh on a slice, and this requires typically a few tens to a hundred thousands elements. In 3D, the volume is sliced in many layers, each layer being meshed roughly like in 2D. Consequently, an equivalent 3D model, requires several millions of elements, leading to serious memory problems.
6.1. EXTENSION TO 3D

- Compared to a 2D case, each node of a 3D mesh is part of many more elements. The result is that the mass matrix (section 2.1) gets many more non-zero elements per lines and its sparsity decreases. This means that even for an equal number of degrees of freedom, a 3D problem is more costly in term of computing time than a 2D problems.

- The equation to be solved is vectorial in 3D: the number of unknowns in the system is roughly tripled.

In practice, one more problem arises: very often models with high memory consumption need to be solved using iterative solvers. Those are memory-efficient but much more costly in term of computing time than fast direct solvers.

Of course, one may always use an extremely coarse mesh to reduce memory requirement, but then what trust can we put into a solution computed that way? Meshing the model on Figure 6.1(a) using 4 or 6 slices along z-axis will surely not model correctly any interface phenomena.

Using an adequate mesh size, one gets the result shown on Figure 6.1(b), scoring over 1.3 million elements. To be solved, such a model requires around 40GB of memory using an iterative - memory efficient - solver, and around 10 hours of CPU-time on the most powerful workstation of the group, for a single wavelength, in a linear version of the model. Non-linearity introduced by gain is likely to multiply this time by 10 ~ 20, and a typical run requires roughly a hundred different wavelengths in order to represent the spectral behavior.

In comparison, a 2D version, with an equivalently accurate mesh, scores just above 20000 elements, requires around 1.5GB of memory — with a direct solver — and roughly 10s of CPU-time per wavelength in a linear version, on a standard computer.

![Figure 6.1: Double hexagonal cavity problem in 3D and corresponding mesh.](image)

As a result, while most of our 2D models require just a few hours of CPU-time for a full parametric study, the same analysis on an equivalent 3D problem...
may take several days or weeks.

Extending a model to 3D is not a mild task. One should think carefully before acting in order not to waste resources. For first investigations of new ideas and concepts like in this work, 2D computations constitute a handful sandbox, relatively inexpensive in terms of time and computer resources.

6.2 The time domain

Time domain formalism is probably the most interesting of all: one can perform wide-band simulations and get information about transient phenomena.

Transient phenomena may be extremely important: some systems may be interesting for their transient behaviors only, other setups may actually reach a different steady state than the one calculated in harmonic mode, or even never reach one at all.

Wide-band allows to perform simulations for multiple wavelengths in one shot as well as to consider interactions between effects taking place in different regions of the spectrum — a very important feature terribly missing so far.

On the other hand, one needs to face new constrains, limitations and technical problems:

- Time domain simulations are computationally more heavy because of time stepping: each small step in time requires to solve a system of linear equations. But fortunately, memory consumption can be maintained low: the system solved at each time step is not significantly bigger than for an equivalent problem in harmonic formalism.

- Comsol tools for time domain are not yet as well developed as for the harmonic mode. The most noticeable problem here being the absence of PML, another is strong numerical dispersion.

- Mathematical expressions of parameters like refractive index, gain and losses in time domain become much more complicated to handle.

This section presents a fully functional absorbing layer for time-domain calculations and introduces basic ideas on how to implement material parameters. A specific scheme based on finite differences (FD) is also briefly discussed.

6.2.1 An absorbing boundary condition

Historical overview

For many years, a general purpose absorbing boundary condition for Maxwell’s equations has been the holy grail of computational electromagnetics. Such a BC still does not exist nowadays. The best we have are a set of BCs which are, as described in section 2.7, non-reflective under some specific circumstances.

In the meanwhile, engineers have been successfully using absorbing layers in anechoic chambers (Figure 6.2). The idea to transpose this concept into
numerical methods and use an absorbing and non-reflective layer rather than a boundary, leading directly to modern PML arrises relatively late.

The very first technique to build such a layer, efficient enough to be called perfectly matched, the split-field PML was proposed by Berenger in 1994 for Yee’s scheme. Its formulation is famous for its complexity and its 27 equations in 3D.

In 1996, Gedney proposed an equivalent but simpler formulation, the uniaxial PML (uPML), based on the use of an artificial anisotropic absorbing material.

Finally, the modern formulation was introduced in 1998 by Teixeira and Weedon, called stretched-coordinates PML. This formulation is based on a mapping of coordinates system from real to complex space and happens to be equivalent but much more general than the previous ones.

Both uniaxial and stretched-coordinates PML have been very successful and are now widely used. Why they are absent for time domain calculations in our software is unknown.

Implementing completely any of the methods above can only be done by modifying software core. However, based on Gedney’s ideas for his uniaxial PML, we may quite easily build an artificial anisotropic material which will be absorbing and only weakly reflective. This technique can be seen as an unperfectly matched or sponge layer.

A sponge layer for time domain in Comsol

Reflection at an interface occurs according to Fresnel’s coefficients (section 1.2). Those are dependent only on the refractive index of the media across the interface and on the angle of incidence of the beam. In general, this refractive index is a complex number combining the three essential material parameters: electric permittivity, magnetic permeability and conductivity (section 4.2).

1Reproduced from Montefiore institute, University of Liège, Belgium — http://www.ulg.ac.be.
Based on those three degrees of freedom, it might be possible to find an interface between different media such that no reflection occurs. An additional difficulty is that those considerations must be valid in the discrete forms of numerical schemes. Gedney’s work showed that strict absence of reflection is possible only at the cost of an artificial material with specific relations between tensors’ components.

For simpler - isotropic - materials, a strictly non-reflective interface cannot be achieved. However, if the refractive index is changed only slightly across the interface, the reflection will be small.

Now, let’s consider the layered medium on Figure 6.3: constant permittivity and permeability, and variable conductivity.

When an electromagnetic wave hits the first interface, partial reflection occurs, but is small since the change in refractive index is low. The transmitted wave travels to the next layer and is damped weakly. At the second interface, we again increase the conductivity but more than at the first step: this will produce stronger reflection, but before this reflected wave reaches our domain, it needs to cross the first layer backwards and is partially damped. Following the same logic, conductivity can be increased more and more at each step, each partially reflected wave being more and more damped on the way back.

Such staircase functions are exactly what happens when we represent an analytical function on a computational grid. Conductivity may be described as a continuous function and the layering appears automatically in the computing process. Often, one chooses a simple polynomial function of the type

$$\sigma(d) = \sigma_0 \ d^\alpha,$$

where $d$ represents the current depth in the layer.

The exponent $\alpha$ is a key parameter: if chosen too low, the function grows too fast close to $d = 0$ and creates strong reflections. If chosen too high, conductivity grows too slowly to efficiently damp the forward wave. This is illustrated on Figure 6.4. The optimal $\alpha$ can be determined for a given problem by trial and errors, and generally lies in the range $[2, 3]$. 63
The parameter $\sigma_0$ is a constant depending on $\alpha$, thickness of the layer, and normalization chosen for $d$. It does not depend on the magnitude of the field to be damped and is dependent on wavelength only for variations across several orders of magnitude.

Finally, a special mesh may be applied onto the sponge layer: the only thing we want is to damp the wave, we do not care about solution in the layer. The mesh size may be increased little by little when going deeper into the layer, as shown on Figure 6.5(a). This has two benefits:

- It reduces number of elements, memory usage and computing time. This can be greatly helpful, especially because such a sponge layer must be notably thicker than a real PML in order to be efficient.

- It is impossible to represent a given wave on a mesh which has a size comparable to or larger than its wavelength. In such a case, the wave must vanish - which is what we want. Oversized mesh elements generate strong numerical error, but, up to some extend, this won’t have any influence on the solution since the resulting waves are damped before reaching the domain.

Figure 6.5 shows a test problem built to analyze the behavior of our sponge layer: a pulse is generated and directed toward the layer, all boundaries are set to PEC. Fig. 6.5(b) and (c) show the electric field at two different time steps. On (c) the wave is strongly damped inside the layer and no reflection is visible. Fig. 6.5(d) shows the electric field in logarithmic scale at the same moment: there is some residual reflection coming from the layer, but the maximum reflection is around 1% in terms of electric field.

A reflection of 1% is acceptable in practice, and might be lowered further by increasing the length of the layer. However, using a real PML, one may reasonably expect the reflection to drop down by several orders of magnitude for layers 10 times shorter than on Figure 6.5.
The sponge layer introduced here is a satisfactory free-space simulating boundary in most of cases where high accuracy is not required. It is a workaround when PMLs are not available, and should be used only then. Figure 6.6 shows how this technique can be applied to a practical model used in the optics group.
Electromagnetic behavior of a material is described in frequency domain by frequency - or wavelength - dependent ($\varepsilon, \mu, \sigma$) or $n$ (section 4.1). Mathematically, those parameters are functions of $\omega$.

Let’s consider only the conductivity $\sigma$, the same procedure being applicable to any other parameter. In harmonic formalism, with strict notations we have the constitutive law

$$\hat{J}(\omega) = \sigma(\omega) \hat{E}(\omega). \quad (6.2)$$

In time domain, the same constitutive law becomes

$$J(t) = \sigma(?) E(t). \quad (6.3)$$

The dependence of $\sigma$ is voluntary left with a question mark. The correct dependence is not time, at least not explicitly. Even in time domain, $\sigma$ remains a function of frequency, or more exactly of the speed of variation of $E$ at time $t$. Thus

$$\sigma(?) = \sigma (\partial_t E(t), \partial_t^2 E(t), \partial_t^3 E(t), ...) . \quad (6.4)$$

From a function of frequency in harmonic formalism, $\sigma$ becomes a differential equation in time domain. This technique is called auxiliary differential equations (ADE).

From the derivation and integration theorem associated to Fourier transform (section 2.6), if $\sigma$ is expressed in frequency domain as a polynomial or a rational function of $\omega$, one can reconstruct analytically an expression for equation (6.4). Similarly, any realistic function for $\sigma(\omega)$ can be expanded into its Taylor series to obtain a polynomial, and experimental data like on Figure 1.5(b) can

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Model taken from the work of Mewael Giday Sertsu.
be fitted with a rational function.

However, practical considerations darken this situation: yet time derivatives are easily accessible in Comsol derivations is a numerically very unfavorable process. Third or fourth order derivatives should be already considered as a hard limit, meaning that the best we can do is to fit a curve like on Figure 1.5(b) with a polynomial of fourth order in the best case. Thus ADE in our case happens to be a very crude method - yet it works in principle.

The differential equation for $\sigma$ in time domain appears because of the form of equation (6.3). We'll now take a radically different approach.

We have

$$\hat{J}(\omega) \xrightarrow{\mathcal{F}^{-1}} J(t).$$  \hspace{0.5cm} (6.5)

Thus

$$J(t) = \mathcal{F}^{-1}\left\{ \sigma(\omega)\hat{E}(\omega) \right\} = (\Sigma \otimes E)(t),$$  \hspace{0.5cm} (6.6)

where

$$\sigma(\omega) \xrightarrow{\mathcal{F}^{-1}} \Sigma(t) \quad \text{and} \quad \hat{E}(\omega) \xrightarrow{\mathcal{F}^{-1}} E(t).$$

and $\otimes$ symbolizes a convolution product. A proper implementation leads to the method called recursive convolution. This is however not applicable in our case since Comsol requires an explicit expression of the type $\sigma = \ldots$.

All this remains valid for permittivity, permeability and refractive index.

### 6.2.3 FDTD - Yee’s scheme

FEM is a very general and powerful technique for solving various differential equations, but it is not the only one. It relies on heavy mathematical machinery and advanced programming techniques for building meshes, performing high-order integrations and solving efficiently linear systems.

Beside FEM, another available method is FD based on a single and extremely simple principle: one defines a regular computational grid with a step size $h$ and approximates all the derivatives by the finite differences

$$\frac{df}{dx}(x) \Rightarrow \frac{f(x + h) - f(x - h)}{2h}.$$

The same holds for higher order and/or partial derivatives in both space and time. Depending on the form of the equations discretized, the process leads to a system of linear equations or an iterative scheme.

Back to section 2.2, it can be shown that, for a scalar partial differential equation in space, choosing as a basis $\mathbb{P}^0$, the ensemble of piece-wise continuous functions, FEM and FD lead to strictly the same system of equations, corresponding to a staircase approximation of the solution, obviously sub-optimal.
FD method is thus often regarded as a simple to understand and easy to implement — almost doable by hand — method for small problems, and FEM is kept for more serious cases.

However, in 1966 Kane Yee introduces a revolutionary iterative scheme for Maxwell’s equations in time domain. The algorithm is based on applying FD to each field component on a different computational grid. The grids are specifically staggered in both space and time (Figure 6.7).

![Figure 6.7: Sample of grids used in Yee’s scheme: (a) 2D TE spatially staggered grids (b) 1D space-time staggered grids. (c) 3D spatial grid.](image)

The discretization leads to a two-step iterative time-stepping scheme based only on explicit update formula — i.e. without a single system of linear equations to be solved — resulting in dramatical boost of performances compared to a FEM-based timestepping.

Further improvements and stronger mathematical basis were brought to Yee’s scheme later, mainly through the work of Allen Taflove, who renamed it to finite differences in time domain (FDTD).

Nowadays, FDTD is the most widespread, efficient and mature algorithm, designed from the beginning for Maxwell’s equations in time domain. Tools like real PML or recursive convolution, absent from Comsol are extensively covered in [21]. The book also supplies a fully working Matlab implementation.

Methods to model properly optical gain - directly from rate equations - exist [22], and the algorithm has been successfully applied on microcavities [23], [24].

While it makes sense to use FEM for Maxwell’s equations in harmonic formalism, this general-purpose algorithm becomes antiquated in time domain where a very specific, much simpler and efficient scheme exists. At the scale of our problems, FDTD - Yee’s scheme outperforms FEM from every point of view. It might worth to give a try to FDTD through other commercial softwares, or maybe by our own implementation.
Conclusions

Following the initial aim of this work, new models, techniques and ideas were introduced and developed towards simulations of polymeric microcavity based lasers. The new cavity design introduced, expected to be a candidate for a laser, eventually showed properties making it more suitable for sensing applications. Those newly discovered properties eventually turned from an apparent half failure into a full success, leading to publication of paper [25].

Other cavity designs will be studied. New ideas and innovative models introduced in this work — while they still need improvements — might play an important role in future projects within the optics group. Some improvements brought to simulation tools during this work are already in use today, the most remarkable being the sponge layer, replacement for the PMLs absent from our main software for time domain simulation.

While all our models were checked against physical coherence in simple cases and qualitatively compared to literature, none was quantitatively checked against experimental results. This is the bitter taste of practical reality: building and experimenting a setup in a lab takes long, much longer than the time available for this master’s thesis. Promising and now well-known results [4] obtained in the group before my arrival are about to be experimented. Hopefully, the present work will be validated or corrected by experiment in near future.
Appendix A

Derivation of the continuous source term described through a density of current

The present appendix derives the form of the RHS of equation (3.1) introduced in section 3.4.2. The proof is essentially based on rewriting Maxwell’s equations under the implemented form with 2D TE assumptions.

In 2D for TE waves in harmonic mode, Comsol solves the following equation :

$$\nabla \cdot (-c \nabla E_z - \alpha E_z + \gamma) + a E_z + \beta \cdot \nabla E_z = f. \quad (A.1)$$

Maxwell’s equations in frequency domain for isotropic homogeneous lossy medium are

$$\begin{align*}
\nabla \cdot E &= \frac{\rho}{\varepsilon}, \\
\nabla \cdot H &= 0, \\
\nabla \times E &= -j \omega \mu H, \\
\nabla \times H &= J + j \omega \varepsilon E.
\end{align*}$$

From this we derive the wave equation :

$$\nabla \times \nabla \times E = -j \omega \mu \nabla \times H. \quad (A.2)$$

From vectorial calculus, we have the following identity :

$$\nabla \times \nabla \times E = \nabla (\nabla \cdot E) - \nabla \cdot \nabla E. \quad (A.3)$$
Combining equation (A.2) with first and fourth Maxwell’s equations and identity from equation (A.3), we get:

\[
\frac{1}{\varepsilon} \nabla \rho - \nabla \cdot \nabla E = -j\omega \mu J + \omega^2 \mu \varepsilon E. \tag{A.4}
\]

Restricting this to our 2D TE case, we get:

\[
\left(\frac{1}{\varepsilon} \nabla \rho \right)_z = -\nabla \cdot \nabla E_z = -j\omega \mu J_z + \omega^2 \mu \varepsilon E_z. \tag{A.5}
\]

And we take

\[J_z = J_z^c + J_z^f\]

With

- \(J^c = \sigma E\) is the physical current density due to material conductivity.
- \(J^f\) is any other arbitrary current density.

From this, equation (A.5) becomes

\[
\nabla \cdot \nabla E_z = j\omega \mu J_z^f - \omega^2 \mu \left(\varepsilon - j\sigma \omega \right) E_z, \tag{A.6}
\]

which can be directly mapped to the coefficient form equation (A.1) by taking

\[
\begin{align*}
  f &= j\omega \mu J_z^f \\
  c &= 1 \\
  a &= \omega^2 \mu \left(\varepsilon - j\varepsilon \omega \right)
\end{align*}
\]

and all the unspecified coefficients equal to zeros.
Appendix B

Acronyms

Comsol  COMSOL Multiphysics®
MAP  Microelectronics and Applied Physics
KTH  Kungliga Tekniska Högskolan - Royal Technical School
FEM  finite element method
PML  perfectly matched layer
FDTD  finite differences in time domain
LOC  lab-on-chip
PMMA  poly(methyl methacrylate)
ADE  auxiliary differential equations
TIR  total internal reflection
GUI  graphical user interface
TE  transverse electric
TM  transverse magnetic
BC  boundary condition
PEC  perfect electric conductor
RHS  right hand side
LHS  left hand side
WGM  whispering gallery mode
ULg  University of Liège
FD  finite differences
References


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