Time-Domain Inverse Electromagnetic Scattering using FDTD and Gradient-based Minimization

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Abstract

The thesis addresses time-domain inverse electromagnetic scattering for determining unknown characteristics of an object from observations of the scattered field. Applications include non-destructive characterization of media and optimization of material properties, for example the design of radar absorbing materials. Another interesting application is the parameter optimization of subcell models to avoid detailed modeling of complex geometries.

The inverse problem is formulated as an optimal control problem where the cost function to be minimized is the difference between the estimated and observed fields, and the control parameters are the unknown object characteristics. The problem is solved in a deterministic gradient-based optimization algorithm using a parallel 2D FDTD scheme for the direct problem. This approach is computationally intensive since the direct problem needs to be solved in every optimization iteration in order to compute an estimated field. Highly accurate analytical gradients are computed from the adjoint formulation. In addition to giving better accuracy than finite differences, the analytical gradients also have the advantage of only requiring one direct and one adjoint problem to be solved regardless of the number of parameters.

When absorbing boundary conditions are used to truncate the computational domain, the equations are non-reversible and the entire time-history of the direct solution needs to be stored for the gradient computation. However, using an additional direct simulation and a restart procedure it is possible to keep the storage at an acceptable level.

The inverse method has been successfully applied to a wide range of industrial problems within the European project, IMPACT (Inverse Methods for Wave Propagation Applications in Time-Domain). The results presented here include characterization of layered dispersive media, determination of parameters in subcell models for thin sheets and narrow slots and optimization problems where the observed field is given by design objectives.

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Chapter 1

Introduction

1.1 Background

In the modern society electromagnetic fields are used in many different devices and for many different purposes. Common examples include wireless communication in antenna systems for mobile phones and satellites, heating in microwave ovens and medical X-ray imaging equipment and tomography. As a result it has become increasingly important to have a good understanding of the electromagnetic field and how it interacts with the environment. The propagation of the field is described by a system of partial differential equations (PDEs) called Maxwell’s equations, [31]. Even though the equations themselves are simple, the added complexity of boundary conditions and materials precludes the exact solution of most realistic problem. Since experiments are usually very costly and time-consuming, numerical simulation often represents the most efficient tool for analysis and design. Computational electromagnetics (CEM) has experienced a tremendous growth in the last decades due to the availability of powerful computers. Some of the applications that receive most attention are

- prediction of radar cross-section (RCS),
- antenna coupling and analysis,
- microwave devices and guided structures,
- electromagnetic compatibility (EMC),
- bioelectromagnetics, e.g. tomography or determination of the specific absorption rate (SAR) for radiation from mobile phones.

The main focus of CEM has previously been the development of efficient solvers for what we refer to as the direct problem. That is, finding the solution to Maxwell’s
Chapter 1. Introduction

Figure 1.1. Anechoic chamber used for reflection experiments at Saab Bofors Dynamics, Linköping. (Courtesy of Erik Söderström, AeroTechTelub AB.)

Equations for a particular problem where all physical parameters are known. Examples include determining the radiation pattern of an antenna or the radar cross section of an aircraft. The computational power of modern computers now makes it possible to address the more difficult and in many cases more interesting tasks of design optimization and inverse problems. In these problems the physical properties are not fully characterized but contain unknown parameters. For example, one may wish to prescribe a desired radiation pattern for an antenna and then determine the characteristic parameters of the antenna to obtain this pattern. Another example is the design of radar absorbing materials to minimize the RCS. Also, reflection measurements are used to determine the characteristics of unknown media. Similar problems arise in medical applications where X-rays are used to investigate the human body, for instance to locate tumors.

This thesis is based on work done within the European project IMPACT (Inverse Methods for Wave Propagation Applications in Time-Domain) where inverse scattering problems in time-domain are considered. The main purpose of our work has been the development of a general inverse code using an existing solver for the direct problem. Several applications have been addressed, including non-destructive characterization of dispersive media and determination of geometrical parameters in so-called subcell models.
We use deterministic gradient-based minimization where the cost function is the difference between estimated and observed fields. This approach is general but computationally intensive since the direct problem needs to be solved in each optimization iteration. Discrete gradients are derived using a Lagrange multiplier formulation. The resulting gradient expressions contain the solution to the adjoint problem which is very similar to the direct problem. The direct and adjoint problems are solved using a parallel finite-difference, time-domain (FDTD) code. The work is based on previous investigations by Stephane Alestra at EADS, in [3].

1.2 Inverse scattering

For any electromagnetic problem we may distinguish between the fundamental part, consisting of the governing equations, and the data i.e. boundary and initial conditions, sources and physical properties, such as geometry and media. Finding the fields from the governing equations with given data is the direct or forward problem. In the inverse problem the field is partially known, for example from measurements or design objectives, and we wish to determine the data from which this observed field originates. In particular, the investigation of an object by measuring the scattered field outside the object is called inverse scattering. Figure 1.2 illustrates an inverse scattering experiment where an unknown object is illuminated by an incident plane wave and the scattered field is observed in a number of receivers. We

![Figure 1.2. The inverse scattering problem.](image-url)
Chapter 1. Introduction

distinguish between two common types of inverse scattering problems. The inverse media problem where we wish to determine the material parameters of the scatterer and the inverse obstacle problem where the geometrical shape of a perfectly reflecting body is sought. In this thesis we will only consider the inverse media problem where the unknown parameters appear in the coefficients of the governing equations.

1.2.1 Difficulties in the inverse problem

The inverse problem is more difficult to solve than the direct problem mainly due to ill-posedness and non-linearity. A problem is called well-posed if the solution exists, is unique and continuous with respect to the data. If any of these properties is not fulfilled the problem is called ill-posed. Inverse problems are usually ill-posed due to a number of reasons. The inverse scattering problem, where the field is only observed outside the scatterer, has inherently non-unique solution since evanescent fields resulting from lossy media or small geometrical features are not observed. Other common difficulties are:

- Lack of data. The observed data is not complete, for example due to limited spatial or frequential information in measurement data.
- Noisy data. Experimental data is contaminated with random perturbations.
- Unreachable observation data. The desired response in an optimization problem may be non-physical or otherwise unattainable by the direct model.
- Inexact method. Numerical approximations may lead to instability (ill-conditioned systems of equations) and limited resolution of discrete models may result in non-physical solutions.

The theoretical analysis of inverse problems has primarily been concerned with the issue of instability, for which a unified treatment using regularization is possible. Most of the available theory is limited to linear inverse problems. In [13] a thorough description of the regularization method is given including convergence results.

The inverse scattering problem is non-linear, i.e. the scattered field depends non-linearly on the parameters of the unknown object. This is a serious practical difficulty since it precludes direct solution methods and leads to non-convex minimization. However, in some cases it is possible to linearize the inverse problem.

1.2.2 Methods

Analytical solutions of inverse electromagnetic scattering problems are possible only in a few special cases, such as scattering from layered media in one dimension. More interesting problems require approximative techniques. The early methods typically involved approximations of the physics in order to obtain a simplified model for the direct problem.
In the Born and Rytov approximations [6] linear relations between the material properties of the scatterer and the scattered field are obtained by assuming that the contrast between the scatterer and the background media is low, so-called weak scattering. The error of the approximation depends on the frequency of the incident wave, see [21] for a discussion of the validity of the approximations. In both cases the scattered field is related to the object through a Fourier integral. The Fourier space is covered by varying the position of transmitter and receiver as well as the frequency and the object is recovered using an inverse transform. This inverse algorithm is called diffraction tomography [11]–[12]. An iterative variant of the Born inverse method, called the Born-iterative method, [43] takes into account multiple scattering effects which are omitted using a linear model. In X-ray tomography the WKB approximation, see [8], is used to linearize the inverse problem. It states that for high frequencies, electromagnetic waves propagate like rays with very little back scattering. The attenuation of the penetrating wave and the material properties of the scatterer are then related by a linear functional which may be expressed as a Radon transform, [36]. Inverse reconstruction using the Radon transform is called back-projection tomography. In case the object is perfectly conducting, the physical optics approximation (PO) may be applied to linearize the inverse problem. The resulting problem may be solved in a diffraction tomography manner, see [25] and [19]. However, the PO approximation is feasible only for convex objects and high frequencies.

In addition to the severe physical approximations, all of the above methods require great flexibility in the measurement procedure since the inverse transform typically relies on observation data for many different angles of incidence and many different frequencies. Further, multiple scattering effects, which are important for non-convex geometries with high contrast between background media and scatterer, are lost in the linearization.

A more general approach is given by minimization where the error between simulated and measured field is minimized by varying the unknown parameters in an iterative optimization algorithm. This method is costly, in particular for higher dimensions, since the direct problem needs to be solved in each iteration. The minimization approach was introduced for acoustic problems in [41]. In most references, deterministic algorithms such as the conjugate gradient and quasi-Newton methods are used but global optimization has also been applied, see [33], [45] and [29] for applications in electromagnetics.

Regarding the choice of solver for the direct problem several possibilities exist. Due to the availability of powerful computers it has become feasible to use exact methods for multi-dimensional problems. Examples include finite-differences (FDTD) and finite-elements where the governing differential equation is discretized on a volume mesh and methods based on the equivalence principle where integral equations are solved on a surface mesh, such as the method of moments. As a rule a volume method is the preferred choice for problems containing different media while the method of moments is more efficient for perfectly conducting structures. Most inverse methods in the literature are formulated in the frequency domain.
However, the possibility to cover a large range of frequencies using pulse excitation makes time-domain approaches attractive. In addition, the time dimension makes it possible to solve inverse problems with limited spatial observation data and further time-gating may be used to filter the observation data. For time-domain minimization approaches see for example [28] and [3]. In [34] FDTD is used in a layer-stripping reconstruction algorithm. We also mention inverse scattering using wave-splitting where the field is decomposed into waves traveling in opposite directions. The inverse problem is solved in a layer-stripping manner using so-called invariant embedding as described in [38] and [17].

1.3 Outline

In the remaining part of the thesis we describe the minimization approach to the inverse scattering problem for Maxwell’s equations in dispersive media.

In Chapter 2 we focus on the non-linear optimization problem and discuss some of the most common algorithms used. The deterministic algorithms require derivative information and we show how accurate gradients are derived using Lagrange multipliers and the adjoint problem.

The numerical solution of the direct problem for Maxwell’s equations using FDTD is described in Chapter 3.

In Chapter 4 we give a general form of Maxwell’s equations suitable for the different types of media encountered in our applications. The adjoint equations and gradients for the continuous two-dimensional equations in simple media are also derived. The corresponding derivations for the discrete problem are done in Chapter 5. A discrete derivation is necessary to avoid introducing errors in the gradient. Due to the absorbing boundary conditions the equations are not reversible and the full time-history of the direct and adjoint fields has to be stored. The memory requirements may be relaxed using an additional direct simulation.

In Chapter 6 we address the inverse problem for subcell parameters and derive gradients using the adjoint approach. The derivation becomes quite technical due to the discrete nature of the subcell models.

Finally, in Chapter 7 we present results from various inverse problems. The main application is the reconstruction of media in multilayer structures. For this case measurement data has been used to validate the approach. Other results include reconstruction of dispersive media and subcell parameters using synthetic observation data. We also study how the cost function is affected by changing the frequency of the incident field and the amount of observation data.
Chapter 2

Minimization

2.1 Introduction

In the minimization approach for inverse scattering the cost function is a measure of the difference between the observed field and the computed field for some trial parameters and an optimizer is applied to improve the solution. Since each evaluation of the cost function requires the solution of the direct problem the computational cost is high, particularly for three-dimensional problems. The resulting optimization problem is non-linear and may contain many local minima. Regularization using a priori information is therefore often employed to obtain a smoother cost function and limit the parameter space. In non-linear optimization there are two basic choices, global optimization where one attempts to find (approximately) the global minimum using stochastic methods, and local, deterministic optimization where gradient information is used to find a local minima. Global techniques, such as simulated annealing [37], [32] and genetic algorithms [18], [16], often require a large number of cost function evaluations and are therefore considered more costly than local methods. We have chosen deterministic, gradient-based optimization using gradients obtained by an adjoint formulation. The resulting gradients require a lot of disk space but the computational cost is independent of the number of parameters. The adjoint approach for the parameter identification problem was introduced in [7] and is also described in for example [42].

2.2 The minimization problem

Let \( A(p) \) be the direct solution operator depending on some unknown parameters \( p \) and let \( y \) denote the observed field. The inverse problem to determine \( p \) from \( y \)
may then be formulated as the least squares minimization

$$\min_p j(p), \quad j(p) = \frac{1}{2} \| A(p) - y \|^2_2$$

(2.1)

In practice the direct problem is discretized and solved using a numerical method. The resulting minimization problem is therefore finite dimensional and we will assume that $p \in \mathbb{R}^n$. In (the unusual) case of a linear direct solution operator $A(p) = Ap$ the cost function becomes a quadratic function in $p$. Provided that $A^T A$ is non-singular this function has a unique minimum given by the solution to the normal equations

$$A^T A p = A^T y$$

(2.2)

For a non-linear operator, $A(p)$ the minimization problem needs an iterative optimization method. The choice of method may vary depending on application. Some important properties to take into consideration are listed below

- differentiability of the cost function,
- number of parameters,
- computational cost of evaluating the cost function and gradient,
- type of constraints,
- accuracy requirements.

For parameter estimation problems for differential equations the evaluation of the cost function is expensive since it requires the solution of the direct problem. The constraints in our applications are mostly simple bounds. In the following section we give a short review of common algorithms in non-linear optimization. For further reading, see for example [14], [10] and [27].

2.3 Unconstrained optimization

Consider the truncated Taylor expansion of $j(p + d)$ around $p$

$$j(p + d) = j(p) + g(p)^T d(p) + \frac{1}{2} d(p)^T H(p) d(p)$$

(2.3)

where $g = \nabla j$ is the gradient and $H = \nabla^2 j$ is the Hessian. A necessary condition for $p^*$ to be a local minimizer is that $g(p^*) = 0$. If in addition the Hessian is positive definite the conditions are sufficient.

A common strategy for gradient-based methods is to iteratively choose a search direction, $d$, and minimize the cost function in this direction

$$\min_{\alpha} j(p + \alpha d)$$

(2.4)

where $\alpha > 0$ is the step length. The one-dimensional minimization problem (2.4) is called the line search problem and is discussed further in Section 2.5.
2.3.1 Conjugate gradient

The conjugate gradient (CG) method was originally formulated for the minimization of a quadratic function with symmetric and positive definite Hessian. In this case it converges in at most \( n \) iterations for a problem of size \( n \). The method has also been found to perform well for more general minimization problems where the cost function is not quadratic. An efficient formulation is the Polak-Ribiere conjugate gradient method (see [14]).

2.3.2 Newton methods

The basic Newton’s method is obtained by minimizing the right-hand side of the Taylor series in (2.3) with respect to \( d \) resulting in \( d = H^{-1}g \). The minimizer is used iteratively according to

\[
p_{k+1} = p_k - H_k^{-1}g_k
\]

which thus converges in one step if the cost function is quadratic. For a general function the iterations converge quadratically close to the minimum. The main drawback of Newton’s method is that it is computationally expensive. In each main iteration the Hessian has to be computed, often using finite differences, and a linear system has to be solved. This has lead to the development of the so called quasi-Newton methods where approximations of the Hessian are constructed during the iterations using function and gradient information. The convergence of these methods is super-linear but they only require derivative information and further the solution of a linear system may be avoided.

Different update formulas have been suggested, the most well-known being the BFGS (Broyden, Fletcher, Goldfarb, Shanno) and the DFP (Davidon, Fletcher, Powell) formulas (see [27]). For general problems the BFGS method, is considered to be the most efficient. The solution of a linear system can be avoided by updating an approximate inverse of the Hessian, \( H_k^{-1} \) instead of \( H_k \). Further, in [26] they show that it is possible to formulate a memory limited update to avoid the storage of the full Hessian.

2.4 Constrained optimization

The main application of the inverse method has been the reconstruction of material parameters. The constraints are then usually on the form of simple bounds. This type of constraints is rather easy to incorporate in the optimization. However, we have also considered problems where the thicknesses of the layers in a multilayer structure are unknown which results in linear parameter constraints.

For constrained minimization problems the sequential quadratic programming (SQP), method [35] has been shown to be one of the most efficient methods. It implements a quasi-Newton update to compute an approximation of the Hessian.
of the Lagrangian of the constrained problem in each main iteration. The search direction is then determined by solving a quadratic programming problem where the Lagrangian is approximated by a quadratic function. Finally, a step size is computed using an inexact line search.

2.5 Line search

In most deterministic algorithms a one-dimensional minimization problem is solved in each iteration to determine the step size in the search direction. The line search problem is typically solved inexactly to save computer time. Let $\phi(\alpha)$ denote the cost function in the search direction, i.e.,

$$\phi(\alpha) = j(p + \alpha d), \quad \alpha > 0. \quad (2.6)$$

The step size, $\alpha$, has to satisfy some criterion to guarantee i) a sufficient decrease in the cost function and ii) a large enough step size. A commonly used criterion is the Wolfe test

$$\begin{align*}
\phi(\alpha) & \leq \phi(0) + \varepsilon \phi'(0) \alpha \\
\phi'(\alpha) & \geq (1 - \varepsilon) \phi'(0)
\end{align*}$$

where $0 < \varepsilon < 0.5$. Once a feasible value is found the step size may be further improved by a minimization strategy. Often, lower degree polynomial interpolation is used since the minimum may then be computed exactly. For a thorough description of the line search problem see, for example [27].

2.6 Computing gradients

The efficiency of deterministic algorithms relies on accurate gradient information. In our case, the cost function depends implicitly on the parameters through the Maxwell’s equations and the gradient may not be computed directly. However, using an optimal control formulation the Fréchet derivative of the cost function may be computed using an additional simulation to solve the adjoint problem. An alternative approach is to approximate the gradient using finite differences, as discussed in Section 2.6.2.

2.6.1 The optimal control formulation

Let the direct problem be described by the equation

$$L(p)u(x, t) = f^{exc}(x, t), \quad x \in \Omega, t \in [0, T], \quad p \in P_{adm}$$

$$u(x, 0) = 0$$

where $L(p)$ is a linear differential operator in time and space including boundary conditions, $p = (p_1, \ldots, p_n)$ are the parameters from the set of admissible parameters $P_{adm}$, $u(x, t)$ is the solution and $f^{exc}(x, t)$ is the excitation source. The
inverse problem is: given the observed field in \( M \) points in space, \( x_m \), determine the unknown parameters \( p^* \) such that the solution to (2.7) coincides with the observed field. Let \( u^\text{obs}_m(t) \) denote the observed time-domain field in \( x = x_m \) and \( u(p, x, t) \) denote the computed field for the parameters \( p \). The difference between the computed and observed fields in observation point \( m \) is denoted by \( d_m \), i.e.

\[
d_m(u(p)) = (u(p, x, t) - u^\text{obs}_m(t))\delta(x - x_m), \quad m = 1, \ldots, M
\]  

(2.8)

where \( \delta \) is the Dirac delta function. We define an inner product and norm associated with (2.7)

\[
(f, g) = \int_0^T \int_\Omega <f, g> \, d\Omega \, dt
\]  

(2.9)

\[
\|f\|^2 = (f, f)
\]  

(2.10)

where \(<\cdot, \cdot>\) is the scalar product between two vectors. The functions \( f \) and \( g \) are real-valued vectors in the time domain. We then introduce a cost function defined as

\[
j(u(p)) = \frac{1}{2} \sum_{m=1}^{M} ||d_m(u(p))||^2
\]  

(2.11)

where we write \( j(u(p)) \) to emphasize the fact that the dependency of the parameters is implicit through the computed solution. The gradient of \( j \) may be derived using an optimal control formulation where the direct equations are included as constraints

\[
\text{find } p^* \text{ such that } j(p^*) \leq j(p) \quad \forall p \in P^{adm}
\]

subject to

\[
Lu = f^\text{exc}, \quad x \in \Omega, \; t \in [0, T]
\]

\[
u(x, 0) = 0.
\]

where we have left out the dependency of the functions to make the notation more compact. The Lagrangian for this problem becomes

\[
\mathcal{L}(p, u, \lambda) = j(u(p)) + (\lambda, Lu - f)
\]  

(2.12)

where \( \lambda \) are called the Lagrange multipliers or adjoint variables. Now, we make a small perturbation of the parameters in (2.12) such that \( p \to p + \delta p \). This implies that \( u \to u + \delta u, \lambda \to \lambda + \delta \lambda \) and \( \mathcal{L} \to \mathcal{L} + \delta \mathcal{L} \). After linearization and using the direct equation (2.7) we obtain
\[
\delta \mathcal{L} = \sum_{m=1}^{M} (d_m(u), \delta u) + (\lambda, L \delta u) + \sum_{i=1}^{n} (\lambda, \frac{\partial L}{\partial p_i} u) \delta p_i
\]  
(2.13)

We now introduce the adjoint operator, \( L^* \) satisfying the relation

\[
(L^* \lambda, u) = (\lambda, Lu)
\]  
(2.14)

Using (2.14) in (2.13) and rearranging the terms we arrive at

\[
\delta \mathcal{L} = (L^* \lambda + \sum_{m=1}^{M} d_m(u), \delta u) + \sum_{i=1}^{n} (\lambda, \frac{\partial L}{\partial p_i} u) \delta p_i
\]  
(2.15)

Since we are interested in the gradient with respect to the parameters \( p_i \) we set the first expression in (2.15) to zero resulting in the adjoint equations

\[
L^* \lambda = - \sum_{m=1}^{M} d_m(u)
\]  
(2.16)

Now, if \( u(p) \) is a solution to the direct equations the second term in the Lagrangian (2.12) vanishes and we have

\[
\mathcal{L}(p, u(p), \lambda) = j(p).
\]  
(2.17)

Hence, \( \delta j = \delta \mathcal{L} \) and the desired gradient is immediately identified in (2.15)

\[
\frac{\partial j}{\partial p_i} = (\lambda, \frac{\partial L}{\partial p_i} u).
\]  
(2.18)

Note that the integrand is non-zero only in the parts of the domain where the direct operator depends on the parameter, \( p_i \).
We make some observations about the adjoint problem:

- The adjoint operator $L^*$ is derived by integration by parts of the right-hand side in (2.14).
- In order for (2.14) to hold, zero terminal conditions have to be used for the adjoint variables, i.e. $\lambda(x,T) = 0$. The adjoint problem is therefore solved backward in time from $T$ to 0.
- The difference between the computed field and the observed field in the observation points (2.8) acts as the excitation in the adjoint equations.

The gradient expression (2.18) is an integral over time and space containing both the adjoint and direct fields. Hence, each gradient computation requires the solution of one direct and one adjoint problem. Figure 2.1 illustrates the minimization procedure using adjoint gradients.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig2_1.png}
\caption{The minimization procedure using adjoint gradients.}
\end{figure}
2.6.2 Finite differences

The adjoint gradient computation requires both the direct and the adjoint equations to be solved in each minimization iteration. Further, the direct and adjoint solutions need to be stored for every time step for the computation of the gradient. It is therefore reasonable to consider an alternative approach where the gradient is computed using the finite-difference approximation

\[
\frac{\partial j}{\partial p_i} \approx \frac{j(p + \Delta p_i e_i) - j(p)}{\Delta p_i}.
\]

We note that one additional cost function value is required for each new parameter. For a problem with \(N\) parameters the gradient therefore requires \(N + 1\) direct solutions. Furthermore, the accuracy of the approximation (2.19) may be poor which could lead to slower convergence of the minimization iterations. Nevertheless, finite-difference approximation may in some cases be more efficient and is also useful for the validation of the exact gradient computation.
Chapter 3

The Direct Problem

Maxwell’s equations are solved numerically using the finite-difference time-domain method (FDTD). This method is well suited for scattering problems due to the availability of efficient absorbing boundary conditions (ABCs), complex material models and subcell models for small geometrical features. Further, the local approximation property makes parallelization using domain decomposition straightforward. The basic FDTD algorithm was formulated by Kane S. Yee in 1966 [44]. Since then there has been extensive development of the method and several books have been published on the subject, see for example [39], [40] and [24].

3.1 The Maxwell equations

The propagation of electromagnetic fields is governed by the Maxwell equations,

\[
\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J} \quad \text{(Ampère’s law)} \tag{3.1}
\]

\[
-\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \mathbf{E} \quad \text{(Faraday’s law)} \tag{3.2}
\]

\[
\nabla \cdot \mathbf{D} = \rho \quad \text{(Gauss’ law)} \tag{3.3}
\]

\[
\nabla \cdot \mathbf{B} = 0 \tag{3.4}
\]

where \( \mathbf{B} \) is the magnetic flux density in \( \text{Vs/m}^2 \), \( \mathbf{D} \) is the electric flux density in \( \text{As/m}^2 \), \( \mathbf{H} \) is the magnetic field in \( \text{A/m} \), \( \mathbf{E} \) is the electric field in \( \text{V/m} \), \( \mathbf{J} \) is the electric current density in \( \text{A/m}^2 \) and \( \rho \) is the electric charge density in \( \text{As/m}^3 \). The divergence equations (3.3) and (3.4) may be seen as resulting from the first
two equations in the following sense. Taking the divergence of (3.1) and (3.2) and 
changing the order of derivation we obtain

\[
\frac{\partial (\nabla \cdot \mathbf{D} - \rho)}{\partial t} = 0 \tag{3.5}
\]

\[
\frac{\partial (\nabla \cdot \mathbf{B})}{\partial t} = 0 \tag{3.6}
\]

where we have used the continuity equation for the charge

\[
\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0. \tag{3.7}
\]

The equations (3.5) and (3.6) show that if the divergence equations are satisfied 
initially, they will continue to be so for all later times.

The fields in Maxwell’s equations are related by so-called constitutive relations. 
In linear, isotropic and non-dispersive (i.e., the material properties are independent 
of the frequency of the field) media they are

\[
\mathbf{B} = \mu \mathbf{H} \tag{3.8}
\]

\[
\mathbf{D} = \varepsilon \mathbf{E} \tag{3.9}
\]

where \( \varepsilon \) is the permittivity, \( \mu \) is the permeability. The corresponding properties of 
vacuum are denoted by \( \varepsilon_0 \) and \( \mu_0 \). Dispersive media is discussed in Section 3.7. 
Lossy media is included through the current density by

\[
\mathbf{J} = \sigma \mathbf{E} \tag{3.10}
\]

where \( \sigma \) is the conductivity. The equations (3.1) and (3.2) may now be recast in 
the form

\[
-\mu \frac{\partial \mathbf{H}}{\partial t} = \nabla \times \mathbf{E} \tag{3.11}
\]

\[
\varepsilon \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \sigma \mathbf{E}. \tag{3.12}
\]

In two dimensions the above system decouples into two independent systems. The 
transverse magnetic (TM) mode:

\[
\mu \frac{\partial H_x}{\partial t} = -\frac{\partial E_z}{\partial y} \tag{3.13}
\]

\[
\mu \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} \tag{3.14}
\]

\[
\varepsilon \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \tag{3.15}
\]

and the transverse electric (TE) mode:
In the following section we will describe how the TE and TM equations are solved numerically using the FDTD method.

3.2 Discretization

FDTD is based on the discretization of the Maxwell curl equations (3.11) and (3.12) using centered finite differences on a uniform Cartesian grid. The resulting scheme is explicit and second-order accurate. The discrete $E$- and $H$-fields are staggered in both time and space which means they are shifted by a half time and space step. The 2D grids for the TE and TM cases are illustrated in Figure 3.1.

![Figure 3.1. The FDTD grid for the TE (left) and TM (right) modes.](image)

Let the spatial grid index $(i,j)$ correspond to the physical coordinates $(i\Delta x, j\Delta y)$ and the temporal index $n$ denote the time $t = n\Delta t$. Half indices are used for the components that are centered between the grid points. Using this notation the FDTD equations for the TM mode (3.13)-(3.15) may be written as
\[
H_x^{n+\frac{1}{2}}_{i,j} = H_x^{n-\frac{1}{2}}_{i,j+\frac{1}{2}} - C_{i,j+\frac{1}{2}} \left[ \frac{E_z^n_{i,j+1} - E_z^n_{i,j}}{\Delta y} \right],
\]
\[
H_y^{n+\frac{1}{2}}_{i,j} = H_y^{n-\frac{1}{2}}_{i,j+\frac{1}{2}} + C_{i+\frac{1}{2},j} \left[ \frac{E_z^n_{i+1,j} - E_z^n_{i,j}}{\Delta x} \right],
\]
\[
E_z^{n+1}_{i,j} = D_a|_{i,j} E_z^n_{i,j} + D_b|_{i,j} \left[ \frac{H_y^n_{i+\frac{1}{2},j} - H_y^n_{i-\frac{1}{2},j}}{\Delta x} - \frac{H_x^n_{i,j+\frac{1}{2}} - H_x^n_{i,j-\frac{1}{2}}}{\Delta y} \right],
\]
where
\[
C = \frac{\Delta t}{\mu},
\]
\[
D_a = \frac{1 - \sigma \Delta t/2\varepsilon}{1 + \sigma \Delta t/2\varepsilon},
\]
\[
D_b = \frac{\Delta t/\varepsilon}{1 + \sigma \Delta t/2\varepsilon}.
\]

Note that the coefficients are associated with grid indices since the material properties ($\varepsilon, \mu, \sigma$) may depend on space. The electric field in the $\sigma E_z$-term in (3.15) is approximated using the centered time average
\[
E_z^{n+\frac{1}{2}} = \frac{E_z^{n+1}_{i,j} + E_z^n_{i,j}}{2}.
\]

For the TE mode, see (3.16)-(3.18), the FDTD equations becomes
\[
E_x^{n+1}_{i+\frac{1}{2},j} = D_a|_{i+\frac{1}{2},j} E_x^n_{i+\frac{1}{2},j} + D_b|_{i+\frac{1}{2},j} \left[ \frac{H_y^n_{i+\frac{1}{2},j+\frac{1}{2}} - H_y^n_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta y} \right],
\]
\[
E_y^{n+1}_{i,j+\frac{1}{2}} = D_a|_{i,j+\frac{1}{2}} E_y^n_{i,j+\frac{1}{2}} - D_b|_{i,j+\frac{1}{2}} \left[ \frac{H_x^n_{i+\frac{1}{2},j+\frac{1}{2}} - H_x^n_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta x} \right],
\]
\[
H_z^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2}} = H_z^{n-\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2}} + C_{i+\frac{1}{2},j+\frac{1}{2}} \left[ \frac{E_x^n_{i+\frac{1}{2},j+1} - E_x^n_{i+\frac{1}{2},j}}{\Delta y} - \frac{E_y^n_{i+1,j+\frac{1}{2}} - E_y^n_{i,j+\frac{1}{2}}}{\Delta x} \right].
\]

In Section 3.1 it was shown that the divergence equations (3.3)-(3.4) were implicitly enforced by the curl equations together with suitable initial conditions. A discrete version of the divergence invariance holds for the FDTD discretization as well, as shown in Section 3.6 in [2]. Given zero initial conditions of the fields it is therefore sufficient to solve the above equations in the numerical simulation.
3.3 Stability and numerical dispersion

The use of an explicit time-stepping scheme for a hyperbolic system implies that the time step has to be chosen sufficiently small for the solution to remain bounded. The stability condition in two dimensions (see for example [40]) is:

\[
\Delta t < \frac{1}{c_{\text{max}} \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}}}
\]

(3.29)

where \(c_{\text{max}}\) is the maximum value of the phase speed \(c = \frac{1}{\sqrt{\varepsilon\mu}}\) in the computational domain. The stability condition does not take into account boundary conditions, dispersive material models, subcell models, etc. Such modifications of the basic scheme may well result in more severe restrictions on the time step.

The dispersion relation relates the numerical phase velocity to the wavelength. In the 2D-TM case on a uniform grid with \(\Delta x = \Delta y = \Delta\) it becomes

\[
\left(\frac{\Delta}{c\Delta t}\right)^2 \sin^2 \left(\frac{\omega\Delta t}{2}\right) = \sin^2 \left(\frac{\tilde{k}_x \Delta}{2}\right) + \sin^2 \left(\frac{\tilde{k}_y \Delta}{2}\right)
\]

(3.30)

where \(\omega\) is the angular frequency, \(\tilde{k}_x\) and \(\tilde{k}_y\) are the \(x\)- and \(y\)- components of the numerical wave vector. Letting \(\Delta\) and \(\Delta t\) approach zero, equation (3.30) approaches the ideal dispersion relation

\[
\left(\frac{\omega}{c}\right)^2 = \tilde{k}_x^2 + \tilde{k}_y^2
\]

(3.31)

showing that the dispersion error may be reduced by improving the resolution. The resolution is often expressed as the number of grid points per wavelength, \(N = \lambda/\Delta\). In the results presented later, we usually have \(N \approx 20\). For large problems and over long times it may be necessary to increase the resolution.

3.4 Sources

Plane waves are generated by impressing electric and magnetic current sources on a surface, called Huygens' surface, surrounding the excited region. Due to the linearity of the equations the field may be decomposed into an incident and a scattered part, i.e.,

\[
E^{\text{tot}} = E^{\text{inc}} + E^{\text{sca}},
\]

(3.32)

\[
H^{\text{tot}} = H^{\text{inc}} + H^{\text{sca}}
\]

(3.33)

and the computational domain is divided in two regions, as illustrated in Figure 3.2. To see how the excitation is implemented in FDTD, consider the \(E_z\)-equation (3.21)
in the 2D-TM case for a Huygens surface with normal in the $x$-direction. The electric current source is added to the $E_z$-field according to

$$E_{z|_{i,j}}^{n+1} = E_{z|_{i,j}}^{n+1} - \frac{\Delta t}{\varepsilon_0} J_{s|_{i,j}}^{n+\frac{1}{2}}$$

(3.34)

where

$$J_{s|_{i,j}}^{n+\frac{1}{2}} = \hat{z} \cdot \frac{1}{\Delta x} \left( \hat{x} \times H_{\text{inc}|_{i,j}}^{n+\frac{1}{2}} \right) = \frac{1}{\Delta x} H_{y|_{i+\frac{1}{2},j}}^{\text{inc}|_{i,j+\frac{1}{2}}}.$$  

(3.35)

The scaling by $1/(\Delta x)$ converts the surface current density into an equivalent volume current density. Due to the staggered grid, the excitation surfaces for the electric and magnetic currents are separated by a half cell. This has to taken into account when evaluating the excitation function to avoid perturbation of the incident wave, see [9].

In some cases we will use a source term in the update equation for a single field component to simulate a point source. For instance, the source in the adjoint equations is of this type. The addition of a term in the equation results in a, so-called, soft source which will not interfere with incoming waves. If, on the other hand, the source is applied by prescribing the field itself a hard source is obtained which acts as a scatterer, see [2].

### 3.5 Absorbing boundary condition (ABC)

In the perfectly matched layer, PML, [5] absorbing boundary condition, a highly absorbing outer layer is used to attenuate outgoing waves, see Figure 3.2. Although it is rather expensive it is still one of the most efficient ABCs due to the low reflection. The U-PML formulation in [15] is a variant of the original PML based
3.6 Inhomogeneous media

In the Maxwell equations in anisotropic media, the frequency-domain Maxwell equations become

\[ \nabla \times \mathbf{E}(r, \omega) = -j\omega\mu\Lambda(\omega)\mathbf{H}(r, \omega) \]
\[ \nabla \times \mathbf{H}(r, \omega) = j\omega\varepsilon\Lambda(\omega)\mathbf{E}(r, \omega) \]

(3.36)
(3.37)

where \( \omega \) is the angular frequency and \( \Lambda \) is a frequency-dependent tensor. In [15] it is shown that the uniaxial tensor

\[ \Lambda(\omega) = \begin{bmatrix} s(\omega)^{-1} & 0 & 0 \\ 0 & s(\omega) & 0 \\ 0 & 0 & s(\omega) \end{bmatrix} \]

(3.38)

where \( s(\omega) \) is a complex valued function. To avoid numerical reflections at the U-PML interface, the conductivity is gradually increased inside the U-PML layer. We use a fourth degree polynomial function of the distance \( \rho \) to the free space interface

\[ \sigma(\rho) = \sigma_{max} \left( \frac{\rho}{d} \right)^4 \]

where \( d \) is the thickness of the U-PML. This particular choice of \( \sigma \) has been found to give good absorption for a wide variety of problems, see [15]. The U-PML layer, which is typically about ten cells thick, is truncated by an outer PEC wall.

3.6 Inhomogeneous media

In the FDTD grid, material properties are associated with cells and boundaries between different media are defined to go through the electric field components as shown for the TM and TE cases in Figure 3.3.

![Figure 3.3. Location of material boundaries in the 2D TE and TM grids.](image)

The convergence of the FDTD scheme for inhomogeneous media was studied in [4] where it was shown that average values have to be used for the material...
parameters on the boundaries to obtain second-order accuracy. The derivation of the modified parameters was done using the integral form of Maxwell's curl equations. In the TM case, where the $E_z$-field is located in the corner of the cell, as illustrated to the left in Figure 3.3, the resulting permittivity becomes the arithmetic average of the permittivities of the four adjacent cells. The value in the grid point $(i, j)$ thus becomes

$$\bar{\varepsilon}_{i,j} = \frac{1}{4} (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4)$$

In the TE case the electric fields are located at the midpoints of the cell sides and the integration surfaces only covers two different permittivities, as shown to the right in Figure 3.3. For the $E_x$-field we have

$$\bar{\varepsilon}_{i+\frac{1}{2},j} = \frac{1}{2} (\varepsilon_2 + \varepsilon_4)$$

and for the $E_y$-field

$$\bar{\varepsilon}_{i,j+\frac{1}{2}} = \frac{1}{2} (\varepsilon_1 + \varepsilon_2).$$

The conductivity is treated equivalently. For the permeability the situation becomes more complicated, at least for the TE mode since in this case the magnetic fields are normal to the material boundary and therefore discontinuous. In [4] they show that harmonic mean values of the permeability should be used. We have not employed any averaging for the permeability, meaning that second order accuracy will not be achieved in the case of inhomogeneous permeability. However, in most real applications $\mu = \mu_0$ everywhere.

### 3.7 Dispersive media

Most real materials are dispersive, i.e., the constitutive relations (3.8)-(3.10) depend on the frequency of the penetrating wave. In case of dispersive permittivity the constitutive relation for the electric field may be written as

$$\hat{D}(\omega) = \hat{\varepsilon}(\omega) \hat{E}(\omega) = \varepsilon_0 (\varepsilon_\infty + \chi(\omega)) \hat{E}(\omega)$$

(3.39)

where $\hat{\varepsilon}$ is the complex dielectric function, $\varepsilon_\infty$ is the asymptotic permittivity when $\omega \to \infty$ and $\chi(\omega)$ is called the susceptibility function. In the time-domain the corresponding relation becomes

$$D(t) = \varepsilon_0 \varepsilon_\infty E(t) + \varepsilon_0 \int_0^t E(t - \tau) \chi(\tau) d\tau$$

(3.40)

where the second term is a convolution. We will consider two different dispersive models. The Debye, or relaxation, model is often used for fluids (for example water)
3.7. Dispersive media

while the Lorentz, or resonance, model is a commonly used model for solid materials (see [23]). The susceptibility functions for these two models are given below

\[
\chi(\omega) = \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega \tau} \quad \text{(Debye)} \tag{3.41}
\]

\[
\chi(\omega) = \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega^2 + 2i\omega \delta - \omega_0^2} \quad \text{(Lorentz)} \tag{3.42}
\]

where \(\varepsilon_s\) is the static permittivity for \(\omega = 0\), \(\tau\) is the relaxation time, \(\omega_0\) is the resonance frequency of the Lorentz model and \(\delta\) is called the damping coefficient. In Figure 3.4 the dielectric functions for two examples of dispersive materials are illustrated. The Debye material is water with \(\varepsilon_s = 81, \varepsilon_\infty = 1.8, \tau = 9.4 \cdot 10^{-12}\) and the Lorentz medium is given by \(\varepsilon_s = 1.2, \varepsilon_\infty = 1, \omega_0 = 10^{10}, \delta = 0.1\omega_0\).

![Figure 3.4. The dielectric function for a Debye material (left) and a Lorentz material (right).](image)

Consider the Debye case and substitute (3.41) into the constitutive relation (3.39) and multiply both sides by \(1 + i\omega \tau\) to obtain

\[
D + i\omega \tau D = \varepsilon_0 (\varepsilon_s E + i\omega \tau \varepsilon_\infty E).
\]

Inverse Fourier transformation to the time domain using the convention \(i\omega \rightarrow \partial/\partial t\) results in the ordinary differential equation (ODE)

\[
\tau \frac{\partial D}{\partial t} + D - \tau \varepsilon_0 \varepsilon_\infty \frac{\partial E}{\partial t} - \varepsilon_0 \varepsilon_s E = 0
\]
In the auxiliary differential equation (ADE) method for dispersive media in FDTD, the \(E\)-field is computed by solving (3.44) together with the Maxwell equation for the \(D\)-field (3.1). Both equations are discretized using the standard FDTD centered differences. This approach, which is used in our code, may be extended to higher-order dispersive relations resulting in higher order of the auxiliary ODE. See [20] for further details.

In the recursive convolution method [22], the convolution integral in (3.40) is discretized and recursively updated to avoid additional storage of the fields.

### 3.8 Subcell models

A uniform grid is poor when the grid size is limited by resolution of small geometrical details and not the wavelength. In this case most of the grid may be unnecessarily fine. An alternative to grid refinement is local modifications of the update equations. Such subcell models may be derived using the integral form of Maxwell’s curl equations

\[
\int \int_S \left( \varepsilon \frac{\partial E}{\partial t} + \sigma E \right) \cdot dS = \oint_C \mathbf{H} \cdot dl
\]

(3.45)

\[
\int \int_S \mu \frac{\partial \mathbf{H}}{\partial t} \cdot dS = -\oint_C \mathbf{E} \cdot dl.
\]

(3.46)

The idea is to derive update formulas by applying (3.45) and (3.46) to the discrete FDTD fields. We consider subcell models for two common geometries, a narrow slot and a thin dielectric sheet.

#### 3.8.1 A narrow slot in a PEC body

Figure 3.5 illustrates the 2D-TE FDTD grid for a narrow slot of subcell width, \(g\) in a large PEC body. For generality, the body is displaced with respect to the grid by the distance \(\alpha\). In [39] a subcell model for this geometry is derived using (3.45) and (3.46). Modified update equations are derived for the field components for which the integration surface contains parts of the PEC object. The integration surface for \(H_z|_{i+\frac{1}{2},j+\frac{1}{2}}\) located above the gap is illustrated in Figure 3.5.

We assume that all fields are zero in the part of \(S\) that lies inside the PEC body. Further, assume that \(H_z\) is constant outside the body and the electric fields are constant along each side of the rectangular domain. Applying Faraday’s law (3.46) to \(H_z|_{i+\frac{1}{2},j+\frac{1}{2}}\) then results in

\[
\mu \frac{\partial H_z|_{i+\frac{1}{2},j+\frac{1}{2}}}{\partial t} (\Delta x \Delta y - \alpha(\Delta x - g))
\]

\[= -gE_x|_{i+\frac{1}{2},j} + \Delta x E_x|_{i+\frac{1}{2},j+1} + (\Delta y - \alpha)(-E_y|_{i+1,j+\frac{1}{2}} + E_y|_{i,j+\frac{1}{2}})\]
Introducing the standard leapfrog discretization in time yields the modified update equation

$$H_{z}^{n+\frac{1}{2}}|_{i+\frac{1}{2},j+\frac{1}{2}} = H_{z}^{n-\frac{1}{2}}|_{i+\frac{1}{2},j+\frac{1}{2}}$$

$$+ \frac{\Delta t}{\mu} \left[ \frac{\Delta x E_{x}^{n}|_{i+\frac{1}{2},j+1} - g E_{x}^{n}|_{i+\frac{1}{2},j} + \alpha \left( E_{y}^{n}|_{i,j+\frac{1}{2}} - E_{y}^{n}|_{i+1,j+\frac{1}{2}} \right) \right]$$

In the same manner we may derive modified update equations for the $H_{z}$ fields inside the slot (for example $H_{z}|_{i+\frac{1}{2},j-\frac{1}{2}}$) and immediately above the structure (for example $H_{z}|_{i-\frac{1}{2},j+\frac{1}{2}}$). The $H_{z}$-components for which $S$ lies entirely in free space are not affected by the structure and are updated using the standard formula (3.28). The $E_{x}$- and $E_{y}$-fields, as illustrated in Figure 3.5, either are zero (inside the structure) or have integration surfaces entirely in free space (for example $E_{x}|_{i+\frac{1}{2},j}$ where the integration surface lies in the $yz$-plane) and thus are not affected by the structure. Consequently, the only modifications to the standard scheme is the update equations for the $H_{z}$-components close to the structure.

### 3.8.2 The thin dielectric sheet

In [30] a subcell model for a thin dielectric sheet was developed. The geometry of the problem is illustrated in Figure 3.6 where $\varepsilon_s$ is the permittivity of the sheet and $\sigma_s$ the conductivity and the surrounding media is free space. The discontinuity in the $E_{y}$-field is modeled by splitting the field in the cells containing the sheet in two components, $\tilde{E}_{y}$ inside the sheet and $E_{y}$ in free space. The $H_{z}$- and $E_{x}$-fields are continuous over the sheet and no splitting is therefore necessary for these components. We will not carry out the derivations here but refer to [30] for the
Figure 3.6. The thin sheet geometry.

details. The thin sheet equations for a similar geometry are given in the discussion of the inverse subcell problem in Chapter 6.
Chapter 4

The Continuous Inverse Problem

The motivation for studying the continuous case is that it gives a clearer picture of the computations involved. Discretization of the continuous results constitutes a possible approach to derive the discrete gradients and adjoint equations although it is not recommended, as will be discussed later. We will introduce a general form of Maxwell’s equations which is valid for dispersive materials and absorbing U-PML media as well as simpler materials and perfectly conducting boundaries. The idea is to avoid special treatment of different media in the derivation of the adjoint equation and illustrate that interfaces between media do not present additional complications. The derivation is done for a specific case, the TM equations in simple media, but it should be obvious how to extend it to the general equations.

4.1 General equations

The scattering problems we are interested in typically include some of the following features:

- absorbing boundary condition (U-PML),
- perfectly conducting boundaries,
- inhomogeneous media,
- dispersive permittivity (Debye or Lorentz) and
- subcell models

In Chapter 3 we have seen the equations for the different types of media. Subcell models must be treated separately due to their inherently discrete nature, but it
is possible to formulate general equations which are valid in both dispersive media and U-PML. In three dimensions the general equations become

\[
\frac{\partial B_i}{\partial t} + c_i B_i + \frac{1}{\mu_0} (\nabla \times E) \cdot e_i = 0 \quad (4.1)
\]

\[
\frac{\partial B_i}{\partial t} + d_{1i} B_i + d_{2i} \frac{\partial H_i}{\partial t} = 0 \quad (4.2)
\]

\[
\frac{\partial D_i}{\partial t} + a_i D_i - \frac{1}{\varepsilon_0} (\nabla \times H) \cdot e_i = 0 \quad (4.3)
\]

\[
b_{1i} \frac{\partial^2 D_i}{\partial t^2} + b_{2i} \frac{\partial D_i}{\partial t} + b_{3i} D_i + b_{4i} \frac{\partial^2 E_i}{\partial t^2} + b_{5i} \frac{\partial E_i}{\partial t} + b_{6i} E_i = 0 \quad (4.4)
\]

where \(i \in \{x, y, z\}\) denotes the component in Cartesian coordinates, and \(e_i\) are the corresponding unit vectors. Different media are distinguished by varying the coefficients. The common system of equations shows that it is possible to give a unified treatment of the entire domain and that the transition between different types of media is taken care of by variable (discontinuous) coefficients. A rewarding property of the system (4.1)-(4.4) is that all terms with spatial derivatives have constant coefficients. The derivation below is greatly simplified due to this fact.

Setting \(\partial/\partial z = 0\) yields the two-dimensional equations. The general equations for the TM mode become:

\[
\frac{\partial B_x}{\partial t} + c_x B_x + \frac{1}{\mu_0} \frac{\partial E_z}{\partial y} = 0 \quad (4.5)
\]

\[
\frac{\partial B_y}{\partial t} + d_{1x} B_x + d_{2x} \frac{\partial H_x}{\partial t} = 0 \quad (4.6)
\]

\[
\frac{\partial B_y}{\partial t} + c_y B_y - \frac{1}{\mu_0} \frac{\partial E_z}{\partial x} = 0 \quad (4.7)
\]

\[
\frac{\partial B_y}{\partial t} + d_{1y} B_y + d_{2y} \frac{\partial H_y}{\partial t} = 0 \quad (4.8)
\]

\[
\frac{\partial D_z}{\partial t} + a_z D_z - \frac{1}{\varepsilon_0} (\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}) = 0 \quad (4.9)
\]

\[
b_{1z} \frac{\partial^2 D_z}{\partial t^2} + b_{2z} \frac{\partial D_z}{\partial t} + b_{3z} D_z + b_{4z} \frac{\partial^2 E_z}{\partial t^2} + b_{5z} \frac{\partial E_z}{\partial t} + b_{6z} E_z = 0 \quad (4.10)
\]

For a translation to physical parameters for the coefficients in (4.5)-(4.10) in the different types of media see Table 4.1.
4.2 Parameters

We now consider an inverse media problem where the material properties of the scatterer constitute the unknown parameters. Further, it is assumed that the geometry consists of piecewise constant media such that the parameters may be represented by a vector with constant elements rather than a continuous function. In the discretized problem this will always be the case since the computational domain is built up by a finite number of elements with constant material properties.

In the non-dispersive case, materials are characterized by the permittivity, conductivity and permeability. The corresponding parameters in the inverse problem are defined as

\[ p_{\text{simple}} = [\varepsilon_r, \sigma, \mu_r]^T \]  

where \( \varepsilon_r \) and \( \mu_r \) relative values with respect to vacuum, \( \sigma_x, \sigma_y \) and \( \sigma_z \) are the lossy parameters of the U-PML and the dispersive parameters are defined in Section 3.7.

\[ p_{\text{Debye}} = [\varepsilon_\infty, \varepsilon_s, \tau, \mu_r]^T \]  

where \( \varepsilon_\infty, \varepsilon_s \) and \( \mu_r \) are the relative values with respect to \( \varepsilon_0 \) and \( \mu_0 \). In order to avoid different magnitudes of the parameters the relaxation time is scaled according

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Media} & c_x & d_{1x} & d_{2x} & c_y & d_{1y} & d_{2y} \\
\hline
\text{Free space} & 0 & 0 & -1 & 0 & 0 & -1 \\
\text{Non-dispersive} & 0 & 0 & -\mu_r & 0 & 0 & -\mu_r \\
\text{Debye} & 0 & 0 & -\mu_r & 0 & 0 & -\mu_r \\
\text{Lorentz} & 0 & 0 & -\mu_r & 0 & 0 & -\mu_r \\
\text{U-PML} & \sigma_y/\varepsilon_0 & \sigma_x/\varepsilon_0 & -1 & \sigma_x/\varepsilon_0 & \sigma_y/\varepsilon_0 & -1 \\
\hline
\end{array}
\]

Table 4.1. Coefficients in the general TM equations
to $\tau_r = \tau / \tau_0$ where $\tau_0$ is the initial value in the minimization. We assume that the Debye media are not conductive i.e. $\sigma = 0$.

In the Lorentz case the parameters are

$$p_{\text{Lorentz}} = [\varepsilon_\infty, \varepsilon_s, \omega_0 r, \delta_r, \mu_r]^T$$

(4.13)

where $\omega_0 r$ and $\delta_r$ are relative to the initial values.

### 4.3 Direct problem

We consider the 2D-TM equations in non-dispersive media (3.13)-(3.15) in the rectangular domain $\Omega = \{0 \leq x \leq L_x, 0 \leq y \leq L_y\}$ with outer boundary $\Gamma$ and the time interval $0 \leq t \leq T$. The scattering geometry is denoted by $S \subset \Omega$ and is modeled by simple media, see (4.11). The surrounding media is free space $(\varepsilon_0, \mu_0)$. We assume PEC outer boundary and zero initial conditions:

$$\begin{align*}
H_x(x, 0) &= 0, \quad H_y(x, 0) = 0, \quad E_z(x, 0) = 0 \quad (4.14) \\
E_z(x, t) &= 0 \text{ if } x \in \Gamma. \quad (4.15)
\end{align*}$$

The direct field vector is denoted by $u = (H_x, H_y, E_z)^T$. The problem is illustrated in Figure 4.1.

![Figure 4.1. The 2D-TM geometry.](image)

### 4.4 Cost function

We wish to determine the material parameters of the scatterer $p = (\varepsilon, \sigma, \mu)$ from the time history of the observed field $E_{\text{obs}}^z$ in $M$ observation points, $x_m$. The cost function is defined as the energy norm of the difference between the computed and
the observed fields as described in Section 2.6.1. The cost function in the TM case is defined as

$$j(u(p)) = \frac{1}{2} \sum_{m=1}^{M} \int_{T} \int_{\Omega} (E^z - E^{obs^z})^2 \delta_m d\Omega dt$$  \hspace{1cm} (4.16)

where $\delta_m$ is the Dirac delta function $\delta(x - x_m)$.

### 4.5 Adjoint equations

Following the approach in Section 2.6.1 the adjoint equations and gradient are obtained by linearization of the Lagrangian. The cost function (4.16) and the direct equations gives the Lagrangian

$$\mathcal{L}(p, u, \lambda) = j(u(p)) + \int_{T} \int_{\Omega} \left\{ H^*_x(\mu \frac{\partial H_x}{\partial t} + \frac{\partial E^z}{\partial y}) + H^*_y(\mu \frac{\partial H_y}{\partial t} - \frac{\partial E^z}{\partial x}) \right.$$  

$$+ \left. E^*_z(\varepsilon \frac{\partial E^z}{\partial t} + \sigma E^z - \frac{\partial H^*_y}{\partial x} + \frac{\partial H^*_x}{\partial y}) \right\} d\Omega dt$$

are the adjoint fields. Perturbing the parameters by $p \rightarrow p + \delta p$ results in $u \rightarrow u + \delta u$, $\lambda \rightarrow \lambda + \delta \lambda$ and $\mathcal{L} \rightarrow \mathcal{L} + \delta \mathcal{L}$. After linearization and using the direct equations (3.13)-(3.15) we obtain the following expression for the perturbation, $\delta \mathcal{L}$

$$\delta \mathcal{L} = \sum_{m=1}^{M} \int_{T} \int_{\Omega} \delta E^z (E^z - E^{obs^z}) \delta_m d\Omega dt$$  

$$+ \int_{T} \int_{\Omega} H^*_x(\mu \frac{\partial \delta H_x}{\partial t} + \frac{\partial \delta H_x}{\partial y} + \frac{\partial \delta E^z}{\partial y}) d\Omega dt$$

$$+ \int_{T} \int_{\Omega} H^*_y(\mu \frac{\partial \delta H_y}{\partial t} + \frac{\partial \delta H_y}{\partial x} - \frac{\partial \delta E^z}{\partial x}) d\Omega dt$$

$$+ \int_{T} \int_{\Omega} E^*_z(\varepsilon \frac{\partial \delta E^z}{\partial t} + \sigma \delta E^z - \frac{\partial \delta H^*_y}{\partial x} + \frac{\partial \delta H^*_x}{\partial y} + \delta \sigma E^z + \sigma \delta E^z) d\Omega dt$$  \hspace{1cm} (4.17)

Integration by parts in time and space results in
\[ \delta \mathcal{L} = \int_{T}^{T} \int_{\Omega} \left\{ \delta \varepsilon E_{z}^{*} \frac{\partial E_{z}}{\partial t} + \delta \sigma E_{z}^{*} E_{z} + \delta \mu \left( H_{x}^{*} \frac{\partial H_{x}}{\partial t} + H_{y}^{*} \frac{\partial H_{y}}{\partial t} \right) \right\} \, d\Omega \, dt \\
+ \int_{T}^{T} \int_{\Omega} \left\{ \delta H_{x} \left( -\mu \frac{\partial H_{x}^{*}}{\partial t} - \frac{\partial E_{z}^{*}}{\partial y} \right) + \delta H_{y} \left( -\mu \frac{\partial H_{y}^{*}}{\partial t} + \frac{\partial E_{z}^{*}}{\partial x} \right) \right\} \, d\Omega \, dt \\
+ \delta E_{z} \left( -\varepsilon \frac{\partial E_{z}^{*}}{\partial t} + \sigma E_{z}^{*} + \frac{\partial H_{y}^{*}}{\partial x} - \frac{\partial H_{x}^{*}}{\partial y} + \sum_{m=1}^{M} \left( E_{z} - E_{z}^{\text{obs}} \right) \delta_{m} \right) \, d\Omega \]
\]
\[ + \int_{T}^{T} \int_{L_{x}} \left[ H_{x}^{*} E_{z} - E_{z}^{*} H_{x} \right]_{0}^{L_{x}} \, dy \, dt + \int_{T}^{T} \int_{L_{y}} \left[ -H_{y}^{*} E_{z} + E_{z}^{*} H_{y} \right]_{0}^{L_{y}} \, dx \, dt \]  
(4.18)

The boundary terms are canceled by the initial and boundary conditions for the
direct field (4.14)-(4.15) and the corresponding conditions for the adjoint fields

\[ H_{x}^{*}(x, T) = 0, \; H_{y}^{*}(x, T) = 0, \; E_{z}^{*}(x, 0) = 0 \]  
(4.19)

\[ E_{z}^{*}(x, t) = 0 \text{ if } x \in \Gamma. \]  
(4.20)

where we note that the “initial” conditions are given at \( t = T \). By setting the
parenthesized expressions in the second integral in (4.18) to zero we obtain the
adjoint TM equations

\[ \mu \frac{\partial H_{x}^{*}}{\partial \tau} - \frac{\partial E_{z}^{*}}{\partial y} = 0 \]  
(4.21)

\[ \mu \frac{\partial H_{y}^{*}}{\partial \tau} + \frac{\partial E_{z}^{*}}{\partial x} = 0 \]  
(4.22)

\[ \varepsilon \frac{\partial E_{z}^{*}}{\partial \tau} + \sigma E_{z}^{*} + \frac{\partial H_{y}^{*}}{\partial x} - \frac{\partial H_{x}^{*}}{\partial y} = -\sum_{m=1}^{M} \left( E_{z} - E_{z}^{\text{obs}} \right) \delta_{m} \]  
(4.23)

where \( \tau = T - t \). Comparing the above system to the direct TM equations (3.13)-(3.15) we note that the only difference is the sign of the spatial derivative terms
and the excitation.

### 4.6 Gradient

Using the adjoint equations (4.21)–(4.22) with boundary and initial conditions
(4.19) and (4.20) the gradient of the cost function is immediately identified in
4.6. Gradient

the first integral in (4.18)

\[
\frac{\partial j}{\partial \varepsilon} = \int_T \int_S E_z^* \frac{\partial E_z}{\partial t} d\Omega dt \quad (4.24)
\]

\[
\frac{\partial j}{\partial \sigma} = \int_T \int_S E_z^* E_z d\Omega dt \quad (4.25)
\]

\[
\frac{\partial j}{\partial \mu} = \int_T \int_S \left( H_z^* \frac{\partial H_x}{\partial t} + H_y^* \frac{\partial H_y}{\partial t} \right) d\Omega dt \quad (4.26)
\]

where we have used that the gradient is nonzero only inside the scatterer \( S \).
Chapter 5

The Discretized Inverse Problem

In the previous chapter the gradient for the minimization problem was derived for the continuous Maxwell equations. The obtained gradient expressions contain the solution of the adjoint equations. These equations were found to be nearly identical to the direct equations. Now we will introduce the numerical approximation and derive the corresponding discrete gradients. The derivation is straightforward for a finite-difference scheme such as FDTD where differentiation is replaced by finite differences and integration by parts becomes summation by parts. By considering the completely discretized problem we ensure that the resulting gradient is algebraically exact. The numerical scheme for the adjoint equations as well as the gradient expressions are thus determined by the direct scheme and not chosen independently. The adjoint scheme will consequently be of the same type as the direct one (e.g. finite-difference or finite-element) which means that typically, only minor modifications are necessary to convert an existing direct solver into an adjoint solver. An alternative to the discrete derivation is to approximate the continuous adjoint equations and gradient. However, this approach leads to grid dependent errors in the gradient. In some cases, for instance if subcell models are present, a fully discrete analysis is the only viable choice.

Unfortunately, the discrete derivation is quite technical. We therefore limit the derivation to the 2D-TM case for simple media and only state the results for the general equations including dispersive media and U-PML.

5.1 Direct problem

The geometry of the problem is illustrated in Figure 4.1. The computational domain is discretized using a 2D-TM FDTD mesh of $N_x \times N_y$ cells as illustrated.
in Figure 3.1. To get a more compact representation of the discrete equations we introduce the finite difference operators

\[ D_x U_{i,j}^n = \frac{(U_{i+1/2,j}^n - U_{i-1/2,j}^n)}{\Delta x}, \]

\[ D_y U_{i,j}^n = \frac{(U_{i,j+1/2}^n - U_{i,j-1/2}^n)}{\Delta y}, \]

\[ D_t U_{i,j}^n = \frac{(U_{i,j}^{n+1/2} - U_{i,j}^{n-1/2})}{\Delta t}, \]

and the time average operator

\[ S_t U_{i,j}^n = \frac{(U_{i,j}^{n+1/2} + U_{i,j}^{n-1/2})}{2}. \]

Using the above notation the direct 2D-TM equations become:

\[ \mu D_x H_x + D_y E_z = 0 \mid_{i,j+1/2, n}, \quad (i,j) \in \Omega_x \] (5.1)

\[ \mu D_y H_y - D_x E_z = 0 \mid_{i+1/2, j, n}, \quad (i,j) \in \Omega_y \] (5.2)

\[ \varepsilon D_t E_z - D_x H_y + D_y H_x + \sigma S_t E_z = 0 \mid_{i,j+1/2, n}, \quad (i,j) \in \Omega_z \] (5.3)

where \( n = 0, \ldots, N - 1 \) in all equations and

\[ \Omega_x : i = 0, \ldots, N_x, \quad j = 0, \ldots, N_y - 1 \]

\[ \Omega_y : i = 0, \ldots, N_x - 1, \quad j = 0, \ldots, N_y \]

\[ \Omega_z : i = 1, \ldots, N_x - 1, \quad j = 1, \ldots, N_y - 1 \]

The indices by the vertical bars in (5.1)-(5.3) denote the discrete point in time and space where the equations are approximated. Note that the material coefficients \((\varepsilon, \mu, \sigma)\) are functions of the spatial index and may vary in inhomogeneous media. As described in Section 3.6 the arithmetic mean values are used for \( \varepsilon \) and \( \sigma \) at the interface between different media. This will affect the gradient expressions derived later.

The discrete electric fields are located at full time and space indexes and the magnetic fields at half increments. The direct field vector \( \mathbf{u} \) for the TM case is defined by

\[ \mathbf{u}^n = \begin{pmatrix} H_x |_{i,j+1/2}^{n+1/2} \\ H_y |_{i+1/2,j}^{n+1/2} \\ E_z |_{i,j}^{n+1/2} \end{pmatrix}. \]
where the index intervals are given above. We have zero initial condition of the fields and perfectly conducting outer boundary such that

\begin{align*}
H_x|_{i,j+\frac{1}{2}} = H_y|_{i+\frac{1}{2},j} = E_z|_{i,j}^0 &= 0 \\
E_z|_{i,j}^n = E_z|_{N_x,j}^n = E_z|_{i,0}^n = E_z|_{1,N_y}^n &= 0.
\end{align*}

(5.4)

The negative time index for the $H$-field may look strange but it is purely a matter of choice of the temporal grid.

5.2 Cost function

The discrete cost function in the TM case is defined as

\[ j(u(p)) = \frac{1}{2} \sum_{m=1}^{M} \sum_{n=0}^{N} (E_z - E_z^{\text{obs}})_{i,j}^n \delta_m \Delta, \]

(5.5)

where the first sum is taken over the $M$ observation points $(i_m, j_m)$ and $E_z^{\text{obs}}$ is the observed field. The scaling, $\Delta = \Delta x \Delta y \Delta t$, is included for simplification of the derivation. The symbol $\delta_m$ denotes the Dirac delta function which has the value 1 in observation grid points $(i_m, j_m)$ and is 0 everywhere else. The parameters are $p = (\varepsilon, \sigma, \mu)$.

5.3 Adjoint equations

The choice of discretization for the adjoint fields is based on the staggered grid used for the direct fields. We use the same spatial grid but shift the time index a half time step to obtain centered gradient expressions. The following notation is used for the adjoint fields

\[ \lambda^n = \begin{pmatrix}
E_z|_{i,j}^{n+1/2} \\
H_x|_{i,j}^{n+1/2} \\
H_y|_{i+1/2,j}^{n+1/2}
\end{pmatrix} \]

(5.6)

As illustrated in Figure 5.1 the adjoint fields are centered in time between the corresponding direct fields.

![Figure 5.1. Temporal grid for the direct and adjoint fields.](image)
Chapter 5. The Discretized Inverse Problem

The adjoint equations and gradients are derived in the same way as in the continuous case, by forming the Lagrangian of the constrained problem and then studying the effect of a perturbation in the parameters. The only difference is that integration by parts is replaced by summation by parts as explained below. Using the adjoint fields (5.6) and the direct equations (5.1)–(5.3) the Lagrangian becomes

\[
\mathcal{L}(p, u, \lambda) = j(u(p)) + \sum_{n=0}^{N-1} \sum_{\Omega_z} E_z^* (\varepsilon D_t E_z - D_x H_y + D_y H_x + \sigma S_t E_z) \bigg|_{t_{i,j}^{n+1/2}}^{t_{i,j}} + \sum_{n=0}^{N-1} \sum_{\Omega_z} H_x^* (\mu D_t H_x + D_y E_z) \bigg|_{t_{i,j+1/2}}^{t_{i,j}} + \sum_{n=0}^{N-1} \sum_{\Omega_y} H_y^* (\mu D_t H_y - D_x E_z) \bigg|_{t_{i+1/2,j}}^{t_{i,j}}
\]

(5.7)

The discrete analogue to integration by parts is summation by parts. Consider the grid functions \( u_{i+1/2} \) and \( v_i \) illustrated in Figure 5.2.

\[ \sum_{i=p}^{q} u_{i+1/2} Dv_{i+1/2} = - \sum_{i=p+1}^{q-1} v_i Du_i - u_{p+1/2} v_p + v_q u_{q-1/2}. \]  

(5.8)
5.3. Adjoint equations

After linearization and then using summation by parts in both time and space we obtain

$$\delta L = \sum_{n=0}^{N-1} \left\{ \sum_{\Omega_x} (\delta \varepsilon D_t E_z^* + \delta \sigma D_t \delta E_z^* S_t) |_{i,j}^{n+1/2} \right. $$

\[ + \sum_{\Omega_y} (\delta \mu H_y^* D_t H_x) |_{i,j+1/2}^{n} + \sum_{\Omega_y} (\delta \mu H_y^* D_t H_y) |_{i,j+1/2}^{n} \} \Delta \]

\[ + \sum_{n=1}^{N} \sum_{\Omega_x} \delta E_z \left( -\varepsilon D_t E_z^* + D_x H_y^* - D_y H_x^* + \sigma S_t E_z^* + \sum_{m=1}^{M} (E_z - E_z^{\text{obs}}) \delta_m \right) |_{i,j+1/2}^{n} \Delta \]

\[ + \sum_{n=0}^{N-1} \sum_{\Omega_y} \delta H_y \left( -\mu D_t H_y^* + D_x E_z^* \right) |_{i,j+1/2}^{n} \Delta , \]  

(5.9)

where we have applied the initial and boundary conditions for the direct fields (5.4) as well the following conditions for the adjoint fields

$$H_x^{N+1/2} |_{i,j+1/2}^{n} = H_y^{N+1/2} |_{i,j+1/2}^{n}, \quad E^*_z |_{i,j+1/2}^{n} = 0 \quad \text{for} \quad i,j \in \Omega_x \quad \text{and} \quad n = 0, \ldots, N-1 \quad \text{(5.10)}$$

$$E^*_z |_{i,j}^{0} = E^*_z |_{i,j}^{N} = 0 \quad \text{for} \quad i,j \in \Omega_y \quad \text{and} \quad n = 0, \ldots, N-1 \quad \text{(5.11)}$$

The adjoint equations are obtained by setting the parenthesized expressions in the last three sums in (5.9) to zero

$$\mu D_t H_y^* - D_y H_x^* = 0 |_{i,j+1/2}^{n+1/2}, \quad (i,j) \in \Omega_x, n = 0, \ldots, N-1 \quad \text{(5.12)}$$

$$-\mu D_t H_y^* + D_x E_z^* = 0 |_{i,j+1/2}^{n+1/2}, \quad (i,j) \in \Omega_y, n = 0, \ldots, N-1 \quad \text{(5.13)}$$

and

$$\varepsilon D_t E_z^* + D_x H_y^* - D_y H_x^* + \sigma S_t E_z^* = -\sum_{m=1}^{M} (E_z - E_z^{\text{obs}}) |_{i,j}^{n} \delta_m. \quad (i,j) \in \Omega_x, n = 1, \ldots, N. \quad \text{(5.14)}$$

The difference between the computed and the observed fields acts as the source in the adjoint equations. Due to the “initial” condition for the adjoint field (5.10) the equations are solved backward in time. The change of variables \( \tau = T - t \) implies that \( \Delta t = -\Delta \tau \) such that the time differences in (5.12)–(5.14) change sign. By
isolating the new iterate we obtain the following update formulas for the adjoint fields

\[
H^*_{x|i,j+\frac{1}{2}} = H^*_{x|i,j+\frac{1}{2}} + C_{i,j+\frac{1}{2}} \left[ \frac{E^*_z|_{i,j+1}^{n'+\frac{1}{2}} - E^*_z|_{i,j}^{n'+\frac{1}{2}}}{\Delta y} \right], \quad (5.15)
\]

\[
H^*_{y|i'+\frac{1}{2},j} = H^*_{y|i'+\frac{1}{2},j} - C_{i'+\frac{1}{2},j} \left[ \frac{E^*_z|_{i+1,j}^{n'+\frac{1}{2}} - E^*_z|_{i,j}^{n'+\frac{1}{2}}}{\Delta x} \right], \quad (5.16)
\]

\[
E^*_z|i,j+\frac{1}{2} = \frac{D_a|i,j E^*_z|i,j^{n'-\frac{1}{2}}}{2} - \frac{D_b|i,j}{2} \left[ H^*_{y|i'+\frac{1}{2},j} - H^*_{x|i,j+\frac{1}{2}} \right] - \frac{M}{2} \sum_{m=1}^M \left( E^*_z|_{i,j}^{n'} - E^{\text{obs}}_z|_{i,j}^{n'} \right), \quad (5.17)
\]

where the coefficients are given in (3.22)-(3.24) and \( n' = N - n \). Compared to the direct equations (3.19)-(3.21) the only difference is the excitation in (5.17) and the sign of the spatial derivative terms. The similarity to the direct equations is expected from the continuous derivation in the previous chapter. However, the discrete derivation is necessary to guarantee a consistent gradient.

### 5.4 Gradient

The gradients are identified in (5.9) as

\[
\left( \frac{\partial j}{\partial \varepsilon} \right)_{\Omega_{\varepsilon}} = \sum_{n=0}^{N-1} \sum_{i,j \in \Omega_{\varepsilon}} w_{\varepsilon,i,j} \left( E^*_z D_t E_z \right)_{i,j+1/2}^{n+1/2} \Delta, \quad (5.18)
\]

\[
\left( \frac{\partial j}{\partial \sigma} \right)_{\Omega_{\sigma}} = \sum_{n=0}^{N-1} \sum_{i,j \in \Omega_{\sigma}} w_{\sigma,i,j} \left( E^*_z S_t E_z \right)_{i,j+1/2}^{n+1/2} \Delta, \quad (5.19)
\]

\[
\left( \frac{\partial j}{\partial \mu} \right)_{\Omega_{\mu}} = \sum_{n=0}^{N-1} \sum_{i,j \in \Omega_{\mu}} \left\{ \left( H^*_{x} D_t H_x \right)_{i,j+1/2}^{n} + \left( H^*_y D_t H_y \right)_{i+1/2,j}^{n} \right\} \Delta \quad (5.20)
\]

where \( \Omega_{\varepsilon} \), \( \Omega_{\sigma} \) and \( \Omega_{\mu} \) denote the spatial domain of the respective parameters. The weight functions \( w_{\varepsilon,i,j} \) and \( w_{\sigma,i,j} \) are necessary due to the averaging of the permittivity and conductivity on the boundaries between different media described in Section 3.6. The weight depends on the material parameters of the four surrounding cells, see Figure 3.3. For example the permittivity weight, \( w_{\varepsilon,i,j}^{m} \), is determined.
by

\[ w_{ij}^m = \begin{cases} 
1, & \varepsilon = \varepsilon_m \text{ in all surrounding cells} \\
\frac{3}{4}, & \varepsilon = \varepsilon_m \text{ in } 3 \\
\frac{1}{2}, & \varepsilon = \varepsilon_m \text{ in } 2 \\
\frac{1}{4}, & \varepsilon = \varepsilon_m \text{ in } 1
\end{cases} \]

In an inhomogeneous material, the permittivity of individual cells may be defined as parameters. Figure 5.3 illustrates a single cell with permittivity \( \varepsilon \) surrounded by free space \( \varepsilon_0 \).

The gradient with respect to \( \varepsilon \) in this case becomes

\[
\frac{\partial j}{\partial \varepsilon} = \frac{1}{4} \sum_{n=0}^{N-1} \left\{ E_z^n D_t E_z^{n+1/2}_{i+1,j} + E_z^n D_t E_z^{n+1/2}_{i,j+1} + E_z^n D_t E_z^{n+1/2}_{i,j} + E_z^n D_t E_z^{n+1/2}_{i+1,j+1} \right\} \Delta
\]

A reconstruction problem with inhomogeneous permittivity is studied in Section 7.1.3.

### 5.5 Verification of the gradients

The adjoint gradients were validated by comparing with finite-difference approximations. The geometry of the test problem consisted of a square region of simple media. The observed field was obtained by simulation and the adjoint gradient was computed in a non-optimal point. The gradient was then compared with a centered finite difference approximations as illustrated for the permittivity below

\[
\frac{\partial j}{\partial \varepsilon} = \frac{j(\varepsilon + \Delta \varepsilon) - j(\varepsilon - \Delta \varepsilon)}{2\Delta \varepsilon}
\]

The step size of the difference approximation was reduced by a factor of two a number of times to make sure the approximation converged. The magnitude of the difference between the adjoint and finite-difference gradients for the three parameters is shown in Figure 5.4.
As illustrated in the figure the error decreases (quadratically as expected) and is of the order of $10^{-7}$ for the smallest step size (somewhat higher for the conductivity gradient). The gradient expression for Debye and Lorentz material were verified in the same way with similar results.

### 5.6 Memory-limited gradient computation

The gradient expressions in (5.18)-(5.19) contains summations of the direct and adjoint fields over all time steps and all grid points in the parameter region. The amount of data required for the gradient computation may therefore become excessively large, particularly in three dimensions. However, it is not necessary to store all the data in advance. Using one additional direct simulation it is possible to reduce the memory requirements significantly.

- Solve the direct problem
  - store the field in the observation points
  - store the full state every $N_R = N/R$ time step, resulting in $R$ restart points
- Compute the excitation for the adjoint problem $(u(t) - u^{\text{obs}}(t))$
- For each restart point, $r = R, R-1, \ldots, 1$
5.6. Memory-limited gradient computation

- Solve the direct problem from \( t = (r - 1)N_R \) to \( t = rN_R \) and store the direct field in the parameter region for each time step, \( U(\Omega_p, t) \)
- Solve the adjoint problem from \( t = rN_R \) to \( t = (r - 1)N_R \) and store the adjoint field \( U^*(\Omega_p, t) \)
- Compute the partial gradient \( (\partial j/\partial p)_r \)
- Add contribution to the total gradient \( \partial j/\partial p = \partial j/\partial p + (\partial j/\partial p)_r \)

The procedure is illustrated in Figure 5.5.

![Figure 5.5. Memory-limited gradient computation.](image)

Note that it is not necessary to store the adjoint fields if the gradient is computed one time step at a time along with the adjoint solution.
Chapter 6

The Inverse Subcell Problem

In the numerical solution of electromagnetic problems a common difficulty is how to model small (compared to the global dimensions), complex devices efficiently. Resolving the small details using a fine mesh is often too costly and may not be necessary since one is typically interested in the field at a distance from the structure. The FDTD method, in particular, is badly suited for modeling complex geometries due to the Cartesian mesh. Subcell models constitute a possible remedy for this problem. However, the local modifications of the numerical scheme need to be derived separately for each type of small structure (narrow gap, thin sheet, etc.). Therefore the method is unpractical for modeling complex structures with many unique features. Inverse scattering provides a different way of using subcell models. In this case the subcell model is seen as a parameterization of the complex device. Using reflection measurements of the real device an inverse problem is solved to find parameters which gives a similar response. By combining a number of subcell models the number of parameters is increased and the quality of the model improved. Of course, the possibility of solving inverse problems for FDTD models containing subcell models is also important by itself.

In this section we derive the gradient of the subcell parameters for a geometry consisting of a thin dielectric sheet with a narrow gap, using the adjoint framework presented in the previous chapters. Due to the discrete nature of the subcell models there are no corresponding continuous results. Although the derivations are somewhat involved the overall approach should be clear.

6.1 Model problem

The geometry under consideration is a dielectric sheet \((\varepsilon_s, \sigma_s, \mu)\) of thickness, \(d\) and with a narrow slot of width \(g\) for the TE mode of the electromagnetic field.

As illustrated in Figure 6.1 the sheet is located in the grid points \(i = i_{\text{min}}, \ldots, i_{\text{max}}\) and \(j = j_s^*\). The index \(j_s^*\) denotes the \(y\)-index of the center of the sheet, i.e. the
corresponding \( y \)-coordinate is given by \( y = j_s^* \Delta y \). We require that the entire sheet lies between \( j_s + 1/2 \) and \( j_s + 1 \) implying that \( d < \Delta y / 2 \). The narrow gap is located at \( x \)-index \( i_g + 1/2 \) and \((\varepsilon, \sigma, \mu)\) are the material properties of the background media. Note that an auxiliary field \( \tilde{E}_y \), located inside the sheet, has been introduced to model the discontinuity of the electric field.

The numbers in the figure indicate the discrete field components that need special attention due to the subcell geometry. The numbers refer to components of a certain type rather than a single component. For example "1" refers to all \( E_x \)-components just above the sheet and not only the one indicated in the figure.

As described in Section 3.8 the modified update equations for these fields are derived by applying the integral form of Maxwell's equations. In the following section we will state the resulting equations without the derivation.

### 6.2 Direct equations

The FDTD mesh for the TE mode is illustrated in Figure 3.1. Due to the different locations of the discrete fields we define the following index spaces

\[
\begin{align*}
\Omega_x : i &= 0, \ldots, N_x - 1, j = 1, \ldots, N_y - 1 \\
\Omega_y : i &= 1, \ldots, N_x - 1, j = 0, \ldots, N_y - 1 \\
\Omega_z : i &= 0, \ldots, N_x - 1, j = 0, \ldots, N_y - 1
\end{align*}
\]
6.2. Direct equations

where $N_x$ and $N_y$ are the number of cells in the $x$- and $y$-directions. As before, we introduce the direct field vector $u$ which in the subcell case becomes

$$u = \begin{pmatrix}
E_x|_{i+1/2,j}^n \\
E_y|_{i,j+1/2}^n \\
\tilde{E}_y|_{i,j+1/2}^n \\
H_z|_{i+1/2,j+1/2}^n
\end{pmatrix}.$$  

To simplify the derivations below we let $\tilde{E}_y$ be defined in the entire region but to be non-zero only inside the sheet, that is for $i = i_{\min}, \ldots, i_{\max}, j = j^*$.

We assume perfectly conducting outer boundary and zero initial conditions of the fields

$$E_x|_{i+1/2,j}^0 = E_y|_{i,j+1/2}^0 = \tilde{E}_y|_{i,j+1/2}^0 = H_z|_{i+1/2,j+1/2}^{-1/2} = 0$$  

In order to limit the number of equations, we define general equations which are applicable in the entire domain and use the coefficients in these equations to distinguish between the field components in different grid points.

First, we consider the $E_x$-field. The only discrete field components affected by the subcell geometry are those just above the sheet, indicated by “1” in Figure 6.1. Using the difference operators introduced in Section 5.1 the discrete equations for these components become

$$\varepsilon_x D_t E_x - D_y H_z + \sigma_x S_t E_x = 0|_{i+1/2,j}^{n+1/2}, \quad (i, j) \in \Omega_x, n = 0, \ldots, N - 1$$  

where

$$\varepsilon_x|_{i+1/2,j} = \begin{cases}
\frac{d}{dx} \varepsilon_s + \left(1 - \frac{d}{dx}\right) \varepsilon, & i = i_{\min}, \ldots, i_{\max}, i \neq i_g, j = j^* \\
\varepsilon, & \text{otherwise},
\end{cases}$$

and correspondingly for $\sigma_x|_{i+1/2,j}$

$$\sigma_x|_{i+1/2,j} = \begin{cases}
\frac{d}{dx} \sigma_s + \left(1 - \frac{d}{dx}\right) \sigma, & i = i_{\min}, \ldots, i_{\max}, i \neq i_g, j = j^* \\
\sigma, & \text{otherwise}.
\end{cases}$$

The $E_y$-field is not affected by the subcell geometry and therefore the ordinary update equations are used for these components.
\[ \varepsilon D_t E_y + D_x H_z + \sigma S_t E_y = 0 \mid_{i,j+1/2}, \quad (i,j) \in \Omega_y, n = 0, \ldots, N - 1 \quad (6.3) \]

For the auxiliary \( \tilde{E}_y \)-field inside the thin sheet we distinguish between three different cases, denoted by "2", "3" and "4" in Figure 6.1:

\[ \varepsilon_y D_t \tilde{E}_y + D_x H_z + \tilde{\sigma}_y S_t \tilde{E}_y = 0 \mid_{i,j+1/2}, \quad (i,j) \in \Omega_y, n = 0, \ldots, N - 1 \quad (6.4) \]

where

\[
\varepsilon_y \mid_{i,j+1/2} = \begin{cases} 
\frac{\varepsilon_s}{\varepsilon + (1 - \frac{\varepsilon_s}{\varepsilon})} & i = i_{\min} + 1, \ldots, i_g - 1, i_g + 2, \ldots, i_{\max}, j = j_s^* \\
\frac{\varepsilon_s}{\varepsilon + (1 - \frac{\varepsilon_s}{\varepsilon})} & i = i_g, i_g + 1, j = j_s^* \\
0 & i = i_{\min}, i_{\max}, j = j_s^* \\
& \text{otherwise.}
\end{cases}
\]

and correspondingly for \( \tilde{\sigma}_y \mid_{i,j+1/2} \).

There are three different cases where the update equations for the \( H_z \)-field need to be modified. Below the sheet, indicated by "5" in Figure 6.1, and at the respective ends of the sheet, i.e. where \( i = i_{\min} \) and \( i = i_{\max} \). Only the one at \( i = i_{\min} \) is illustrated in Figure 6.1 where it is denoted by "6". The \( H_z \mid_{i_{\min} + 1/2,j_{s},+1/2} \)-component just below the gap is updated using the same equation as component "5" since the permeability is \( \mu \) everywhere. Using variable coefficients we may form a common equation for all the \( H_z \)-components

\[ \mu D_t H_z - D_y E_x + a_{1z} D_x E_y + \tilde{a}_{1z} D_x \tilde{E}_y + a_{2z} E_y \mid_{i+1/2} + \tilde{a}_{2z} \tilde{E}_y \mid_{i+1/2} = 0 \mid_{i+1/2,j+1/2}, \quad (i,j) \in \Omega_z, n = 0, \ldots, N - 1 \quad (6.5) \]

where the additional indexes for the last two terms overrides the index of the equation to the right. Four regions with different coefficients in the \( H_z \)-equation are identified

1) \( i = i_{\min}, \ldots, i_{\max} - 1, \quad j = j_s \) (below sheet)
2) \( i = i_{\min} - 1, \quad j = j_s \) (left end-point)
3) \( i = i_{\max}, \quad j = j_s \) (right end-point)
4) everywhere else.

The corresponding coefficients are

1) \( a_{1z} = (1 - d/(\Delta y)), \quad a_{2z} = 0, \quad \tilde{a}_{1z} = d/\Delta y, \quad \tilde{a}_{2z} = 0, \)
2) \( a_{1z} = (1 - d/(\Delta y)), \quad a_{2z} = -d/(\Delta x \Delta y), \quad \tilde{a}_{1z} = d/\Delta y, \quad \tilde{a}_{2z} = d/(\Delta x \Delta y) \)
3) \( a_{1z} = 1, \quad a_{2z} = d/(\Delta x \Delta y), \quad \tilde{a}_{1z} = 0, \quad \tilde{a}_{2z} = -d/(\Delta x \Delta y) \)
4) \( a_{1z} = 1, \quad a_{2z} = 0, \quad \tilde{a}_{1z} = 0, \quad \tilde{a}_{2z} = 0. \)
6.3 Cost function

The discrete cost function in the TE case is given by

\[
\begin{align*}
\frac{1}{2} \sum_{m=1}^{M} \sum_{n=0}^{N} \left\{ \sum_{\Omega_x} \left( E_x(p) - E_{x,\text{obs}} \right)^2 \right\} + \sum_{\Omega_y} \left( E_y(p) - E_{y,\text{obs}} \right)^2 \left| i_{n+1/2,j} \right| \delta_m \right\} \Delta, \quad (6.6)
\end{align*}
\]

where \( E_{x,\text{obs}} \) and \( E_{y,\text{obs}} \) are the \( x \)- and \( y \)-components of the observed electric field in the observation points, \( \Delta = \Delta x \Delta y \Delta t \) and \( \delta_m \) is the Dirac delta function that picks out the observation points in space. Note that due to the staggered grid, the discrete \( E_x \)- and \( E_y \)-fields are located in different grid points.

6.4 Parameters

The parameters of the inverse problem in the subcell case are the permittivity and conductivity of the sheet, \( \varepsilon_s \) and \( \sigma_s \), the width of the narrow gap \( g \) and the thickness of the sheet, \( d \). The parameter vector \( p \) thus becomes

\[
p = [\varepsilon_s, \sigma_s, g, d]^T \quad (6.7)
\]

6.5 Adjoint equations

The adjoint fields for the inverse subcell problem are defined in the same way as was done for the TM case in Section 5.3. This means the adjoint fields are located in the same grid points as the corresponding direct fields but are staggered by a half time step. The adjoint field vector is thus defined as

\[
u = \begin{pmatrix}
E_x^{n+1/2}_{i+1/2,j} \\
E_x^n_{i,j+1/2} \\
E_y^{n+1/2}_{i,j} \\
E_y^n_{i+1/2,j} \\
H_z^n_{i+1/2,j+1/2}
\end{pmatrix}, \quad (6.8)
\]

where the adjoint auxiliary field \( \tilde{E}_{y,s}^* \), like its direct counterpart, only is non-zero inside the sheet, i.e. \( i = i_{\text{min}}, \ldots, i_{\text{max}}, j = j_s^* \). Boundary terms will appear in
the derivation of the discrete adjoint equations. The following initial and boundary conditions for the adjoint fields are needed for these terms to vanish

\[ E^x_{i+1/2,j} = E^y_{i+1/2,j} = E^a_{i+1/2,j} = 0 \]

\[ E^x_{i+1/2,0} = E^y_{i+1/2,N_y} = E^a_{i+1/2,0} = 0. \]  

Using the direct subcell equations (6.2)-(6.5) and the adjoint fields (6.8) the Lagrangian becomes

\[
L(p, u, A) = \left( u^T p \right) + 
\sum_{n=0}^{N-1} \sum_{i,j} \left( E^x_i \left( \varepsilon_{ij} D_i E_j - D_y H_z + \sigma_x S_i E_x \right) \right) \nabla_{i+1/2,j} + 
\sum_{n=0}^{N-1} \sum_{i,j} E^y_i \left( \varepsilon_{ij} D_i E_j + \sigma_y S_i E_y \right) \nabla_{i+1/2,j} + 
\sum_{n=0}^{N-1} \sum_{i,j} \tilde{H}_y \left( \mu D_i H_z - D_y E_x + a_{1z} D_x E_y + \tilde{a}_{1z} \tilde{D}_z E_y \right) + 
\sum_{n=0}^{N-1} \sum_{i,j} \left( a_{2z} E_y |_i + \tilde{a}_{2z} \tilde{E}_y |_i \right) \nabla_{i+1/2,j+1/2} \Delta
\]

Linearizing and using the direct equations yields

\[
\delta L = \sum_{n=0}^{N-1} \sum_{i,j} \left( \delta E^x_i \left( E^x_i - E^{obs}_i \right) \nabla_{i+1/2,j} + \delta E^y_i \left( E^y_i - E^{obs}_i \right) \nabla_{i+1/2,j} + \delta H^y_i \left( \mu D_i H_z - D_y E_x + a_{1z} D_x E_y + \tilde{a}_{1z} \tilde{D}_z E_y \right) \nabla_{i+1/2,j} + \delta E^x_i \left( a_{2z} E_y \right) + \delta E^y_i \left( \tilde{a}_{2z} \tilde{E}_y \right) \right) \Delta
\]
The adjoint equations are obtained by summation by parts of the above expression. The main difference compared to the inverse media case in Chapter 5 is found in the $H_z$-equation (6.5) where the coefficients in front of the $D_x$-terms are space dependent. These coefficients will “spread out” to the equations for the adjacent adjoint fields. We illustrate for the $E_y$-component. The $\delta E_y^*$-terms in (6.11) are

$$\sum_{i,j=1}^{N-1} \sum_{\Omega y} E_y^* (\varepsilon D_t \delta E_y + \sigma S_t \delta E_y)^{n+1/2} \Delta +$$

$$\sum_{i,j=1}^{N-1} \sum_{\Omega z} H_z^* (a_{1z} D_x \delta E_y + a_{2z} \delta E_y || i) \big|_{i+1/2,j+1/2} \Delta$$

Using summation by parts in time and space and using the initial and boundary conditions for the direct and adjoint fields to cancel the boundary terms results in

$$\sum_{i,j=1}^{N-1} \sum_{\Omega y} \delta E_y \left\{ -\varepsilon D_t E_y^* + \sigma S_t E_y^* - D_x (a_{1z} H_z^*) + a_{2z} \delta E_y \right\} \big|_{i,j+1/2}^{n+1/2} \Delta$$

Now, consider for example the $E_y^*$ field in the grid point $i_{min} - 1, j_{s} + 1/2$, i.e. one cell to the left of the sheet. The update equation for the corresponding direct field, $E_y$, is not affected by the sheet since the integration surface (see Section 3.8) lies entirely in the background medium. For the adjoint field, using the coefficients defined in Section 6.2 we obtain

$$- \varepsilon D_t E_y^* + \sigma S_t E_y^* - \frac{\Delta y - d}{\Delta y} D_x H_z + \frac{d}{\Delta x \Delta y} H_z^* \big|_{i-3/2} = 0 \big|_{i_{min}-1,j_{s}+1/2}$$

which clearly depends on the subcell parameter $d$ (the sheet thickness). For the remaining adjoint equations we state the results without derivation. The equation for the $E_x^*$-field becomes

$$-\varepsilon_x D_t E_x^* + D_y H_z^* + \sigma_x S_t E_x^* = 0 \big|_{i+1/2,j}, (i,j) \in \Omega x, n = 1, \ldots, N$$

and for the $E_y^*$-field

$$-\varepsilon D_t E_y^* + \sigma S_t E_y^* - D_x (a_{1z} H_z^*) + a_{2z} \delta E_y \big|_{i,j+1/2} = 0 \big|_{i_{min}-1,j_{s}+1/2}$$
Finally, the adjoint equation for the \( H_x^* \)-field becomes:

\[
-\mu D_t H_x^* + D_y E_x^* - D_x E_y^* - D_x \bar{E}_y^* = 0 \mid_{i+1/2}^{n+1/2}, (i, j) \in \Omega_y, n = 1, \ldots, N
\]  

(6.15)

### 6.6 Gradients

The gradient is obtained by identification in (6.11). To obtain the gradient with respect to the original parameters in (6.7) we need to use that

\[
\frac{\delta \varepsilon_x}{\delta \varepsilon_s} = \frac{\partial \varepsilon_x}{\partial \varepsilon_s} \delta \varepsilon_s + \frac{\partial \varepsilon_x}{\partial d} \delta d
\]

and similarly for the other coefficients. The following partial derivatives of the coefficients are needed,

\[
\frac{\partial \varepsilon_x}{\partial \sigma_s} \bigg|_{i+1/2,j} = \frac{\partial \varepsilon_x}{\partial \sigma_s} \bigg|_{i+1/2,j} = \begin{cases} 
\frac{d}{\Delta y}, & i = i_{\text{min}}, \ldots, i_{\text{max}}, i \neq i_y, j = j_s \\
\frac{d}{\Delta x} (\Delta x - g); & i = i_y, j = j_s \\
0, & \text{otherwise}
\end{cases}
\]

(6.16)

\[
\frac{\partial \varepsilon_x}{\partial \delta d} \bigg|_{i+1/2,j} = \begin{cases} 
\frac{(\varepsilon - \varepsilon_s)}{\Delta y}, & i = i_{\text{min}}, \ldots, i_{\text{max}}, i \neq i_y, j = j_s \\
\frac{\varepsilon_s}{\Delta y}, & i = i_y, j = j_s \\
0, & \text{otherwise}
\end{cases}
\]

(6.17)

The derivatives of \( \sigma_y \) with respect to \( d \) is obtained by substituting \( \varepsilon \) and \( \varepsilon_s \) with \( \sigma \) and \( \sigma_s \) in the expressions for \( \partial \varepsilon_x / \partial d \).

\[
\frac{\partial \varepsilon_y}{\partial \sigma_s} \bigg|_{i,j+1/2} = \begin{cases} 
1 & i = i_{\text{min}} + 1, \ldots, i_y - 1, i_y + 2, \ldots, i_{\text{max}}, j = j_s \\
\frac{\varepsilon_y}{\Delta y} & i = i_y, j = j_s \\
\frac{\varepsilon_s}{\Delta y} & i = i_{\text{min}}, j = j_s \\
0 & \text{otherwise}
\end{cases}
\]

(6.18)

\[
\frac{\partial \varepsilon_y}{\partial g} \bigg|_{i,j+1/2} = \begin{cases} 
\frac{1}{2\Delta x} (\varepsilon - \varepsilon_s) & i = i_y, j = j_s \\
0 & \text{otherwise}
\end{cases}
\]

(6.19)

Again, the derivatives of \( \sigma_y \) with respect to \( d \) and \( g \) are obtained by substituting \( \varepsilon \) and \( \varepsilon_s \) with \( \sigma \) and \( \sigma_s \). The coefficients in \( a_{1z}, a_{2s}, \tilde{a}_{1z}, \tilde{a}_{1s} \) depend on the sheet thickness \( d \) which means we need to compute the corresponding derivatives.
6.6. Gradients

1) \( a_{1z}' = (1 - d/\Delta y), \quad a_{2z}' = 0, \quad \bar{a}_{1z}' = d/\Delta y, \quad \bar{a}_{2z}' = 0, \)

2) \( a_{1z}' = (1 - d/\Delta y), \quad a_{2z}' = -d/(\Delta x \Delta y), \quad \bar{a}_{1z}' = d/\Delta y, \quad \bar{a}_{2z}' = d/(\Delta x \Delta y) \)

3) \( a_{1z}' = 1, \quad a_{2z}' = d/(\Delta x \Delta y), \quad \bar{a}_{1z}' = 0, \quad \bar{a}_{2z}' = -d/(\Delta x \Delta y) \)

4) \( a_{1z}' = 1, \quad a_{2z}' = 0, \quad \bar{a}_{1z}' = 0, \quad \bar{a}_{2z}' = 0 \)

where the \( ' \) denotes the derivative with respect to \( d \). Using the partial derivatives above the gradient for the subcell parameters becomes

\[
\begin{align*}
\frac{\partial j}{\partial \varepsilon_x} &= \sum_{E_x} E_x^s \frac{\partial \varepsilon_x}{\partial \varepsilon_x} D_t \tilde{E}_x|_{i+1/2,j}^{n+1/2} \Delta + \sum_{E_y} \tilde{E}_y^s \frac{\partial \varepsilon_y}{\partial \varepsilon_x} D_t \tilde{E}_y|_{i,j+1/2}^{n+1/2} \Delta \\
\frac{\partial j}{\partial \sigma} &= \sum_{E_x} E_x^s \frac{\partial \sigma_x}{\partial g} S_t E_x|_{i+1/2,j}^{n+1/2} \Delta + \sum_{E_y} \tilde{E}_y^s \frac{\partial \sigma_y}{\partial g} S_t \tilde{E}_y|_{i,j+1/2}^{n+1/2} \Delta \\
\frac{\partial j}{\partial \varepsilon_y} &= \sum_{E_x} E_x^s \left( \frac{\partial \varepsilon_x}{\partial d} D_t \tilde{E}_y + \frac{\partial \sigma_y}{\partial d} S_t \tilde{E}_y \right)|_{i+1/2,j}^{n+1/2} \Delta + \\
&+ \sum_{E_y} \tilde{E}_y^s \left( \frac{\partial \varepsilon_y}{\partial d} D_t \tilde{E}_y + \frac{\partial \sigma_y}{\partial d} S_t \tilde{E}_y \right)|_{i,j+1/2}^{n+1/2} \Delta + \\
&+ \sum_{H_y} H_y^s \left( a_{1z}' D_x \tilde{E}_y + \bar{a}_{1z}' D_x \tilde{E}_y + a_{2z}' \tilde{E}_y|_i + \bar{a}_{2z}' \tilde{E}_y|_i \right)|_{i+1/2,j+1/2}^{n+1/2} \Delta
\end{align*}
\] (6.20)

(6.21)

(6.22)

(6.23)

The above gradient expressions were verified using finite differences as described in the previous chapter.
Chapter 7

Results

As we have seen in the previous sections, the inverse minimization algorithm consists of several different parts and careful validation is necessary to ensure correct results. During the validation synthetic data from numerical simulations play an important role. In these cases synthetic reflection data is obtained by simulation and the inverse algorithm is applied to reconstruct the original values from an arbitrary initial guess. This approach has the advantage that the exact solution is known. Furthermore, different sources of error such as noise and lack of data may be isolated and studied separately.

An important application of the inverse modeling is non-destructive testing. Typically, reflection measurements of the tested structure are carried out and the inverse algorithm is applied to determine the unknown parameters from the observed field. In Section 7.1 we show examples of media reconstruction of multilayer structures using synthetic data, both non-dispersive media and Debye media are considered. We also give an example where the scattering geometry is completely unknown and a large number of parameters is used to model a general inhomogeneous permittivity. In Section 7.2 reconstruction using measured data is addressed. The experimental setup for reflection measurements at Saab Bofors Dynamics is described. The data is obtained in frequency domain and has to be transformed to fit into the time-domain framework. The transformation procedure is validated using analytical data. Finally, we show results for the characterization of a three layer panel of simple media using measured data.

In some cases the thicknesses of the panel layers are not known and needs to be reconstructed simultaneously with the material parameters. To be able to compute the cost function and gradient of the thickness parameters we use quadratic interpolation of the cost function in the discrete mesh. This approach is validated using both synthetic and measured data in Section 7.3.

Another application of inverse modeling is design optimization. In this case a desired scattered field is specified and the minimization is applied to determine the optimal parameters for a given model. Two different optimization problems
are considered in Section 7.4, minimization of the field in a composite box and frequency filtering of a reflected wave using a simple conductivity model.

The reconstruction of subcell parameters in a model containing a thin sheet and a narrow slot is studied in Section 7.5. In Section 7.6 we study how the frequency of the excitation affects the behavior of the cost function. We also study the effect of changing the number of observation points and adding noise. Finally, in Section 7.7 we describe the parallel implementation and show some performance results.

In all the presented results the minimization problem was solved by the optimization routine \texttt{nag\_nlp\_sol} from NAG (Numerical Algorithms Group), [1]. It implements an SQP algorithm for general constrained non-linear optimization. The termination criterion for the gradient was set to $10^{-6}$.

In order to improve readability, each test case is given a four letter label which is repeated in the corresponding figures and tables.

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{figure7_1.png}
\caption{SSIM FDTD model of the multilayer panel.}
\end{figure}
7.1 Characterization of media using synthetic observation data

7.1.1 Layered structure of simple media (SSIM)

In the first test case we consider the reconstruction of the relative permittivities and permeabilities of a multilayer structure. The geometry consists of five layers with different media, resting on a perfectly conducting table, as illustrated in Figure 7.1. The thickness of each layer is fixed to 0.1 m, resulting in a total of ten parameters. The incident field consists of a plane wave Gaussian pulse with the \( \vec{E} \)-field polarization in the xy-plane (i.e. the TE mode) and propagating in the (-1,-1) direction. The cutoff frequency of the pulse is 7.5 GHz, corresponding to a free space wavelength of about 0.04 m. The cell size is \( \Delta = 0.001 \) m and the number of cells in each direction \( N_x = 40 \) and \( N_y = 80 \). The \( x \)- and \( y \)-components of the electric field are observed in two points located at grid indices \( i = 5, j = 65, 75 \), as indicated in Figure 7.1. The initial parameter values are chosen as \( \varepsilon_r = 2.5 \) and \( \mu_r = 1.5 \) in all layers.

![Figure 7.2. SSIM Reconstruction of a multilayer panel using synthetic data.](image-url)
Chapter 7. Results

The result of the minimization is illustrated in Figure 7.2. The termination criterion for the gradient is reached in 45 main iterations. The maximum relative error in the final parameters is below $10^{-6}$. The problem was also solved using the built-in finite-difference approximation of the gradient in the optimizer. The relative error of the difference approximation in the initial point was of the order $10^{-6}$. In this case the iterations did not converge to the correct solution and terminated in a local minima after 45 iterations. At this point the relative error in some parameters exceeded 100% and the decrease in the cost function was only a factor three. This indicates the sensitivity of the minimization procedure even for a synthetic test case.

In case measured data is used there are additional difficulties, for example due to noise in the observation data. The sensitivity with respect to noise was studied by adding Gaussian noise to the time-domain observation data. Different noise levels were tested and the convergence of the minimization iterations for the different levels are found in Figure 7.3. In case of ten percent noise the convergence to the correct solution is lost. It is hard to draw any general conclusions from a specific test case but similar experiments for other problems indicate that noise levels of a few percent is often not critical. To obtain a more reliable solution one may use multiple initial points in the minimization.
7.1. Characterization of media using synthetic observation data

7.1.2 Layered structure of dispersive media (SDEB)

In this test case we consider the reconstruction of the dielectric function for three material layers of different Debye media for the TM mode. The computational domain is similar to the previous example in Figure 7.1 with a cell size of $\Delta = 0.001 \text{ m}$ and 50 by 60 cells. Each layer has a thickness of ten cells and a width of 30 cells. The excitation consists of a plane wave Gaussian pulse with cutoff frequency of 7.2 GHz and traveling in the (-1,-1) direction. A single observation point located close to the upper left corner is used and the observed $E_z$-field is obtained by simulation. The unknown parameters consist of the three Debye parameters (see Equation 3.41) in each layer resulting in nine parameters. Since the parameters have widely different scales we use the relative value for the relaxation time (with respect to the initial guess), as described in Section 4.2.

The results from the minimization are illustrated in Figure 7.4. All parameters were reconstructed correctly in about 115 main iterations. Note that $\varepsilon_s$ is recovered.
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faster than the other parameters, implying that the cost function depends strongly on this parameter. Furthermore, the parameters in the top layer converge faster than those of the layers below. This is expected since a large amount of the incident energy is reflected by the top layer.

7.1.3 General inhomogeneous permittivity (SGEN)

In this test case the inverse algorithm is applied to the reconstruction of a material structure of unknown shape. Since no information about the shape is given the relative permittivity is completely inhomogeneous, i.e., $\varepsilon_r = \varepsilon_r(x, y)$. The observed field is obtained for a “z”-shaped object with permittivity $\varepsilon_r = 5.0$ using twelve observation points surrounding the unknown domain. The problem is solved for the TM case of Maxwell’s equations using a Gaussian pulse plane wave excitation with a cutoff frequency of 14 GHz.

![Figure 7.5. SGEN Computational domain for the general inhomogeneous permittivity reconstruction example.](image)

The size of the FDTD grid is 40 by 40 cells the cell size is $\Delta = 0.001 \text{m}$ and the permittivity is varied within a 21 by 21 cells square resulting in 441 unknown parameters. The dimensions of the unknown region corresponds to one by one wavelength for the cutoff frequency. The permittivity is initially set to free space.
In Figure 7.6 the permittivity profile in different minimization iterations is illustrated. We note that the “z”-shape is apparent after just a few iterations. The convergence of each parameter is however quite slow and the accuracy is about three digits after 800 iterations. The same problem was studied with noisy observation data (10%) and the results are shown in Figure 7.7. The effect of the added noise becomes more pronounced as the number of iterations grows. For this type of problem regularization by penalization of the spatial variation of the material parameters may be efficient. However, this would lead to a “smeared out” solution where the location of discontinuities will be less sharp.
7.2 Characterization of a multilayer panel using measured data

In this section we consider non-destructive characterization of the material properties of an unknown panel using measurements of the reflected field. Several modeling issues have to be solved before the inverse algorithm can be applied, for example how to use the frequency domain reflection data. The measurements were carried out at Saab Bofors Dynamics and the simulations were conducted by AeroTechTelub AB in Linköping.

7.2.1 Description of the measurement equipment

The material sample consists of a square panel with a side length of 300 millimeters and a total thickness of 2 to 30 millimeters. The panel is built-up by several layers, typically three to five, with different dielectric properties. The measurements are
conducted in an anechoic chamber where the sample is placed on a metallic table located in the middle of the chamber, as illustrated in Figure 7.8. The table is perforated with small holes and connected to a vacuum pump to ensure that the sample is tightly fit onto the table. Two pairs of horn antennas (only one is shown in Figure 7.8) mounted in fixed positions at angles 17.5 deg and 60 deg at a distance of 1.25 m from the center of the table are used for emitting and receiving waves. The excitation consists of a continuous harmonic wave in the frequency range 4–18 GHz (corresponding to wavelengths between 1.7–15 cm). The frequency may be chosen in increments of 20 MHz resulting in a maximum of 701 frequencies. Absorbers reduce reflections from the walls of the chamber and an absorber placed between the two antennas makes sure that the direct field from the emitter to the receiver is absorbed. The receiver antenna measures the amplitude and phase of the reflected electric field for each frequency. To avoid capturing undesired reflections, only a limited time-interval of the registered field is taken into account, as illustrated in Figure 7.9.

7.2.2 Numerical model

The experimental setup is modeled using 2D FDTD for the TE mode. The reduction to two dimensions relies on the fact that the main contribution to the registered field comes from the first reflection, denoted by “1” in Figure 7.9. The effect of
reflections at the edges of the panel is small due to the absorbing walls and the time gating. Further simplification is possible since the table is located in the far field of the emitter antenna as discussed in Appendix A. The incident field may then be approximated by a plane wave. The advantages of this approach is that we avoid detailed modeling of the antennas and a significant reduction of the problem size is possible. The latter factor is important since a fine grid is necessary to resolve the material sample. The computational domain is illustrated in Figure 7.10.

Typically, the cell size is limited by the thickness of the layers in the material sample (usually only a few millimeters) rather than by the shortest wavelengths. Therefore a coarser grid may be used in the horizontal direction where only the wavelength has to be resolved. In the simulation in Section 7.2.5 the cell size was $\Delta x = 0.001$ m and $\Delta y = 0.0002$ m.
7.2. Characterization of a multilayer panel using measured data

7.2.3 Transformation of measurement data

The minimization requires observation data in the time domain, see (5.5). The measurement data thus has to be transformed using an inverse Fourier transform. We will define a time-domain excitation with the desired frequency content, and then use the measured reflection coefficient to compute the corresponding observed reflected field.

The frequency content of the excitation should be limited to the frequencies of the measurement data since there is no information about the response of frequencies outside this interval. The following function is well suited for this purpose

\[
    f_{\text{exc}}(t) = \gamma \left( \frac{\sin(\omega_{\text{max}}(t - t_0))}{t - t_0} - \frac{\sin(\omega_{\text{min}}(t - t_0))}{t - t_0} \right). \tag{7.1}
\]

The Fourier transform becomes a rectangular pulse which is non-zero in the interval \([\omega_{\text{min}}, \omega_{\text{max}}]\). The parameter \(t_0\) is a translation in time and \(\gamma\) is a scaling of the amplitude. In practice the function (7.1) has to be truncated to fit in the simulation, which destroys the finite spectrum. However, if the simulation time is large the amplitude outside the desired frequency interval becomes small. In Figure 7.11 we give an example of a truncated pulse in the time and frequency domains where \(f_{\text{min}} = 4 \cdot 10^9\) Hz, \(f_{\text{max}} = 18 \cdot 10^9\) Hz, \(T = 40/(2\pi f_{\text{min}})\) s, \(\Delta t = T/1000\) s and \(t_0 = 0.5(T - \Delta t)\) s.

\[\text{Figure 7.11. The approximative frequency domain square pulse (7.1)}\]
Chapter 7. Results

The output from a reflection experiment consists of the complex frequency domain reflection coefficients for the chosen frequencies. Two experiments are carried out, one for the unknown panel and a reference measurement where the panel is removed. In the latter case the field is reflected by the PEC table. By scaling the panel data with the reference data we limit the influence of corner reflections, etc., since these should be of similar magnitude in both experiments. Denoting the measured panel data by $R_{\text{meas}}^{\text{panel}}(k)$ and the reference data by $R_{\text{meas}}^{\text{PEC}}(k)$ the normalized reflection data is computed by:

$$R_{\text{meas}}^{\text{norm}}(k) = \frac{R_{\text{meas}}^{\text{panel}}(k)}{R_{\text{meas}}^{\text{PEC}}(k)}$$

where $k$ is a frequency index. The simulated excitation is defined in the time domain according to (7.1) and is denoted by $E_{\text{sim}}^{\text{inc}}(n)$ where $n$ is a time index. The excitation is then transformed to the frequency domain using an FFT resulting in $E_{\text{sim}}^{\text{inc}}(k)$. For the chosen excitation, the computed field for the panel $E_{\text{sim}}^{\text{panel}}(k)$ may then be expressed as

$$E_{\text{sim}}^{\text{panel}}(k) = R_{\text{meas}}^{\text{norm}}(k)E_{\text{sim}}^{\text{inc}}(k)$$

(7.2)

where linear interpolation of the measured data is used to compute intermediate values. Finally, the corresponding time-domain field, $E_{\text{sim}}^{\text{panel}}(n)$ is obtained by an inverse Fourier transform. This field becomes the observed field in the cost function, as defined in (5.5).

### 7.2.4 Validation using analytical data, (ASIM)

The scattering problem for a one-dimensional layered structure with oblique incident field is possible to solve analytically by enforcing continuity of the field over the material boundaries. In order to validate the transformation procedure, analytically computed data for a two-layer panel was computed analytically and used in place of measurement data. In the numerical simulation a two-dimensional model of the geometry is used. The simulation time and the location of the observation point were chosen to avoid contributions from corner reflections.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial value</th>
<th>Final value</th>
<th>Correct value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permittivity, layer 1</td>
<td>0.1</td>
<td>5.13</td>
<td>5.0</td>
</tr>
<tr>
<td>Conductivity, layer 1</td>
<td>5.0</td>
<td>0.11</td>
<td>0.1</td>
</tr>
<tr>
<td>Permittivity, layer 2</td>
<td>3.0</td>
<td>2.19</td>
<td>2.0</td>
</tr>
<tr>
<td>Conductivity, layer 2</td>
<td>2.0</td>
<td>3.01</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Table 7.1. ASIM Results for the multilayer reconstruction with analytical data.

In Figure 7.12 the convergence of the minimization iterations is shown and the final values of the permittivities and conductivities of the two layers are given in
7.2. Characterization of a multilayer panel using measured data

Table 7.1. Due to the approximations made in the solution process, for example when using one-dimensional observation data and in the numerical solution of the direct problem, the accuracy of the final values (between one and two digits) is acceptable.

![Figure 7.12. ASIM The multilayer reconstruction with analytical data.](image)

7.2.5 Reconstruction of a three layer panel using measured data (MSIM)

In this case experimental data is used to determine the material characteristics of a layered panel. The panel consists of three layers, numbered from the layer closest to the PEC table. The measured physical characteristics of the different layers are given in Table 7.2. Reflection measurements were conducted in the range between

<table>
<thead>
<tr>
<th>Description</th>
<th>Thickness (mm)</th>
<th>Permittivity</th>
<th>Conductivity</th>
<th>Permeability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 1</td>
<td>1.1</td>
<td>3.6</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Layer 2</td>
<td>0.9</td>
<td>5</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>Layer 3</td>
<td>2.0</td>
<td>3.6</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 7.2. Physical characteristics of the measured panel.
Table 7.3. MSIM Results from the multilayer reconstruction using measured data.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial Value</th>
<th>Final Value</th>
<th>Measured Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_1$, $\varepsilon_3$</td>
<td>5.22</td>
<td>3.67</td>
<td>3.6</td>
</tr>
<tr>
<td>$\sigma_1$, $\sigma_3$</td>
<td>9.62</td>
<td>0.00</td>
<td>0</td>
</tr>
<tr>
<td>$\varepsilon_2$</td>
<td>3.66</td>
<td>5.23</td>
<td>5</td>
</tr>
<tr>
<td>$\sigma_2$</td>
<td>0.00</td>
<td>9.62</td>
<td>10</td>
</tr>
</tbody>
</table>

4–18 GHz in steps of 20 MHz for a single antenna configuration (17.5 deg), see Figure 7.8. The measured amplitude and phase of the reflection coefficients for the panel and the reference PEC plate are shown in Figure 7.14. We wish to reconstruct the permittivity and the conductivity of the two different media in the panel (top and bottom layers are the same media) resulting in four unknown parameters. The result of the minimization is shown in Table 7.3 and the convergence of the parameters is illustrated in Figure 7.13. The relative error between measured and simulated value is less than 5% for all parameters.
7.2. Characterization of a multilayer panel using measured data

Figure 7.14. MSIM The measured amplitude and phase of the reflection coefficient for the material (above) and for the reference metal plate (below).
7.3 Structure characterization

In the testing of multilayer panels the layer thickness is sometimes not known but has to be included as an unknown parameter in the reconstruction. In this case, quadratic interpolation of the cost function for the geometrical parameter is used. The results were provided by AeroTechTelub AB.

![Figure 7.15. SSTR Convergence history for the synthetic structure characterization case.](image)

**Figure 7.15. SSTR Convergence history for the synthetic structure characterization case.**

7.3.1 Reconstruction of structure and media from synthetic data (SSTR)

In this experiment we consider the reconstruction of both material and structure parameters. The geometry consists of a two-layer panel, resting on a PEC table. We wish to determine the conductivity of each layer as well as the location of the interface between the layers. The latter parameter is defined as the vertical distance from the table. The total thickness of the structure is known, resulting in three parameters.

Due to the finite resolution of the FDTD grid the geometrical parameter may only be varied in steps corresponding to whole increments of the cell size. To be able
to compute the cost function for intermediate values we use quadratic interpolation. That is, for each parameter value supplied by the optimizer, we compute three cost function values corresponding to the three closest discrete grid points in the vertical direction and interpolate to obtain a quadratic polynomial. The resulting polynomial is also used for computing the gradient of the cost function. Note that the maximum step size of the geometrical parameters should be limited to ensure the validity of the interpolation.

The results from the minimization are given in Table 7.4. In Figure 7.15 we illustrate the convergence of the parameters during the iterations. The increase in the cost function in some iterations is explained by the fact that values from subiterations in the optimizer are included. All three parameters were recovered accurately.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial value</th>
<th>Final value</th>
<th>Correct value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity, layer 1</td>
<td>3.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Conductivity, layer 2</td>
<td>3.0</td>
<td>6.0</td>
<td>6.0</td>
</tr>
<tr>
<td>Distance, layer 1 (mm)</td>
<td>3.0</td>
<td>4.0</td>
<td>4.0</td>
</tr>
</tbody>
</table>

Table 7.4. SSTR Parameters for the synthetic structure characterization case.

### 7.3.2 Reconstruction of structure from measured data (MSTR)

In this case measurement data is used to determine the position of the interior interfaces in a three layer structure with known material properties. The total thickness as well as the thickness of the middle layer is known. Two parameters are included in the minimization, the distances to the two interior interfaces. A linear constraint has to be added to keep the thickness of the middle layer constant. The results from the minimization are shown in Table 7.5 and Figure 7.16. We see that both parameters were accurately recovered.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial value</th>
<th>Final value</th>
<th>Correct value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance, layer 1 (mm)</td>
<td>2.6</td>
<td>1.1</td>
<td>1.1</td>
</tr>
<tr>
<td>Distance, layer 2 (mm)</td>
<td>3.5</td>
<td>2.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Table 7.5. MSTR Parameters for the measured structure characterization case.

### 7.4 Characterization of media from optimized data

The previous examples have all been reconstruction problems, where the observed field was given by real or simulated data obtained for the object to be reconstructed. In optimization the observed field is rather given by design objectives and may well be unobtainable or even non-physical. The solution method is the same as in a
Chapter 7. Results

Figure 7.16. MSTR Convergence history for the measured structure characterization case.

reconstruction case. The main difference lies in the interpretation of the results, since it is not possible to verify that the obtained solution is the optimal one. The quality of the solution may be improved by using multiple initial points.

7.4.1 Composite box optimization (OBOX)

We will consider the problem of minimizing the field inside a composite box subject to a Gaussian pulse plane wave. This problem is solved for the TE mode and the geometry is illustrated in Figure 7.18. The box consists of two different dielectrics: a metallic part and an aperture in the left wall. An antenna modeled by a Gaussian pulse point source is used as excitation and the field ($E_x$ and $E_y$) is observed in seven points inside the box. The desired observed field is set to zero for the duration of the simulation. The convergence history of parameters and cost function are shown in Figure 7.17. The parameters and bounds in the optimization as well as the final values are found in Table 7.6. The minimization results in a significant reduction of the cost function. The results in Figure 7.17 indicate that the conductivity is more important than the permittivity in this case.
7.4. Characterization of media from optimized data

7.4.2 Optimization of layered media (OLAY)

The geometry of the problem consists of a three-layer panel where the conductivity of the middle layer is varied to obtain a certain reflection in the frequency domain. In this example, provided by AeroTechTelub AB, the goal is to have total reflection
### Table 7.6. OBOX Results for the composite box optimization.

<table>
<thead>
<tr>
<th>Description</th>
<th>Min</th>
<th>Max</th>
<th>Initial</th>
<th>Final</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permittivity, dielectric 1</td>
<td>1</td>
<td>25</td>
<td>1</td>
<td>12.1</td>
</tr>
<tr>
<td>Conductivity, dielectric 1</td>
<td>1</td>
<td>$10^6$</td>
<td>1</td>
<td>16.6</td>
</tr>
<tr>
<td>Permittivity, dielectric 2</td>
<td>1</td>
<td>25</td>
<td>5</td>
<td>25 (on bound)</td>
</tr>
<tr>
<td>Conductivity, dielectric 2</td>
<td>$10^{-6}$</td>
<td>$10^3$</td>
<td>0.5</td>
<td>2.72</td>
</tr>
</tbody>
</table>

Figure 7.19. Desired, initial and final reflection coefficient for the optimization experiment.

up to 10 GHz and only ten percent reflection above that frequency. Using the transformation procedure described in Section 7.2.3 a time-domain goal function is obtained. The inverse algorithm is then applied to find the optimal conductivity. In Figure 7.19 the desired reflection is illustrated together with the initial and final reflection coefficients in the minimization. As expected, we are not able to get the desired reflection but nonetheless the solution has improved significantly from the initial guess. By increasing the number of parameters in the model, for example allowing dispersive materials, it should be possible to improve the solution further.
7.5 Subcell reconstruction from synthetic data (SSUB)

In this test case we wish to reconstruct the geometrical parameters of a subcell model consisting of a thin sheet with a small gap. The geometry is the same as illustrated in Figure 6.1 where the surrounding media is free space. The initial parameter values and bounds as well as the final values resulting from the optimization are given in Table 7.7. The convergence of the parameters is illustrated in Figure 7.20. The sensitivity of the cost function with respect to the subcell parameters is of entirely different scales. While the cost function is highly sensitive to the thickness of the sheet it is extremely insensitive to changes in the gap width. This is reflected by the fact that the thickness is recovered after only about ten iterations while the remaining iterations are required to determine the gap width to the given precision.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial Value</th>
<th>Final Value</th>
<th>Correct Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sheet thickness, d</td>
<td>$0.5 \cdot 10^{-3}$</td>
<td>$1.0 \cdot 10^{-3}$</td>
<td>$1.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Gap width, g</td>
<td>$0.5 \cdot 10^{-3}$</td>
<td>$1.0 \cdot 10^{-3}$</td>
<td>$1.0 \cdot 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 7.7. SSUB Results for the subcell reconstruction test case.

Figure 7.20. SSUB Convergence history for the subcell reconstruction test case.
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7.6 Sensitivity of the cost function

7.6.1 Sensitivity vs frequency

The frequency spectrum of the incident wave strongly affects the characteristics of the minimization problem. In general a short wavelength gives sharper minima, in the sense that a small deviation from the minima results in a large increase of the cost function. The drawback is that short wavelengths also tend to generate many local minima. Longer wavelengths on the other hand give a smoother cost function with less distinct minima. To illustrate this behavior we studied the cost function for the synthetic multilayer case (see Section 7.1.1). Only two parameters were used, the relative permittivities of layer 1 and 3. The observed field was obtained by a direct solution with $\epsilon_1 = 5$ and $\epsilon_3 = 3$. Both parameters were then varied between 1 and 10 in increments of 0.1 and the cost function was computed for each combination resulting in a two-dimensional array of cost function values. Two different excitations were used, both Gaussian plane waves with cutoff frequencies $0.02$, $0.04$, $0.06$, $0.08$, $0.1$.
of about 1 GHz in the low-frequency case and 30 GHz in the high-frequency case. Figure 7.21 illustrates the cost function for the two excitations.

The figure indicates that for long wavelengths the convergence will be initially fast and then slow down as the iterations approach the minima. This is preferable if little or nothing is known about the media such that the initial guess may be far away from the correct solution. In case the quality of the a priori data is better a short wavelength will give faster convergence. One could also think of using a combination of two excitations, a longer wavelength to get a rough estimate of the solution and then a short wavelength to improve the accuracy. The effect of varying the frequency is illustrated for the multilayer reconstruction example in Section 7.1.1. The problem was solved for six different excitations. In Figure 7.22 we show the cost function for the different cases. For the two excitations with the highest cutoff frequencies the iterations converge to local minima. For the lower frequencies the global minimum is found but the number of main iterations increases when the frequency becomes too low. The minimum number of main iterations is obtained for a cutoff frequency of 4 GHz. These results correspond well to the observations made above.
7.6.2 Sensitivity vs observation data

The quality of a solution to an inverse problem naturally depends on the amount of observation data. If it is insufficient we may have multiple solutions or no solutions at all. In our case the observation data is given in the time domain, typically for a wide range of frequencies. Since the response from different parts of the geometry are separated in time, the temporal data contain spatial information which is not present in the frequency domain. In many cases it is therefore sufficient to have a small number of observers. Nonetheless, it may be extremely hard to find the global minimum using a locally converging minimization algorithm.

The dependence on observation data was studied for the multilayer reconstruction case with two parameters, described in Section 7.6.1. In the cost function plots in Figure 7.21 two observation points were used. The corresponding plots where the number of observation points have been increased to 19, distributed around the multilayer structure, are found in Figure 7.23.

![Figure 7.23. The cost function for 19 observers. Compare with Figure 7.21.](image)

In the high frequency case we note significant reduction of the number of local minima and the global minimum becomes more distinct. The low frequency case
seems to benefit less from the increased number of observers and the cost function around the minimum is still rather flat.

### 7.7 Parallelization by domain decomposition and MPI (SPAR)

Due to the local property of the FDTD scheme, it is well suited for parallelization using domain decomposition where the computational domain is divided along the Cartesian axes, as illustrated to the left in Figure 7.24. To illustrate the parallelization strategy, consider the 2D-TM equations (3.19)-(3.21). The $E_z$-field is advanced in time using the surrounding $H_x$- and $H_y$-fields and the $H$-fields are correspondingly updated using the surrounding $E_z$-fields. In Figure 7.24 (to the right) the communication over a processor boundary in the $y$-direction is illustrated. Processor 2 sends the $H_y$-field located at the right of the boundary, to processor 1 where it is used in the update of the $E_z$-field to the left of the boundary. The $E_z$-field is then sent to Processor 2 where it is needed in the update of the $H_y$-field.

Both the direct and adjoint solvers were parallelized using this approach and the communication is handled by MPI (Message Passing Interface). The computation of the gradient requires data from the entire parameter region in space, see for example the expressions (5.18)-(5.20), and therefore requires parallelization. For simplicity, the same decomposition is used as in the direct and adjoint solvers. The spatial summation is thus carried out on different processors and the contributions are finally added to form the desired gradient, as shown for the permittivity below:

$$
\left( \frac{\partial j}{\partial \varepsilon} \right)_{\Omega_x} = \sum_{p=0}^{N_{\text{proc}}-1} \left( \frac{\partial j}{\partial \varepsilon} \right)_{\Omega_x, p} (7.3)
$$
where $\Omega_{\varepsilon,p}$ denotes the grid points belonging to processor $p$ that lies within the parameter region. When solving an inverse problem using the minimization approach, most of the time is spent solving the direct and adjoint problems. Each evaluation of the cost function requires a solution of the direct problem and each gradient evaluation requires an additional adjoint solution. The performance of the direct solver is therefore studied separately below. We will also show results for a full optimization where the gradient computation is included. All parallel simulations were carried out at the Center for Parallel Computers (PDC) at KTH on the IBM SP cluster, Strindberg.

### 7.7.1 Direct solver

The parallel efficiency of the direct solver was evaluated using up to 16 processors. Two different measures of the efficiency of the parallelization were used, scale-up, where the problem size for each processor remains constant and speed-up where the total problem size is constant. In the first case the problem size for each processor was $2500 \times 2500$ cells and in the second case the total problem size was $2500 \times 2500$. The results are illustrated to the left in Figure 7.25. Note that in these simulations no significant I/O is performed as opposed to the minimization results.

### 7.7.2 Gradient computation

Here, we consider a synthetic reconstruction case where we wish to determine the permittivity and conductivity of a thin dielectric layer lying on a perfectly con-
ducting plate. The size of the computational domain is 2500 by 2500 cells and it is divided in a uniform processor grid as illustrated for the 16 processor case in Figure 7.26. The corners of the rectangular material sample are located in the grid coordinates (300,2000) and (2150,2080). The speed-up for the different parts of the minimization are shown to the right in Figure 7.25. Since most of the I/O takes place in the processors which contain parts of the unknown material, the load balance will be quite poor. This is reflected in the results which vary quite a lot depending on the number of processors and distribution. Comparing with the results for the direct solver above, the performance is significantly degraded due to the additional I/O. The gradient computation shows very irregular speed-up. This is likely due to the fact that most of the time is spent performing I/O. The data is stored locally on each processor, which means that the I/O should be possible to perform in parallel, however, caching effects and poor load balance may still ruin the speed-up. These issues were not investigated further.

Figure 7.26. SPAR Computational domain for the inverse problem.
Appendix A

Far-field limit

The figure illustrates the experimental situation where $R$ is the radius of the antenna aperture, and $P$ is a point on the measured panel. The phase difference between two points at the aperture is given by:

$$k = \frac{R^2}{2L\lambda}$$

where $\lambda$ is the wavelength. In our case the shortest wavelength is $\lambda_{\text{min}}=1/60\text{ m}$, $L=1.25\text{ m}$ and $R=0.05\text{ m}$ resulting in

$$k_{\text{max}} = 0.06$$

which is well within the conventional limit for the farfield, $k=1/4$. 
Bibliography


