Analysis of Photonic Crystal Waveguides by the use of FDTD with Regularization

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The figure on the previous page shows the magnitude of the x-component of the electric field of light after 24000 time steps when simulating the W1 PC photonic crystal waveguide. This is only a plane cut through the middle of the W1 PC waveguide. Totally there are 75 such planes in the computational domain. When simulating the W1 PC waveguide the program has to deal with approximately 450 times more information than what is illustrated, and this information changes several thousands of times during the simulation.
Abstract

A photonic crystal waveguide is an arrangement of dielectric materials with the ability to function as a guide for light. The amount of light which is propagated through the waveguide depends on the frequency, the color, of the light. This can be utilized in optic fiber technology to filter out signals with specific frequencies. Instead of sending signals in just one frequency it is possible to send different signals with different frequencies in one single fiber, and to use photonic waveguides to filter out the signals.

In this thesis it is explained how to simulate photonic waveguides with computer assistance with the help of a numerical algorithm called the Finite Difference Time Domain method, (FDTD). To improve the numerical computations regularization has been used, that is, discontinuous functions are replaced with continuous ones. We have investigated how to apply regularization effectively.

The main result of the investigation is that the total error becomes remarkably smaller with regularization than without. The accuracy when computing with regularization and a cell size of 50 nanometers is close to the accuracy when computing without regularization but a cell size of 25 nanometers.

Sammanfattning

En fotonisk kristallvägledare är ett arrangemang av dielektriska material som kan vägleda ljus. Andelen av det ljus som fortplantas genom vägledaren beror på frekvensen på ljuset, d.v.s. ljusets färg. Detta kan utnyttjas i optisk fiber-teknologi för att filtrera ut signaler med specifika våglängder. I stället för att sända signaler med en enda våglängd är det möjligt att sända signaler med olika våglängder samtidigt i en enda fiber, och filtrera ut dessa med fotoniska kristallvägledare.

I avhandlingen förklaras hur fotoniska kristallvägledare simuleras med datorberäkningar med hjälp av en numerisk algoritm som på svenska kallas Finita Differens Tids Domän metoden, (FDTD). För att förbättra de numeriska beräkningarna har regularization använts, vilket innebär att diskontinuerliga funktioner ersätts med kontinuerliga. Vi har undersökt hur regularization bör appliceras för att fungera effektivt.

Acknowledgments

This project was performed at PDC, Parallelldatorcentrum (Center for Parallel Computers), at KTH (PDC is hosted by NADA, Department of Numerical Analysis and Computing Science, KTH) and was a collaboration between PDC and IMIT, the Department of Microelectronics and Information Technology at KTH.

This project was a continuation on a master thesis project performed by Jing Gong, finished in January 2003 [5]. However, Jing used parallelization to improve the program by help of parallel computers, we have not used parallelization, but instead investigated the numerical methods.

I deeply would like to thank my main supervisor Dr. Ulf Andersson at PDC for his helpfulness and willingness in spending time discussing the problems and answering all my questions.

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Chapter 1

Introduction

This thesis deals with how to implement a numerical method that describes how light (i.e. electromagnetic waves) is propagating through a photonic waveguide. A photonic waveguide is an arrangement of dielectric materials that guides light. Since light consists of electromagnetic waves the propagation of light satisfies Maxwell’s equations.

1.1 Maxwell’s equations

Maxwell’s equations was introduced by James Clerk Maxwell in 1873,

\[\nabla \cdot \mathbf{D} = \rho \quad \text{(Gauss’ law for the electric field),}\n\]

\[\nabla \cdot \mathbf{B} = 0 \quad \text{(Gauss’ law for the magnetic field),}\n\]

\[\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \quad \text{(Faraday’s law),}\n\]

\[\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}_e \quad \text{(Ampere’s law),}\n\]

(1.1)

\(\rho\) is the charge density, \(\mathbf{D}\) the electric flux density vector, \(\mathbf{E}\) the electric field vector, \(\mathbf{H}\) the magnetic field vector, \(\mathbf{B}\) the magnetic flux density vector and \(\mathbf{J}_e\) is the electric conduction current density. Any electromagnetic field must satisfy these equations everywhere [9].

Usually we can assume that we have a linear, isotropic and nondispersive material (properties independent of field, direction and frequency). Then we have the relations:

\[\mathbf{B} = \mu \mathbf{H} = \mu (H_x, H_y, H_z) \quad \text{and}\n\]

\[\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon (E_x, E_y, E_z).\n\]

(1.2)

\(\mathbf{J}_e\) is the electric current density, we assume that it is proportional to \(\mathbf{E}\),

\[\mathbf{J}_e = \sigma \mathbf{E}.\n\]

(1.3)
The components in Faraday’s and Ampere’s laws can thereby be written,

\[\begin{align*}
\epsilon \frac{\partial E_x}{\partial t} &= \frac{\partial H_y}{\partial y} - \frac{\partial H_z}{\partial z} - \sigma E_x, \\
\epsilon \frac{\partial E_y}{\partial t} &= \frac{\partial H_z}{\partial z} - \frac{\partial H_x}{\partial x} - \sigma E_y, \\
\epsilon \frac{\partial E_z}{\partial t} &= \frac{\partial H_x}{\partial x} - \frac{\partial H_y}{\partial y} - \sigma E_z, \\
\mu \frac{\partial H_x}{\partial t} &= \frac{\partial E_y}{\partial y} - \frac{\partial E_z}{\partial z} H_x, \\
\mu \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial z} - \frac{\partial E_x}{\partial x} H_y, \\
\mu \frac{\partial H_z}{\partial t} &= \frac{\partial E_x}{\partial x} - \frac{\partial E_y}{\partial y} H_z. 
\end{align*}\]

Now we have a coupled system of six first-order differential equations which is suitable for numerical computations [1]. How to treat (1.4) numerically to finally develop the FDTD scheme is described in Chapter 3.

1.2 The numerical method - FDTD

The method we use to solve Maxwell’s equation is called FDTD or Yee’s algorithm. It was introduced by Kane Yee in 1966 and further improved by Allen Tafove in the 1970s. Yee’s algorithm is a second-order finite-difference time-domain (FDTD) method and very efficient for simple geometries.

The FDTD method for solving Maxwell’s equations has been the workhorse of computational electromagnetics in the time domain, due to its simplicity. However, the original FDTD method is efficient only for regular geometries of small or moderate size, without dielectric interfaces. The problems often include difficulties, complex geometries, large and complex domains et cetera, and the second-order accuracy is reduced to first order. During the past two decades, much progress has been made in improving the FDTD method. Modern computers has, of course, simplified, but not as much as one may think, since many problems are 4-dimensional\(^1\). If the resolution is doubled in each dimension, the problem size becomes 16 times larger [17].

FDTD applications is not limited to photonic waveguides. For example, in 1987 SAAB performed lightning analysis on the fighter aircraft JAS 39 Gripen on a grid with \(60 \times 30 \times 30\) cells (approximately) [1].

1.3 Photonic waveguides - the W3 PC waveguide and the W1 PC waveguide

Two waveguides have been analyzed, the \(W3\) PC waveguide and the \(W1\) PC waveguide. Both waveguides are constructed in similar ways, by layers of dielectric materials with air-holes etched in a triangular array all over the waveguide except a straight line through the whole waveguide. This line of no air-holes ”guides” the light [5]. The distance between the holes is 450 nanometers in both the W1 PC and the W3 PC waveguide. This gives the waveguide a band gap at a wavelength of approximately 1550 nanometers.

Figure 1.1 shows a schematic diagram of how a photonic waveguide could look like, this is an illustration of the W1 PC waveguide. Figure 1.2 shows the W3 PC waveguide enlarged a couple of 1000:s times.

\(^1\)Three dimensions in space and one dimension in time
Photonic waveguides are usually very small, due to the frequency of the light. It is both expensive and complicated to construct these. Therefore it is of great interest to analyze the properties with computer simulations by the use of FDTD. The problem that arises when simulating photonic waveguides is that the geometry of waveguides contains lots of discontinuities and the second-order accuracy is reduced to first-order [1]. The discontinuities appears in the function $\varepsilon_r(\vec{r})$, the permittivity. The speed of light in a media depends on the permittivity. The method we will use to improve our computations is called regularization.

Regularization means that we replace the discontinuous function $\varepsilon_r(\vec{r})$ with a continuous function $\tilde{\varepsilon}_r(\vec{r})$. This procedure will decrease the error caused by the numerical computations, the discretization error, but we also introduce another error, the model error. This thesis will try to explain how to find a balance between the discretization error and the model error [1][3].
Chapter 2

Brief description of the physical phenomena in photonic waveguides

The propagation of light in photonic waveguides are based on Maxwell’s equations. This chapter motivates the structure of a photonic waveguide.

2.1 Photonic band gap material

A photonic crystal is an artificial structure with the electromagnetic properties periodically modulated on a length scale comparable to a light wavelength. A photonic crystal might possess a photonic band gap (PBG), in which the light, with its frequency in the band gap, can not propagate in the photonic crystal. Waves with other wavelengths may propagate through the structure with low losses [12]. The frequency of the band gap is here referred to as \( \lambda_0 \). All photonic crystals described in this thesis do have a photonic band gap.

The PBG effect was proposed in 1987 by Yablonovitch and John, and the subject has received an increasing interest since then. One of the most interesting application of photonic band gap materials are when constructing photonic band gap waveguides, with properties different from conventional waveguides (TIR-based waveguides). The most interesting technical application is currently in optical fiber configurations [13].

2.2 Distributed Bragg reflector

In one dimension, a PBG structure may consist of multiple layers of alternating high- and low-index materials, even called a distributed Bragg reflector (DBR). In Chapter 22 of [14] there is a detailed description of how to compute the transmission of the DBR when waves (i.e. light) propagate through the layers but here we just state the result:

\[
T(\lambda) = \left| \frac{B(L, \lambda)}{B(0, \lambda)} \right|^2, \quad B(z, \lambda) = B(0, \lambda) \frac{\cosh[\kappa(z - L)]}{\cosh(\kappa L)}, \quad \kappa = \kappa(\lambda). \tag{2.1}
\]

The thicknesses of the layers in the DBR have to satisfy following relationship:

\[
n_1a = n_2b = \frac{\lambda_0}{4}. \tag{2.2}
\]

How the transmission could look like is shown in Figure 2.1. We see that there is a range of wavelengths around \( \lambda_0 \) for which almost no waves are allowed to
2.3 3D photonic crystals

The three dimensional analogue to the DBR have to include a periodicity of the dielectric constant, similarly as the DBR. The most usual way to construct this is to etch holes with a two-dimensional periodicity in a plane of dielectric or metallic material (see Figure 2.2). This structure may possess a photonic band gap similar to that seen in Figure 2.1. The frequency of the photonic band gap depends on the distance between the holes.

If we introduce a defect in an otherwise perfect crystal, the result may be that some frequencies of the light that are in the PBG, may propagate through the waveguide with low loss. An example of such a defect is that we omit etching holes in a line through the whole structure, providing a path for the light. This is illustrated in Figure 2.2. [16]

Figure 2.1: Left figure: The distributed Bragg reflector, DBR, alternating layers with different index. Right figure: Transmission diagram of the DBR.

propagate, instead they are reflected or diffracted. This is called the band gap [14][15].

2.4 The principle of wave guidance

One way to explain why the line defect act as a waveguide is to imagine the fields (or the photons) as bouncing between the “walls” of the guide where
it cannot propagate because of the PBG. The theory of this is analogue to conventional waveguides, where the photonic crystal structure (the walls) is replaced by conducting plates.

![Diagram of wave guidance](image)

Figure 2.3: *The principle of wave guidance. The walls reflect the wave to and fro.*

The fields have to obey Maxwell’s equations as well as boundary conditions at all points of the wall. There are two boundary conditions, for the first the tangential component of the electric field has to be zero and for the second the normal component of the magnetic field also has to be zero. By imaging the fields as linearly polarized plane waves one can show that the following relationship has to be fulfilled:

\[ kb \sin \theta = n \pi, \quad n \in \mathbb{N}. \]  

(2.3)

The meaning of \( \theta \) and \( b \) is defined in Figure 2.3. However, for a specific frequency of the fields there is an upper limit of the integer \( n \), i.e. a limited number of fields are able to propagate through the waveguide. These different waves are called *modes*. There is also a *cut-off frequency* below which no waves can be propagated, each mode has its own cut-off frequency,

\[ v_n = \frac{nc}{2b} \]  

(2.4)

A more detailed explanation can be found in a book about electromagnetism, for example in Chapter 12 of [9].
Chapter 3

The FDTD scheme

In this chapter we continue with investigating Faraday’s and Ampere’s laws (the equation system (1.4)) numerically. This will result in a numerical algorithm known as the FDTD scheme, describing the time development of the, in this case, electric and magnetic fields.

3.1 Approximating derivatives

An often used approximation of a first-order derivative is:

\[
\frac{df(x)}{dx} \approx \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}.
\] (3.1)

The error is proportional to \(\Delta x^2\) i.e. the error is \(O(\Delta x^2)\). To treat the equation system (1.4) with numerical methods we have to discretize the functions in, say \(N_xN_yN_z\) discrete variables. The first idea maybe would be to introduce systems of variables like

\[
H_{x|_{i,j,k}}^n = H_x(i\Delta x, j\Delta y, k\Delta z, n\Delta t)
\]

and

\[
E_{x|_{i,j,k}}^n = E_x(i\Delta x, j\Delta y, k\Delta z, \Delta t), \quad i, j, k, n \in \mathbb{N},
\]

and the first expression in (1.4) would then by use of (3.1) be:

\[
\frac{E_{x|_{i,j,k}}^{n+1} - E_{x|_{i,j,k}}^{n-1}}{\Delta t} = \frac{1}{\Delta z} \left[ H_{y|_{i,j,k+1}}^n - H_{y|_{i,j,k-1}}^n \right] + \frac{1}{\Delta y} \left[ H_{z|_{i,j+1,k}}^n - H_{z|_{i,j-1,k}}^n \right] - \sigma E_{x|_{i,j,k}}^n.
\] (3.2)

The order of accuracy is two\(^1\) [2].

But here we can use a simple trick. Examining equation (1.4) we find that the space derivative in the three upper equations only involve expressions of the magnetic field (\(H\)) whereas the three lower only involve expressions of the electric field (\(E\)). Therefore, we do not need to have the grids of \(E\) and \(H\) at the same points in space. A better choice of discretization which we will use is the FDTD grid, a Cartesian grid with the electric and magnetic components

\(^1\)Convergence is of order \(k\) if \(|a_{n+1} - a| < |a_n - A|^{k}\) for some \(N\) and \(A\), \(\lim_{n \to \infty} a_n = a\) [10]
staggered from each other (both in time and space) [1]:

\[
E_x^n_{i+\frac{1}{2},j,k}, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_y + 1, \quad k = 1, \ldots, N_z + 1, \\
E_y^n_{i,j+\frac{1}{2},k}, \quad i = 1, \ldots, N_x + 1, \quad j = 1, \ldots, N_y, \quad k = 1, \ldots, N_z + 1, \\
E_z^n_{i,j,k+\frac{1}{2}}, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_y + 1, \quad k = 1, \ldots, N_z, \\
H_x^n_{i,j,k+\frac{1}{2}}, \quad i = 1, \ldots, N_x + 1, \quad j = 1, \ldots, N_y, \quad k = 1, \ldots, N_z, \\
H_y^n_{i+\frac{1}{2},j,k}, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_y + 1, \quad k = 1, \ldots, N_z, \\
H_z^n_{i+\frac{1}{2},j+\frac{1}{2},k}, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_y, \quad k = 1, \ldots, N_z + 1. 
\]

(3.3)

For example \(E_x^n_{i+\frac{1}{2},j,k}\) is the \(x\) component of the electric field at \((x, y, z) = ((i + 1/2 - 1)\Delta x, (j - 1)\Delta y, (k - 1)\Delta z)\) at time \(t = n\Delta t\). (This notation agrees with that used in [1] but differs slightly from that used in [2].)

Figure 3.1 illustrates the location of the field components in one space-dimension.

Figure 3.1: The FDTD grid in one space dimension \((x)\), \(E_z\) components symbolized as arrows and \(H_y\) components symbolized as circles. The fields \(E_x, E_y, H_x\) and \(H_z\) do not interact with \(E_z\) and \(H_y\) according to Maxwell’s equations. Note that this is components of vectors, the algorithm deals with scalars and does not understand that these are components of vectors.

The reason for this choice of grids is that we can replace \(\Delta x\) in \((3.1)\) with \(\Delta x/2\). With almost the same number of unknown variables we have achieved a resolution twice as high.
3.2 The FDTD scheme

If we express (1.4) with the discretization (3.3) we will obtain the FDTD scheme for Maxwell’s equations, also known as the Yee’s algorithm:

\[
H_x^{n+1}_{i,j+1,k+1} = H_x^n_{i,j+1,k+1} + \frac{\Delta t}{\mu \Delta z} \left[ E_y^n_{i,j+1,k+1} - E_y^n_{i,j,k+1} \right] - \frac{\Delta t}{\mu \Delta y} \left[ E_z^n_{i,j+1,k+1} - E_z^n_{i,j,k+1} \right] \tag{3.4}
\]

\[
H_y^{n+1}_{i+1,j,k+1} = H_y^n_{i+1,j,k+1} + \frac{\Delta t}{\varepsilon \Delta x} \left[ H_z^n_{i+1,j+1,k+1} - H_z^n_{i+1,j,k+1} \right] - \frac{\Delta t}{\varepsilon \Delta z} \left[ H_x^n_{i+1,j+1,k+1} - H_x^n_{i+1,j,k+1} \right] \tag{3.5}
\]

\[
H_z^{n+1}_{i+1,j+1,k+1} = H_z^n_{i+1,j+1,k+1} + \frac{\Delta t}{\varepsilon \Delta x} \left[ E_x^n_{i,j+1,k+1} - E_x^n_{i+1,j,k+1} \right] - \frac{\Delta t}{\varepsilon \Delta y} \left[ E_y^n_{i,j+1,k+1} - E_y^n_{i,j,k+1} \right] \tag{3.6}
\]

\[
E_x^{n+1}_{i,j+1,k} = E_x^n_{i,j+1,k} - \frac{\Delta t}{\varepsilon_{i,j+1,k} \Delta z} \left[ H_y^{n+1}_{i,j+1,k+1} - H_y^n_{i,j+1,k} \right] + \frac{\Delta t}{\varepsilon_{i,j+1,k} \Delta y} \left[ H_z^{n+1}_{i,j+1,k+1} - H_z^n_{i,j+1,k} \right] \tag{3.7}
\]

\[
E_y^{n+1}_{i,j+1,k} = E_y^n_{i,j+1,k} - \frac{\Delta t}{\varepsilon_{i,j+1,k} \Delta x} \left[ H_z^{n+1}_{i,j+1,k+1} - H_z^n_{i,j+1,k} \right] + \frac{\Delta t}{\varepsilon_{i,j+1,k} \Delta z} \left[ H_x^{n+1}_{i,j+1,k+1} - H_x^n_{i,j+1,k} \right] \tag{3.8}
\]

\[
E_z^{n+1}_{i,j+1,k} = E_z^n_{i,j+1,k} - \frac{\Delta t}{\varepsilon_{i,j,k+1} \Delta y} \left[ H_y^{n+1}_{i,j,k+1} - H_y^n_{i,j,k} \right] + \frac{\Delta t}{\varepsilon_{i,j,k+1} \Delta x} \left[ H_x^{n+1}_{i,j,k+1} - H_x^n_{i,j,k} \right] \tag{3.9}
\]

It is straightforward to obtain the expressions for lossy materials with nonzero \( \rho \) and \( \sigma \).

So the situation would be that we know all the field components \( \mathbf{H}(t - \Delta t/2) \) and \( \mathbf{E}(t) \). With equations (3.4) to (3.6) we compute the new \( \mathbf{H}(t + \Delta t/2) \) components. Then we can use these to compute the new \( \mathbf{E}(t + \Delta t) \) components and so on.

To compute all the components we have to include all possible combinations of \( (i, j, k) \). This means we have to compute approximately \( 6N_xN_yN_z \) expressions at each step in time. The problems can thus become very large and hence we may need large computer capacity.

**Example of a FDTD update in one dimension:** In one dimension the field components do not vary with \( y \) or \( z \), only (3.9) and (3.5) is necessary with that reservation. The update of the \( E_{z,1.5}^5 \) component would be:

\[
E_{z,1.5}^5 = E_{z,1.5}^4 + \frac{\Delta t}{\varepsilon_{1.5} \Delta z} \left[ H_{y,2}^{1.5} - H_{y,1}^{1.5} \right] \tag{3.10}
\]

(see also Figure 3.1).
3.3 The Yee cell

Figure 3.2 shows the Yee cell, an illustration of the FDTD scheme defined in (3.3). The computational region is divided in $N_xN_yN_z$ such Yee cells.

3.4 The Wave equation

Before we continue with the numerical computations we will try to solve Faraday’s and Ampere’s laws analytically. If we consider the fields in $y$ and $z$-direction to be independent (i.e. the one-dimensional case, as in the example before). The system (1.4) becomes:

$$\begin{align*}
\epsilon \frac{\partial E_z}{\partial t} &= -\frac{\partial H_y}{\partial x}, \\
\epsilon \frac{\partial E_y}{\partial t} &= \frac{\partial H_z}{\partial x}, \\
\mu \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial x}, \\
\mu \frac{\partial H_z}{\partial t} &= -\frac{\partial E_y}{\partial x},
\end{align*}$$

which we can rewrite as two systems,

$$\begin{align*}
\epsilon \frac{\partial E_z}{\partial t} &= -\frac{\partial H_y}{\partial x}, \\
\mu \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial x}, \\
\epsilon \frac{\partial E_y}{\partial t} &= \frac{\partial H_z}{\partial x}, \\
\mu \frac{\partial H_z}{\partial t} &= -\frac{\partial E_y}{\partial x},
\end{align*}$$

These two systems are not coupled with each other, i.e. the time development of $E_z$ and $H_y$ is completely described by the two upper equations in (3.11). We differentiate the first equation in (3.11) with respect to $x$ and the second with respect to $t$,

$$\begin{align*}
\epsilon \frac{\partial^2 E_z}{\partial x^2 \partial t} &= \frac{\partial^2 H_y}{\partial x^2}, \\
\mu \frac{\partial^2 H_y}{\partial t^2} &= \frac{\partial^2 E_z}{\partial x^2 \partial t},
\end{align*}$$

Figure 3.2: The positions of the electric and magnetic field components when using the FDTD grid in three dimensions. Reprinted from [1] with permission.
In (3.12) we see that \(\frac{\partial^2 E_x}{\partial x \partial t}\) appears both in the upper and lower expression. We put these together and obtain,

\[
\frac{\partial^2 H_y}{\partial t^2} = \frac{1}{\epsilon \mu} \frac{\partial^2 H_y}{\partial x^2}.
\]  

(3.13)

We see that the \(H_y\)-component satisfies the scalar wave equation\(^2\). From this we understand that, assuming \(\epsilon\) and \(\mu\) is non-zero, the speed of propagation is limited, this is the speed of light, \(c = \frac{1}{\sqrt{\mu} \epsilon}\) [1][9].

The solution to the wave equation is \(Ce^{i\omega(x+ct)}\) for an arbitrary constant \(C\). Therefore the general solution of \(H_y\) can be written as,

\[
H_y(t) = \int_{-\infty}^{+\infty} \hat{H}_y(\omega)e^{i\omega t} d\omega,
\]  

(3.14)

for a specific function \(\hat{H}_y\). If the problem is simple this could be a way to solve the problem, but for nontrivial structures, varying \(\epsilon\), (3.13) is rather a reformulation of the original problem than an attempt to solve the problem. Due to Fourier analysis any function can be written as (3.14) [7].

### 3.5 Boundary conditions

Setting \(i\) to \(N_x + 1\) in (3.9) we obtain an expression involving\(^3\) \(H_{i=N_x+1}\), which is not defined. Similar problems occurs for \(i = 1\). In addition to that we usually have special conditions on the internal boundaries of the problems region. Therefore we need boundary conditions.

In this thesis we will only deal with absorbing boundary conditions, ABCs. This means that if a wave is propagating through an area where there is an absorbing boundary condition, the wave will disappear with no reflections at all, as if the wave had continued without reflection. However this is not as simple as it sounds, there are lots of different ABCs with different properties. In Chapter 4.6 of [1] there is a summary of some different boundary conditions, here we will only deal with an ABC called Mur. An example of how it is implemented, for low \(x\) (the edge at \(x = 0\)):

\[
E_{n+1}^{y|i=1} = E_{n+1}^{y|i=2} - \frac{c\Delta t}{c\Delta t + \Delta x} \left( E_{n}^{y|i=1} - E_{n}^{y|i=2} \right).
\]  

(3.15)

### 3.6 Stability for FDTD

#### 3.6.1 Definition of the CFL-number

We cannot choose \(\Delta x\), \(\Delta y\), \(\Delta z\) and \(\Delta t\) arbitrarily without stability problems. For example, investigating (3.4) one may imagine that if the factor \(\Delta t(\mu \Delta z)^{-1}\) would be too large, then \(H_x\) may receive a too large part in each step in time. \(H_x\) could then grow towards infinity.

The stability limit is given by:

\[
\Delta t < \frac{1}{c\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}.
\]  

(3.16)

\(^2\)In the same manner it can be shown that even the \(E_z\)-component satisfy exactly the same wave equation.

\(^3\)Note that the electric field has \((N_x + 1)(N_y + 1)(N_z + 1)\) components.
CHAPTER 3. THE FDTD SCHEME

Figure 3.3: Illustration of the model used in the program. The absorbing boundary conditions (ABC) would ideally not reflect anything, but they do anyway. However, the reflection does not seem to have caused problems in this master project.

$c$ is the propagation speed of the wave. Most often this is written as $CFL < 1$, where $CFL$ is the CFL-number defined as (from [1]):

$$CFL = c \Delta t \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}.$$  (3.17)

3.6.2 The magic time step

Consider the wave equation in one dimension:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \quad (3.18)$$

If we define $u(i\Delta x, n\Delta t)$ as $u^n_i$, (3.18) may be written as:

$$\frac{u^{n+1}_i - 2u^n_i + u^{n-1}_i}{(\Delta t)^2} + O[(\Delta t)^2] = c^2 \left( \frac{u^{n+1}_i - 2u^n_i + u^{n-1}_i}{(\Delta x)^2} + O[(\Delta x)^2] \right) \quad (3.19)$$

$O[(\Delta t)^2]$ and $O[(\Delta x)^2]$ represents the errors, let us try to minimize these.

Observe that $O[]$ represents exactly the same function to the left and the right in (3.19). The reason for this is that they have exactly the same origin, a derivative of second order in (3.18) (a strict mathematical proof of this would probably become more complicated). Assuming that $\Delta t$ is related to $\Delta x$ as $\Delta t = \Delta x/c$ which is called the magic time step, (3.19) reduces to simply:

$$u^{n+1}_i - 2u^n_i + u^{n-1}_i = c^2 \left( u^{n+1}_i - 2u^n_i + u^{n-1}_i \right). \quad (3.20)$$

This may look a little bit strange in connection to numerical computations. We tried to minimize the error terms, but in fact the error terms cancelled out completely. (3.20) is not a numerical approximation, but the analytic solution of the wave equation in one dimension. In connection to CFL-numbers, $\Delta t = \Delta x/c$ means that $CFL = 1$, the limit of stability [2].

In this thesis we deal with three dimensions. We do not have a magic time step when $CFL = 1$, but the effect is appearing even in three dimensions, the larger the value of CFL, the less will the total error become. However, we will not plunge deeply in this phenomena. $CFL = 1$ was also the limit of stability, so the program is mostly set to work with $CFL = \sqrt{3}/2 \approx 0.86$. 

Chapter 4

Numerical problems - how to treat discontinuities

Here the problems caused by discontinuities will be discussed. Regularization, the method used to make the functions more regular, will be introduced.

4.1 Discontinuities

As was mentioned in Chapter 2, the structure that the FDTD scheme will be applied on contains lots of discontinuities in $\epsilon$. We are therefore concerned with the effect on numerical computations.

Consider a function $f(x)$ with a discontinuity between $x = x_k$ and $x = x_{k+1}$ with a “jump” of, say, $J$.

An example of a function with a discontinuity between $x=x_k$ and $x=x_{k+1}$.

\[f_k\]
\[f_{k+1}\]
\[f_{k+2}\]

\[\text{Figure 4.1: A discontinuous function.}\]

The estimation of the function where it really is continuous, for example when interpolating between $x = x_{k+1}$ and $x = x_{k+2}$, has an error $e_{\text{max}}(x) = \max(f(x)) - \min(f(x))$, $x \in [x_{k+1}, x_{k+2}]$. First-order Taylor expansion gives:

$e_{\text{max}}(x) \propto (x_{f_{\text{max}}} - x_{f_{\text{min}}}) = \{\text{for some resolution}^1\} = |x_{k+1} - x_{k+2}| = \Delta x$.

If we on the other hand choose an interval involving a discontinuity, the error becomes $e_{\text{max}} = \max(f(x)) - \min(f(x)) = \max(x_k - x_{k+1}, J) \approx \Delta x + J$ [10].

\[^1\text{For the most functions we can assume that the we can chose a resolution so fine that the function is monotonically increasing or decreasing between } x = x_{k+1} \text{ and } x = x_{k+2}. \text{ Then } e_{\text{max}} = |f_{k+1} - f_{k+2}|.\]
Comparing this with the expressions for the second-order FDTD scheme ((3.4) - (3.9)), we can imagine that the accuracy no longer is of second order. Considering that we do have a finite number of discontinuities, then for a specific point in the computational domain the probability of a discontinuity is appearing there is proportional to $1/N$, where $N$ is the total problem size$^2$. From this we can imagine that the second order accuracy is destroyed due to the discontinuities.

The error should therefore become: $e_{tot} = c_1 \Delta x + c_2 \Delta x^2$. The constant $c_1$ could of course for some problem be so small that it is negligible at normal choices of $\Delta$. This was definitely not the case in this master project, as can be understood by examining Figure 1.2.

4.2 Regularization

Now we have arrived at one of the main subjects in this report. The appearing problem is to solve Maxwell's equations in a structure perforated with cylindrical holes, resulting in a discontinuous $\varepsilon(r)$.

In an attempt to achieve better numerical properties we replaces the discontinuous $\varepsilon(r)$ with a continuous function which we will call $\tilde{\varepsilon}(r)$ or transition region function. A couple of such functions are shown in Figure 4.2. The region in which $\varepsilon(r)$ differs from $\tilde{\varepsilon}(r)$ is called the transition region and the width of it is called $\delta_{\text{reg}}$.

The properties of different transition region functions in one dimension is discussed and examined in [3].

![Figure 4.2: A couple of transition region functions $\tilde{\varepsilon}$, here the transition region spans from -0.25 to 0.25, and the width of it, $\delta_{\text{reg}}$, is therefore 0.5. The original function, $\varepsilon(x)$, is a step function with a step from 10 to 1 which could be the case for the permittivity in a perforated material.](image)

$^2$In three dimensions, $N = N_x \times N_y \times N_z$
With \( \epsilon(r) \) replaced by \( \tilde{\epsilon}(r) \), the functions in the numerical algorithms no longer are discontinuous. The discretization error should be smaller. On the other hand we have changed the model, which introduces an error, a model error. Hopefully, but not for sure, we are able to find a minimum of the sum of these errors, the total error. The relationship of how the errors depend on the width of the transition region for a specific problem in one dimension is illustrated in Figure 4.3 [1][3]. In the case of waveguides there is a similar relationship, but it is not trivial to make a diagram of this. By the results we will find that it is possible to find a transition region function that makes the total error remarkably smaller.

![Graph](image)

**Figure 4.3:** Model error, discretization error and the total error as function of \( \delta \). The cell-size is constant. The total error is equal to the sum of the model error and the discretization error. The relationship may differ from problem to problem. The figure is reprinted from [3] with permission from the authors.
Chapter 5

Transmission and reflection properties

The main topic of this master’s project was to find out the transmission and reflection properties of waveguides. We are therefore more interested in the power flow rather than the actual component values of the fields.

5.1 Power flow

The energy flux at a specific time is defined by Poynting’s vector,

\[
S(r, t) = E(r, t) \times H(r, t) =
\]

\[
= (E_y H_z - E_z H_y, E_z H_x - E_x H_z, E_x H_y - E_y H_x)
\]

(5.1)

This is the energy per square meter propagating in the \(x\), \(y\) and \(z\) direction, respectively [8].

However, in this project we are interested in the transmission and reflection for specific frequencies. The field components are expressed as functions of the frequency instead of time, i.e. we take the Fourier transform of the components,

\[
E_x(r, \omega) = \int_{-\infty}^{\infty} E_x(r, t) e^{i\omega t} dt.
\]

(5.2)

Numerically we are not able to integrate over infinity, therefore the Fourier transform has to be approximated for some interesting values of \(\omega\) (which has to agree with the properties of the source),

\[
E_x(r, \omega_k) = \sum_{k=1}^{N_t} E_x(r, t_k) e^{i\omega_k t_k} \Delta t, \ t_k = k\Delta t.
\]

(5.3)

In the frequency domain, Poynting’s vector is defined as [19],

\[
S(r, \omega) = \frac{1}{2} E(r, \omega) \times H^*(r, \omega) =
\]

\[
= \frac{1}{2} (E_y H_z^* - E_z H_y^*, E_z H_x^* - E_x H_z^*, E_x H_y^* - E_y H_x^*).
\]

(5.4)

A problem that arises here is that the electric and magnetic fields are staggered from each other. Therefore the field components are interpolated to the center of every twinkle (a twinkle is the side of a Yee cell, see [18] for details).

Poynting’s vector describes the energy propagating in the \(x\), \(y\) and \(z\) direction. Considering a surface \(\mathcal{S}\), the energy passing through that surface, the power flow, is obtained by integrating the normal component of (5.4),

\[
P_{\mathcal{S}}(\omega) = \int_{\mathcal{S}} S(r, \omega) \cdot \hat{n} \, d\mathcal{S}.
\]

(5.5)
Considering $\mathcal{S}$ as a square in the $xz$-plane (as applied in this thesis for two different values of $y$) the power flow $P_y(\omega)$ becomes,

$$P_y(\omega) = \int_{z_1}^{z_2} \int_{x_1}^{x_2} S_y(r, \omega) \, dx \, dz,$$

(5.6)

numerically,

$$P_y(\omega) = \sum_{k_{x_1}} \sum_{i_{x_2}} S_y(r, \omega) \Delta x \Delta z,$$

(5.7)

Note that power flow may be positive or negative, in difference from energy.

## 5.2 Transmission

Two methods has been used to estimate the transmission. The source is the same in both methods.

### 5.2.1 Method 1: Comparing incident and transmitted energy

This method was mainly used for the W3 PC waveguide. The transmission is computed as,

$$T(\omega) = \frac{P(y_{trans}, \omega)}{P(y_{inc}, \omega)}$$

(5.8)

$y_{inc}$ is a value of $y$ at the very beginning of the waveguide and $y_{trans}$ at the very end (see Appendix A2 for details).

### 5.2.2 Method 2: Comparing with a reference structure

There may be numerical problems computing transmission with (5.8), for example unexpected reflections. An alternative way is to use a reference structure. Then we compute the power flows $P^{ref}(y_{trans})$ and $P^{ref}(y_{inc})$ for a structure where the subject of interest is not appearing in the specified problem, for example a waveguide without holes. Then we do the computations once again, with the interesting subject appearing. Now we can separate the transmission and reflection that is due to the interesting subject (for example how the holes is affecting the transmission and reflection properties).

The transmission becomes:

$$T(\omega) = \frac{P(y_{trans}, \omega)}{P^{ref}(y_{trans}, \omega)} \cdot$$

(5.9)

This is the fraction of energy that passes through an area at $y = y_{trans}$ with and without a specific subject. When analyzing the W1 PC waveguide this specific subject will consist of mirrors, and we thereby estimate the effect of the mirror.

## 5.3 Reflection

Figure 5.1 shows the reflection, the $E_x$-component as function of time at the detector closest to the source. The incident wave packet should be separated from the reflection, otherwise they may cancel each other out, and information is destroyed. For simplicity, we use reference structures whenever we compute reflections. The reflection is by definition:

$$R(\omega) = \frac{P^{ref}(y_{inc}, \omega)}{P(y_{inc}, \omega)},$$

(5.10)
We have to find an expression of $P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})$, the reflected energy. $P(y_{\text{inc}}, \omega_{\ell})$ is the sum of the incident and reflected wave, from this we have to subtract the incident wave. This can be done by subtracting $P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})$, the incident wave in the reference structure (defined in the section before this one),

$$R(\omega_{\ell}) = \frac{P(y_{\text{inc}}, \omega_{\ell}) - P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})}{P(y_{\text{inc}}, \omega_{\ell})} = 1 - \frac{P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})}{P(y_{\text{inc}}, \omega_{\ell})}. \quad (5.11)$$

It is not for granted that we should subtract $P^{\text{ref}}(y_{\text{inc}})$. Almost the same result is achieved if we subtract $P^{\text{ref}}(y_{\text{trans}})$. The reflection is mostly of interest when we are dealing with mirrors in waveguides. Then we might be interested in how efficient the mirror is in relation to a perfect mirror, that reflects the whole wave. In (5.11) we include numerical reflections and losses of the wave. An alternative way of computing the reflection would be:

$$R_{\text{eff}}(\omega_{\ell}) = \frac{P(y_{\text{inc}}, \omega_{\ell}) - P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})}{P^{\text{ref \ perfect \ mirror}}(y_{\text{inc}}, \omega_{\ell}) - P^{\text{ref}}(y_{\text{inc}}, \omega_{\ell})}. \quad (5.12)$$

$P(y_{\text{inc}}, \omega_{\ell})$ is the incident power flow in the waveguide we are interested of, which includes a mirror. $P^{\text{ref \ perfect \ mirror}}$ is the power flow in a reference structure with a perfect mirror located at the same place as the mirror in the waveguide. $P^{\text{ref}}$ is the power flow in a waveguide without mirrors.

However, the method with perfect mirrors has not been tested at all in this master project, it may contain secondary effects.

5.4 The loss

The loss, $L(\omega_{\ell})$, is the part of the wave that is neither transmitted nor reflected, i.e. the part of the wave that passes the first detector and then disappear from
the computational region without passing some of the detectors (probably emitted through some of the sides, making the waveguide a little bit “shining”). The definition is simply:

\[ L(\omega_l) = 1 - T(\omega_l) - R(\omega_l). \]  
(5.13)
Chapter 6

The source

To have some use at all for the equations describing time development of the fields we need either initial values for the fields (i.e. $E(t_0)$ and $H(t_0)$) or some kind of source that adds energy to the system. In this project a time dependent plane source has been used.

The natural choice of a source would be a signal consisting of sinusoidal waves. But we do also want the signal to appear as a wave packet (partially depending on the problems discussed in Section 5.3), therefore we multiply the signal with a Gaussian pulse,

$$E_{\text{source}}(x, z) = k(x, z) \cos(\omega_0 t) e^{-\frac{\omega_0^2}{2}(t-t_0)^2}, \quad \omega_0 = \frac{2\pi c_0}{\lambda_0}.$$  

(6.1)

When updating the fields, the electric field is given by (6.1) for the whole plane of a specific $y$ in the computational region (see Appendix A2, Chapter 9 on page 46).

(6.1) was the signal used for the W3 PC waveguide and is illustrated in Figure 6.1, with $k(x, z) = 1$, $\lambda_0 = 1550$ nm and $t_0 = 32/\omega_0$ (these parameters was used in the program, except that $k(x, z)$ was more complicated). The signal that was used for the W1 PC waveguide is slightly different and is illustrated in Figure 6.2.

Figure 6.1: To the left we see the time dependence of the pulse used as source when computing on the W3 PC waveguide in this project. To the right we see the Fourier transform of the pulse. There is a peak at $\lambda_0 = 1550$ nm, approximately 200 THz, in later transmission diagrams the frequency will be normalized by a constant $a = 450$ nm, then 200 THz corresponds to 0.29.

Analyzing the Fourier transform of the pulse (the right parts of Figures 6.1 and 6.2) we see that the signal will mainly involve frequencies around 150-250
Figure 6.2: To the left the pulse used when computing on the W1 PC waveguide. Because the properties of the waveguides are a bit different the pulses should be different as well. To the right the Fourier transform of the pulse.

Figure 6.3: $k(x, z)$ that was used in the W1 PC waveguide, a similar function was used when computing on the W3 PC waveguide.

THz (1200-2000 nm, or 0.23-0.38 in normalized frequency $(a/\lambda)$). This is the spectra we are interested in [6][5][7].

In (6.1) there is also a space dependent function $k(x, z)$, this function is displayed in Figure 6.3. The values of $k(x, z)$ was computed by Dr. Min Qiu at IMIT by help of the software FIMMWAVE - a vectorial 2D waveguide solver, Photon Design [20].
Chapter 7

Technical information

7.1 The GEMS-project

GEMS stands for General Electro Magnetic Solvers. The main objective with this project was to develop software for solving Maxwell’s equations. The software aims to on the international level be state of the art and form a platform for future development by Swedish industry and academia [1].

The GEMS-code was and is still developed by PSCI. See [22] for more information.

This master project was not a part of the GEMS project. However, the time domain part of the GEMS-code has been used and updated to handle regularization when computing on photonic waveguides. This part will be included in the GEMS-code.

More information of how to use regularization with the GEMS-code can be found in [24].

7.2 Computing resources

The computers at PDC have been used to run the program. Mostly the Linux cluster Lucidor has been used. This cluster consists of 90 nodes, each with two 900 MHz Itanium2 64-bit processors and 6 GB of main memory (RAM-memory). Only one node has been used at the time has been used [23].

When using regularization, the program has to handle with the information about $\varepsilon_{i,j,k}$. This requires a little bit more RAM-memory, but this is negligible in comparison to all the other variables the program handles with. In fact, the part of the code that handles with the structure had to be rewritten to handle with regularization, so running without regularization requires less RAM-memory than running with regularization.

A typical execution on Lucidor with the GEMS-code and regularization requires 420 MB of RAM-memory and takes 2 hours, 59 minutes and 7 seconds, the initialization procedure takes 3 seconds. Running the GEMS-code without regularization takes approximately the same time as with regularization. A typical execution (made by Dr. Ulf Andersson) takes 2 hours, 42 minutes and 24 seconds, the initialization procedure takes 1 minute and 52 seconds. Both examples was data for the W3 PC waveguide with a cell-size of 50 nm and 25 000 steps in time, Mur ABC was used in both cases.
Chapter 8

Results

Here the results are stated in form of transmission and reflection diagrams. Two types of waveguides have been used, “W3 PC” which has three rows free from air-holes and “W1 PC” with one single row free.

8.1 The W3 PC waveguide

The W3 PC waveguide consists of three layers of dielectric material with air holes etched in a triangular pattern. Three rows of holes are removed providing a path for the light.

8.1.1 Linear transition region function

The first transition region function to be used is $\tilde{\varepsilon}_1$, a linear function, i.e. the easiest possible function. Figure 8.1 shows the transmission when using $\tilde{\varepsilon}_1$ and four different values of $\delta_{\text{reg}}$.

One issue we should study is whatever we really achieve better accuracy with regularization. Figure 8.2 displays the transmission diagrams computed with and without regularization. As reference we have transmission diagrams computed without regularization and a cell-size of $dx = dy = dz = 50$ nm and also with $dx = dy = dz = 25$ nm, these were made by Dr. Ulf Andersson. Note that a cell-size of 25 nm compared to 50 nm results in 8 times as many variables and therefore approximately 8 times as much RAM-memory, the computational time is approximately 16 times as long, since also $\Delta t$ is half as large. When using regularization the cell-size is 50 nm.

The results seems to be better with a large value of $\delta_{\text{reg}}$. The transmission diagram when $\delta_{\text{reg}} = 80$ nm is no doubt closer to the transmission diagram with $dx = dy = dz = 25$ nm compared to $\delta_{\text{reg}} = 35$. This is definitely an indication telling us that regularization really may be a good method.
Figure 8.1: Transmission diagram for W3 PC using \( \tilde{\epsilon}_1 \) as transition region function, \( dx = dy = dz = 50 \text{nm} \).

Figure 8.2: Transmission diagram for W3 PC using \( \tilde{\epsilon}_1 \) as transition region function, \( dx = dy = dz = 50 \text{nm} \). As reference (solid black curve) there is the result when computing with \( dx = dy = dz = 25 \text{nm} \) and \( dx = dy = dz = 50 \text{nm} \), but without regularization (the references was made by Dr. Ulf Andersson).
8.1.2 Non-linear transition region function

The next transition region function to be used is $\tilde{\epsilon}_{3C}$. The result seems to be roughly the same as for $\tilde{\epsilon}_1$. One should keep in mind that the cell size is about the same size as $\delta_{reg}$. Maybe the difference would have been larger for other kinds of problems.

Figure 8.3: Transmission diagram for W3 PC using $\tilde{\epsilon}_{3C}$ as transition region function, $dx = dy = dz = 50\text{nm}$.

Figure 8.4: Comparison, transmission diagrams for $\tilde{\epsilon}_{3C}$ with $dx=dy=dz=50\text{nm}$, and transmission diagrams without transmission with $dx=dy=dz=50\text{nm}$ resp. $dx=dy=dz=25\text{nm}$. As reference (solid black curve) there is the result when computing with $dx = dy = dz = 25\text{nm}$ and $dx = dy = dz = 50\text{nm}$, but without regularization (the references were made by Dr. Ulf Andersson).
8.1.3 Transition region chosen as huge as possible

Since the results seem to be better with large values of $\delta_{\text{reg}}$, the next figure shows the result when $\delta_{\text{reg}}$ is chosen as large as possible, namely two times the radius, 126 nm. The transmission diagrams (Figure 8.5) seem to be close to

![Transmission diagram for W3 PC, $\delta_{\text{reg}}$ chosen as large as possible, 126 nm. Five different transition region functions. As reference (dotted curve) there is the result when computing with $dx = dy = dz = 25\text{nm}$ without regularization (the reference was made by Dr. Ulf Andersson)](image)

the reference at a normalized frequency of 0.28, but differs at other frequencies. The reason for this may be the properties of the source. The source produces waves centered at 0.29 (see Chapter 6 on page 20).

$\tilde{\epsilon}_{3M}$ and $\tilde{\epsilon}_{5CM}$ seems to be the least good transition region function around a frequency of 0.28, but on the other hand these are the best around 0.35. Once again we should keep in mind that the cell-size is about the same size as $\delta_{\text{reg}}$.

8.1.4 Conical air-holes

The holes in the waveguides are not perfectly cylindrical, but a little bit conical, as one can imagine when investigating Figure 1.2 on page 3. To investigate how this may affect the transmission, the holes were divided in a couple of layers with different radius, as shown in Figure 8.7.
From the results in Figure 8.6, it is clear that the transmission may be remarkably influenced by the conical shape. The dip at 0.28 is moved to the left and the transmission is not as close to 1.0 as it is with completely cylindrical holes.

The holes are not completely parallel to each other either. This has not been investigated.

Figure 8.6: Transmission diagrams when the air holes are a bit conical. Three different slopes and the normal, cylindrical hole. The shape of the holes are shown in Figure 8.7.

Figure 8.7: The shape of the air holes when they are conical.
8.1.5 The dependence of the depth of the holes

We are also interested in how the depth of the holes affects the transmission. Figure 8.8 shows the transmission in the case of four different depths of the holes (usually the depth is 2000 nm).

The influence on the transmission is remarkably small when the depth is changed from 2000 to 1000 nm. On the other hand, the influence is large when changing from 1000 to 650 nm. The reason for this is that most part of the wave is propagating in the upper part of the waveguide.

In connection to conical holes, one understands that the holes could be cylindrical between a depth of 0 to 1000 nm, and conical below 1000 nm, with limited effects on the transmission.

![Transmission diagrams. Different depth of the holes: 2000 nm (usual), 1500, 1000 and 650 nm.](image)

Figure 8.8: The dependence of depth. Completely cylindrical holes (once again).

8.1.6 25 nanometers precision

We may be interested in how the result would be with both regularization and 25 nanometers precision. Figure 8.9 shows that the transmission diagrams when computing with and without regularization are very close to each other. The reason could be that we are rather close to the true transmission of this model.

It would be interesting to divide the cell size once again, to 12.5 nm, but the computer resources do not allow this since this requires 64 times as much RAM-memory and 256 times as long computational time (approximately) as with 50 nm.
8.1. THE W3 PC WAVEGUIDE

Figure 8.9: Transmission diagram for W3 PC with a cell-size of 25 nm and 50 nm, respectively. $\delta_{\text{reg}}$ has the same value as the cell-size. As reference (solid black curve) there is the result when computing with a cell-size of $dx = dy = dz = 25$ nm, but without regularization (reference made by Dr. Ulf Andersson).

8.1.7 Comparison with experimental results

Independently of how much we compute on the problems, we still cannot be sure that we have taken everything into account. Therefore it is of great interest to compare the computations done with FDTD with experimental results, done by experimental physicists at IMIT. As we see in Figure 8.10 the experimental

Figure 8.10: Comparison with experimental results. The figure maybe looks a bit strange, it is two different graphs with independent axes suited together. Data taken from [5].
results are definitely not completely in agreement with the results from FDTD. Both the author as well as Dr. Ulf Andersson have noticed that the dip around 0.27-0.28 moves to the left the better the resolution is. On the other hand Jing Gong, the former master project student, have recognized the opposite behavior, that the dip is approaching the experimental results from the left instead of from the right. The reason may be that Jing wrote a separate code at IMIT. Maybe we have used slightly different sources or something [5]. In other moments in this project it has been recognized that the results may be very dependent of changes in the source.

The movement of the dip may also depend on the conical shape of the air-holes. In fact, comparing Figure 8.10 with Figure 8.6 at page 27, the experimental results seem to agree better with a transmission diagram computed with conical holes.

Finally, one should keep in mind that even the experimental results may include errors.

8.2 W1 PC

According to communication with Dr. Min Qiu, the research on the W3 PC waveguide made by IMIT turned to show that it was difficult to get the waveguide function in a proper way. Therefore another waveguide was introduced, the W1 PC waveguide.

The W1 PC waveguide consists of just one layer of dielectric media, and has one row free from air holes, or almost free. The air holes is pass through the whole layer, in difference from the W3 PC waveguide.

Here we will mainly deal with the influence of mirrors in the waveguide. The transition function will be \( \tilde{c}(r) \) and the width of the transition region, \( \delta_{\text{reg}} \) will be 135/2 nm all the time. The radius of the holes is 135 nm, slightly smaller than in the W3 PC waveguide. The distance between the holes, \( a \), is 450 nm, as for W3 PC. The grid size has been \( \Delta x = \Delta y = \Delta z = 20 \) nm, compared to 50 nm for W3 PC. The CFL-number is the same as before.

8.2.1 W1 PC without mirrors

With no mirrors in the path the light is permitted to propagate quite unhindered. The left part of Figure 8.11 shows the W1 PC waveguide without mirrors,
the right part shows one of the field components as function of time at three different positions. Figure 8.12 shows that 70-90% of the light passes the waveguide.

Figure 8.11: Left figure: The structure of W1 PC. Right figure: The probes, showing the x-component of the electric field in the middle of the guide as function of time for three different points, three different values of y: 34\(dy\), 360\(dy\) and 821\(dy\).

Figure 8.12: Left figure: The transmission diagram of the W1 PC waveguide. The transmission is computed as the transmitted energy divided by the incident. Right figure: The transmitted energy and the incident energy. We see that these energies are very close to each other, which causes trouble when dividing these with each other. As a result of this, the transmission seems to oscillate. We note that the transmission and reflection diagrams may not be reliable for frequencies below 0.28 and above 0.305 (approximately).
8.2.2 Mirrors

The simplest way to include a mirror in the waveguide is by letting one single air-hole be present in the guide. It is of significance that the holes that a mirror consists of is arranged in the same triangular pattern as all the other holes. The left part of Figure 8.13 shows the structure with one single-hole mirror. The right part shows the probes. From now on the transmission and reflection will be computed by the second method, by the use of a reference waveguide, namely the waveguide without mirror displayed in Figure 8.11.

A mirror may also consist of two air holes, here we will refer to this as a “double mirror”. This mirror will reflect more of the wave than a single hole mirror, Figure 8.14 shows the structure with one double-hole mirror and the probes of this.

![Figure 8.13](image1.png)

**Figure 8.13**: Left: The structure, one single mirror. Right: The probes, showing the x-component of the electric field at three points: one probe in the middle of each detector (see Appendix for more information) and one in between.

![Figure 8.14](image2.png)

**Figure 8.14**: Left figure: The structure, one double mirror, consisting of two air holes. Right figure: The probes, showing the same information in correspondence to Figure 8.13.

At first, we investigate how the properties depends on the radius that the mirrors consists of. Figures 8.15 and 8.17 shows transmission and reflection diagrams for single and double mirrors, respectively. It is also of interest to know how much of the wave that is lost, i.e. either transmitted or reflected. Figures 8.16 and 8.18 shows the loss as a function of the wavelength.
8.2.3 W1 PC with a mirror consisting of one air hole - dependence of radius

Figure 8.15: Transmission and reflection diagrams, the dependence of the radius of the air hole that the mirror consists of.

Figure 8.16: The loss, i.e. $1 - T - R$, $T$ is the transmission, $R$ the reflection.
8.2.4 W1 PC with a mirror consisting of two air holes - dependence of radius

Figure 8.17: Transmission diagrams, the dependence of the radius of the two air holes that the mirror consists of.

Figure 8.18: The loss, i.e. \(1 - T - R\), \(T\) is the transmission, \(R\) the reflection.
8.2. W1 PC

Figure 8.15 appears to have been computed with 100 000 steps in time all over, but in some cases only 50 000 steps was used. A number of 50 000 steps were not really enough to minimize non-physical oscillations, but the trouble is that these kinds of computations are very time consuming and deserves compromises.

It is clear that the reflection is higher with a “two air holes mirror” (double mirror). At the same time the transmission is much smaller. Therefore the total loss is less with a single air hole mirror. As expected the transmission is higher with small air holes.

8.2.5 The effect of moving the mirror

Another way to affect the properties of the waveguide is to move the mirror a little bit in comparison to the other air holes. The triangular lattice the air holes is arranged in is necessary in order to achieve a band gap effect. Moving the mirror away from this lattice may exhibit interesting phenomena.

![Diagram of mirror movement](image)

Figure 8.19: *How the mirror is moved by a distance b. When dealing with double-mirrors the two air holes are moved together, keeping the distance between them constant.*

Figures 8.20 and 8.22 shows transmission and reflection diagrams for single and double mirrors, respectively. Figures 8.21 and 8.23 shows the loss as a function of the wavelength.
8.2.6 W1 PC with a mirror consisting of one air hole - dependence of the mirrors position

Figure 8.20: The reflection and the transmission.

Figure 8.21: The losses.
8.2.7 W1 PC with a mirror consisting of two air holes - dependence of the mirrors position

Figure 8.22: The reflection and the transmission.

Figure 8.23: The losses.
It is definitely clear that the transmission and the reflection are affected by the value of $b$. When $b$ is equal to 0.5 the reflection is very close to zero for some frequencies (around 0.29) whereas the reflection is around 0.9 for the same frequencies when $b$ is equal to 0.1. The transmission shows the opposite behavior.

The minimum loss is obtained in the case when $b = 0.5$. The reason for this could be that the mirror is not effective as a mirror and therefore more light is transmitted. Of course less light is reflected at the same time but obviously this effect is smaller than the effect on the transmission.

### 8.2.8 The dependence on the number of air holes in a mirror

So far, all mirrors have consisted of one or two air holes. A question arises concerning how many air holes a mirror should consist of, and what the differences are between these.

A mirror could of course be arranged in a more complex way to achieve specific properties. Figure 8.24 shows a structure with 4 air holes with different radius. According to the results, the reflection increases with the radius, but

![Figure 8.24: A mirror consisting of 4 air-holes with increasing radius, see the result in Figure 8.25.](image)

the difference seems small between 2, 3 and 4 mirrors. The transmission seen in 8.25 is close to zero in all cases but the case of one mirror.

The loss (Figure 8.26) is smallest with one mirror.
Figure 8.25: Transmission and reflection with one, two, three and four mirrors. The appearance of “increasing radius mirror” is clear from Figure 8.24.

Figure 8.26: The losses. The appearance of “increasing radius mirror” is clear from Figure 8.24.
8.3 W1 PC waveguide with two mirrors

A very interesting phenomena occurs if the waveguide includes two mirrors, with a specific distance between them, as seen in 8.27. When the wave hits the mirrors, one part of the wave will be reflected and one part will be transmitted, as we have seen earlier. Between the mirrors the wave is captured, bouncing between the mirrors.

8.3.1 Single-hole mirrors

In the simplest case the mirrors consists of two air holes. The distance between the holes is 5400 nm. The right part of Figure 8.27 shows that the wave has not really left the waveguide when the simulation was interrupted after ap-

Figure 8.27: Left: the structure, the holes acts like mirrors, and “captures” the wave. Right: How the field between the mirrors is decreasing (the $E_x$ component at $x = nx \Delta x/2, z = nz \Delta z/2$ and $y = 7200 \text{ nm}$ as function of time)

Figure 8.28: The transmission through the W1 PC waveguide with two mirrors. Two different method used. The left holes of the mirrors are located at and nm, the distance between the mirrors is 5400 nm.

Between the holes is 5400 nm. The right part of Figure 8.27 shows that the wave has not really left the waveguide when the simulation was interrupted after ap-
proximately 250 000 steps in time. However it was not possible to continue the simulation due to the rules of the computer usage\(^1\).

Figure 8.28 shows the transmission diagram. Both methods for computing the transmission has been used. Probably the solid line is a better estimation than the dash-dotted line but they are obviously close to each other.

It is remarkable how narrow the peaks are. This could probably be used in technical applications to filter out signals with different wavelengths, but of course there are other problems in constructing a functioning system. For example it is a problem to have a usage at all for the reflected wave.

### 8.3.2 Double-hole mirrors

Here each of the mirrors consists of two mirrors. The distance between the holes is 8100 nm, i.e., a bit longer then the computations with single-hole mirrors. The peaks seems to be even sharper. The right part of Figure 8.29 shows that an even greater part of the wave is still left between the mirrors when the computations are interrupted. The transmission diagram is shown in Figure 8.29. It would be desirable to use a computation longer than 60 hours.

\[
\begin{array}{c}
\text{Figure 8.29: Left: The structure, the holes acts like mirrors, and “captures” the wave. Note that the distance between the holes is a little bit different from the example before. Right: How the field between the mirrors is decreasing (The } E_x \text{ component at } y=7200 \text{ nm).}
\end{array}
\]

Figure 8.30 shows the transmission diagram.

### 8.3.3 Experimental results of the W1 PC waveguide

In [21], experimental results of the W1 PC waveguide is presented. I have tried to verify these with computer simulation, but by some reason the computations became unstable after approximately 50000 steps in time. The problem was that this waveguide required a larger computational area, which requires larger computer capacity or simplifications.

The right part of Figure 8.31 shows the transmission diagram from the experimental results, the left part a SEM micro graph picture of the real waveguide. It is possible to see similarities with this diagram and the diagrams of the simulations of the W1 PC waveguide with two mirrors, the amplitude is around

\[^1\text{I’m not permitted to execute computations longer then 60 hours.}\]
Figure 8.30: The transmission computed by help of a reference waveguide without mirrors. The left holes of the mirrors are located at 4500 and 13050 nm, the distance between the mirrors is 8100 nm.

0.01-0.03 and there are three distinct peaks. Somewhat surprising, the agreement is better in comparison with the single-hole mirrors than the double-hole mirrors. The reason should be that there are other parameters than the number of holes in the mirrors that are different.

Figure 8.31: To the left a “SEM micrography picture” of the W1 PC waveguide. To the right experimental results of this waveguide. A wavelength of 1560 nm corresponds to a normalized frequency of 0.29. Pictures reprinted from [21] with permission.
Chapter 9

Summary and conclusions

Regularization has been showed to improve the accuracy when computing on photonic waveguides with the FDTD method. However there seems not to be an easy way to decide which is the best way to do this. Different transition region functions has different effects on different problems.

The best choice of $\delta_{reg}$, the width of the transition region, seems to be to choose this as large as possible. This indicates that the discretization error is huge compared to the model error that regularization causes. In other words one could say that the accuracy becomes better the more regularization that is used.

Experimental results seems to confirm the computations, but far away from exactly. A higher resolution could solve this problem, but not for sure.

The FDTD method with or without regularization should primarily be used to analyze effects of different positions of mirrors and similar, rather than designing a whole system and hope it will work. When analyzing specific effects, one could use a much smaller structure, which would result in shorter computational time and less memory consumption.

The capacity of the computer systems is definitely a limit, especially the RAM-memory. Therefore it would be interesting to use parallel computations on the problems, i.e. connect several computers with each other.

We have seen examples that indicate that the properties of the source seem to affect the transmission and reflection properties remarkably, at least according to my subjective opinion. It could be interesting to test different types of sources. It could also be interesting to study the convergence. This could be done with three different cell-sizes, for example $\Delta x = \Delta y = \Delta z = 50$ nm, 25 nm, and 12.5 nm in the W3 PC waveguide. From this it would be possible to get an estimation of the order of convergence. However, for the W3 PC waveguide used in this project, the computers does not allow a higher resolution than 25 nm, approximately. It would be possible to use other cell-sizes, for example, $\Delta x = \Delta y = \Delta z = 50$ nm, 37.5 nm, and 25 nm, but then it would be a bit troublesome to create a source file for 37.5 nm (describing the space dependent function $k(x, z)$, see Chapter 6 on page 20).

One have to keep in mind that the resolution has to be so high that it describes the shape of the structure well enough. A cell-size of 50 nm means that the distance between the holes is 9 times the cell-size, 25 nm means 18 times the cell-size. There is definitely a difference in the result from these two cell-sizes. The choice of $\delta_{reg}$, the width of the transition region, has been of almost the same size as the cell-size. We have not been able to observe that one particular transition region function is better than the others, which could be due to the resolution.

In all simulations that has been done, the structure as well as the source has been symmetric. From this follows that even the solution is symmetric.
Therefore it would be possible to simulate just the right part of the waveguide
and reflect this solution to the left part of the waveguide. Thereby the number
of variables would be divided by two, with no loss of accuracy.

Since Maxwell’s equations are linear, it is possible to divide the function of
permittivity, \( \epsilon(r) \), in a way that the sum of the functions is approximating the
permittivity, i.e. \( \epsilon(r) \approx \epsilon_A(r) + \epsilon_B(r) + \epsilon_C(r) \). The function of permittivity is a
step function, it could be approximated as the sum of sinusoidal functions (due
to fourier analysis). Then the program could be used for each of the sinusoidal
functions. The solution (the fields) is the sum of the sub-solutions. However, the
expression of the Poynting’s vector is not linear, the program has to be rewritten
to compute the transmission and reflection properly. This has therefore not been
tested and may not work good in the reality.

The part of the Fortran 90 code that has been written will be included in
the GEMS code.

Parallel with this master project, two abstracts have been written by Ulf
Andersson, Min Qiu and the author of this thesis: one two-page abstract sub-
mitted to ECOC2004 [25] and one one-page abstract submitted to EMB04 [26].
Both abstracts has been accepted.
Appendix

A1. The detector plane of W1 PC

Figure 9.1: The detector area (as a dotted square) of the W1 PC waveguide used in the program (the xz-plane). The detector area is nine times as large as the area of the real “guide” (the boundary to the holes is symbolized with a dashed line).
A2. W1 PC from above

Figure 9.2: Location of the detectors and the source for the W1 PC waveguide
A3. The indata file used by the program - the W3 PC waveguide

file=reg_W3PC.dat:

Data read from reg_material.f90.

DELTA_REG (nm): ('value * r' or 'value * 1')
65 * 1

TRANSITION_FUNCTION (1,3M,3C,5CM or 5MM)
5MM

DEPTH_OF_THE_HOLES (nm):
2000.0

DISTANCE_BETWEEN_HOLES
450.0

RADIUS_OF_HOLES ('value * a' or 'value * 1')
0.36 * a

LENGTH_L1 (nm): (OBS:L2 = L1 and L3 = ny*dy-L1-L2)
5000.0

WIDTH_W1 (nm): (OBS:W2 = (nx*dx-W1)*0.5_rfp)
1200.0

CONICAL_HOLES ENABLED

CONICAL_NR_OF_SEGMENTS nr of segments the hole is divided in (1 is default)
1

CONICAL_RADIUS_AT_DEPTH The radius of the holes at depth prop to the radius (0<= r <=1)
1

HEIGHT_OF_THE_LAYERS Height of the layers (from z=0)
4950 5400 5600

EPSILON_OF_THE_LAYERS
10 11.2 10

ORDER_OF_ACCURACY the order of accuracy in the FDTD-loop
2

CONSTANTS
1 1

EPSILON_ZERO
8.8541878

PART_OF_R
1
DISABLE_ALL_HOLES
FALSE

WAVE_GUIDE
W3PC

MIRROR_W1PC
DISABLED

NUMBER_OF_MIRRORS
0

MIRRORS_Y_POSITIONS
1000
2000

EOF
A4. The indata file used by the program - the W1 PC waveguide

file=reg_W1PC.dat:

Data read from reg_material.f90. NOTE: all distances in nanometers!

DELTA_REG (nm): ('value * r' or 'value * 1')
0.5 * r

TRANSITION_FUNCTION (1,3M,3C,5CM or 5MM)
3C

DEPTH_OF_THE_HOLES (nm):
1500.0

DISTANCE_BETWEEN_HOLES (nm):
450.0

RADIUS_OF_HOLES ('value * a' (i.e. unitless) or 'value * 1' (nm))
135 * 1

LENGTH_L1 (nm): (OBS:L2 = L1 and L3 = ny*dy-L1-L2)
0.0

WIDTH_W1 (nm): (OBS:W2 = (nx*dx-W1)*0.5_rfp)
400.0

CONICAL_HOLES
DISABLED

CONICAL_NR_OF_SEGMENTS nr of segments the hole is divided in (1 is default)
1

CONICAL_RADIUS_AT_DEPTH The radius of the holes at depth prop to the radius (0<= r <=1)
1

HEIGHT_OF_THE_LAYERS Height of the layers (from z=0)
600 900 1500

EPSILON_OF_THE_LAYERS
1.0 10.0489 1.0

ORDER_OF_ACCURACY the order of accuracy in the FDTD-loop
2

CONSTANTS
1 1

EPSILON_ZERO
8.8541878

PART_OF_R
1.0

DISABLE_ALL_HOLES
FALSE

WAVE_GUIDE
W1PC

MIRROR_W1PC
DISABLED

NUMBER_OF_MIRRORS
2

MIRRORS_Y_POSITIONS
1000
2000

MIRRORS_RADIUS_Q
1.0
1.0

EDF
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