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FINITE ELEMENT TIME DOMAIN AND ITS APPLICATIONS
METODA KONEČNÝCH PRVKŮ V ČASOVÉ OBLASTI A JEJÍ APLIKACE

DOKTORSKÁ PRÁCE
DOCTORAL THESIS

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ABSTRACT

The thesis deals with modeling dispersive media by the finite-element time-domain method. Mathematical model including dispersive models is proposed and finite element approximation of this model is presented. Three of the most commonly used dispersive models are investigated, namely the Debye model, the Lorentz model and the Drude model. The techniques for implementing these dispersive models are described. Presented techniques are incorporated into a finite element method. Finally, a new method based on a digital filtering technique is presented. Various test examples are used to verify all the developed methods. Achieved results are discussed, and possible improvements of methods are suggested.

KEYWORDS

Finite element time domain, mathematical model, dispersive media, Debye model, Lorentz model, Drude model.

ABSTRAKT

Disertační práce se zabývá modelováním dispersních materiálů metodou konečných prvků v časové oblasti. V práci jsem navrhl matematický model zahrnující dispersní modely a aplikoval jsem na něj metodu konečných prvků. Pozornost jsem věnoval třem nejvíce používaným dispersním modelům. Jedná se o Debyeho model, Lorentzův model a Drudův model. Dále jsem se zabýval technikami implementace těchto dispersních modelů. Techniky jsem zabudoval do metody konečných prvků. Navíc jsem vyvinul novou metodu založenou na technice digitální filtrace. Funkčnost vyvinutých metod a technik jsem ověřil na řadě testovacích příkladů. Diskutoval jsem dosažené výsledky a navrhuji jejich možná vylepšení.

KLÍČOVÁ SLOVA

Metoda konečných prvků, matematický model, dispersní prostředí, Debyeho model, Lorentzův model, Drudeho model.

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DECLARATION

I declare that I have written my doctoral thesis "Finite element time domain and its applications" independently, under the guidance of the doctoral thesis supervisor and using the technical literature and other sources of information which are all quoted in the thesis and detailed in the list of literature at the end of the thesis.
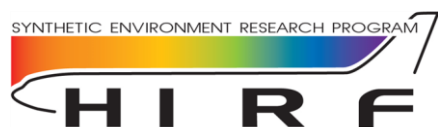
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Brno, the 7$^{\text{th}}$ of May, 2014 _____

Jan Cigánek

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Jan Cigánek

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LIST OF ABBREVIATIONS

EM	Electromagnetic
FETD	Finite Element Time Domain
FDTD	Finite Difference Time Domain
FEM	Finite Element Method
HIRF-SE	High Intensity Radiated Fields – Synthetic Environment
BUTFE	Brno University of Technology Finite Elements
ABC	Absorbing Boundary Condition
RC	Recursive Convolution
ADE	Auxiliary Differential Equation
PEC	Perfect Electric Conductor
FD	Finite Difference
FV	Finite Volume
IE	Integral Equation
CEM	Computational Electromagnetic
IBVP	Initial-Boundary Value Problem
DTI	Direct Time Integration

1   INTRODUCTION

Analysis of general electromagnetic (EM) problems such as wave propagation, scattering or waveguide simulation has been a topic in engineering for a long time. With growing speed of computers, some of these problems have been successfully solved by numerical methods [1]. But there are still many real problems which are necessary to be solved at this time [2].

One of the most useful numerical methods is the finite element time domain (FETD) method. Even though the FETD has lots of advantages, the method is not as developed as the most similar finite difference time domain (FDTD) method where lots of techniques has been proposed.

Finite element method (FEM) appropriately solves particular electromagnetic problems [3]. In order to obtain more precise results, it is necessary to use sophisticated physical and mathematical models. In another step, we have to develop appropriate techniques for solving these models. Improvement of older algorithms and development of new ones is a critical task for solving complex structures which mainly demand lots of memory storage, and computational processes require lots of running time. Although almost all measurements are defined in frequency domain, it is highly useful to solve these problems numerically in time domain [4].

Complex structures to be analyzed cover a large computational domain, and moreover, are often made from various materials (i.e., are strongly inhomogeneous). A simple model, which includes constant coefficients of properties of materials, is usually poorly suitable for obtaining sufficient results [1]. Employing loss, anisotropy or dispersion into solved numerical models distinctly improves required accuracy. On the other hand, corresponding mathematical models become more complicated, and approaches for solving them require additional improvement.

If a standard Finite-Element Time-Domain (FETD) code is assembled, it is relatively effortless to implement techniques for modeling the losses and anisotropy. On the other hand, the process for the implementation of a dispersive medium brings more troubles. In order to model various real materials, we have to use different dispersive models. An insufficient work has been published on modeling dispersive media by FETD methods [5].

1.1   Motivation for the Finite Element Approach

In electromagnetics, the finite element method has been used for over forty years. Although lots of techniques have been developed for this method, there are still issues in electromagnetics that need to be solved [2].

HIRF-SE

Exploitation of numerical methods for solving electromagnetic compatibility (EMC) problems is one of major unsolved tasks [6]. The European project *High Intensity Radiated Fields – Synthetic Environment* (HIRF-SE) was aimed to develop

a computer framework for numerical techniques, which would be suitable for aeronautical industry [7]. This project involved 44 participants including Brno University of Technology (BUT). Our responsibility included the development of a tool based on the finite element time domain method.

BUTFE solver

For purposes of the HIRF-SE project, we developed a tool called BUTFE (Brno University of Technology Finite Elements). The tool is a full-wave solver based on the FETD method. The BUTFE was mainly developed for the simulation of electrically large structures such as a whole aircraft [8]. Required test cases were properly solved with an appropriate accuracy during the HIRF-SE project [9]. Successful results proved that the solver is able to handle with specific electromagnetic structures.

Some test cases for the HIRF-SE verification involved dispersive materials. This was the strongest challenge because there is a lack of appropriate approaches for analyzing electromagnetic fields in dispersive media by finite element time domain methods [5].

The lack of approaches for creating dispersive models by FETD in a combination with model requirements formulated in the HIRF-SE project motivated us to develop suitable approaches for the FETD method.

2   STATE OF THE ART

In this chapter, we will present the state of the art in the field of the finite element time domain method for analyzing electromagnetic problems. We will concentrate mainly on approaches developed for analyzing electromagnetic fields in dispersive materials.

2.1   General description of FEM

Generally, the finite element method (FEM) is a numerical method for solving boundary-value problems. FEM is widely used in various engineering fields [10]. FEM is a part of so-called variational methods [11]. The origin of the method can be found in work of Courant published in 1942 [12]. There are many books describing FEM from a mathematical point of view [13]. Some commercial solvers for the design of electromagnetic structures are based on this method like ANSYS, COMSOL, HFSS and PAM-CEM.

2.2   Finite element method in electromagnetism

Mathematical models suitable for the analysis by FEM can be found in many books about electromagnetic fields [14]. The fundamental information about the exploitation of FEM in electromagnetism can be found in papers and books [15], [16]. The excellent book dealing with the implementation of FEM for electrical engineers is surely [17]. Lots of useful approaches for electromagnetic problems are described in [3] and [18]. There are many articles focused on specific aspects of FEM like basis functions [19], accuracy [20], stability [21], applications [22] etc. Advantages and disadvantages with respect to other numerical methods can be found in various papers and books, for instance [23].

2.3   Finite element time domain

A relatively low number of articles and books have been published on the utilization of finite element time domain (FETD) method for the analysis of electromagnetic problems compared to other numerical methods. A general overview including important references for the FETD method was published in [24].

The most cited contribution to FETD with the widely used numerical scheme called the Newmark method was published in [25]. A detailed description of time schemes for different equations is available in the book [26]. An approach for time discretization of the wave equation is described in [27].

Since the finite element method is suitable for so-called closed problems, we have to introduce special boundary conditions when solving open-space problems. A useful method for an accurate plane-wave excitation in scattering problems is called the total-and-scattered-field decomposition [28]. Gerrit Mur proposed a method called Absorbing

Boundary Condition (ABC) for the finite-difference time-domain (FDTD) method which has been successfully implemented into FETD [29] too. This approach can be employed for the total-and-scattered-field decomposition technique [30]. A proper description of ABC for FEDT can be found in the book [20].

An important article about the stability for the most commonly used time schemes can be found in the paper [31]. New and improved techniques for the finite element time domain method were described in the book [4].

Nowadays, FETD is often hybridized with other numerical methods. This hybridization has been developed for solving complex problems [32]. New methods based on finite element methods have been developed in [33].

2.4   Dispersive media

Methods of the time-domain analysis of electromagnetic fields in environments, which can contain dispersive materials, have been investigated for a long time [34]. Since the main difference between the FETD and the FDTD is the spatial discretization, the same approaches used for implementing frequency dispersive media in FDTD could be employed for FETD after certain modifications. Therefore, we can consider methods for FDTD as a potential approach for FETD.

Behavior of electromagnetic fields in dispersive media is described in many papers [35]. Propagation of the plane wave in dispersive media is studied for instance in [36]. There are exact solutions of certain problems related to electromagnetic fields in dispersive media [37]. Some of these methods have been developed for specific applications in the time domain based on reflection data [38].

Generally, we have to use full-wave methods such as FDTD or FETD [39] for the solution of wave propagation in dispersive media.

The major problem with the time-domain analysis of electromagnetic fields in dispersive materials can be specified as follows [4]. In the time domain, the constitutive relation between the electric field **E** and the displacement field **D** is given by [40]

$$\mathbf{D}(\mathbf{r},t) = \int_{-\infty}^{t} \varepsilon(\mathbf{r},t-\tau)\mathbf{E}(\mathbf{r},\tau)\,d\tau \qquad (2.1)$$

where **r** is the position vector and t denotes time.

The expression describes a convolution between the electric field intensity **E** and the permittivity ε. As mentioned above, this expression is difficult to be evaluated by analytical methods.

The discrete form of (2.1) consists of the following approach. The time variable is discretized as $t = n\Delta t$ where n is a natural number. The field quantity is denoted as $E(n\Delta t) = E^n$. A direct implementation of (2.1) requires the storage of the entire past time series of E^n. This approach is obviously not efficient to be used [41].

Different dispersive models such as the Debye model, the Lorentz model or the Drude model are used for modeling of electromagnetic fields in a real dispersive material [42]. Each model describes fields in a real medium with specific properties

[43]. The Debye model is the simplest one. Therefore, there are several possible methods for analyzing fields with the Drude model compared to other models [44].

There are basically three main approaches for all models to obtain update equations with frequency-dependent media: (1) the *Recursive Convolution* (RC), (2) the *Auxiliary Differential Equation* (ADE) and (3) the method based on the inverse-transformation [45]. Some approaches have no clear physical background. Some approaches for FDTD techniques were published in the overview [46]. A complex summary and an analysis of approaches for numerical methods have been presented in a relatively new paper [5]. Obviously, there are much more approaches for FDTD than for FETD.

Approaches for FETD and FDTD analysis of fields in dispersive media are mostly based on using the recursive convolution [47]. FETD methods based on the recursive convolution were described in [48]. An easily implemented scheme for FETD, but only for the Debye model, was described in [49]. The use of ADE to implement dispersive models is shown in [50]. A relatively good method based on the Inverse Fourier transform, which was first employed for FDTD [51], was described in [52]. The authors concentrated on applications which can be simplified into 1-D problems. This method elegantly avoids solving the time convolution by defining the dispersive polarization [53].

A proper way of implementing update schemes for dispersive models into a hybrid solver is proposed in [54]. Some papers describe approaches for dealing with dispersive models in special applications [55].

3 OBJECTIVES

The finite element method (FEM) is a powerful numerical method for solving boundary-value problems. Even though this approach is highly developed, there are still some weaknesses which can cause problems to achieve acceptable results in a reasonable computational time.

Each dispersive material can be described by a specific dispersive model but there is a lack of effective algorithms for solving an interaction of electromagnetic fields with dispersive materials by finite element time domain (FETD) methods.

The dissertation is aimed to develop new techniques and improve existing techniques which will be suitable for the analysis of electromagnetic fields in dispersive media by finite element time domain methods. Especially, we turn our attention to:

- Developing a FETD method for the analysis of electromagnetic fields in dispersive media using the Debye model;

- Developing a FETD method for the analysis of electromagnetic fields in dispersive media using the Lorentz model.

- Developing a FETD method for the analysis of electromagnetic fields in dispersive media using the Drude model.

- Solving initial-boundary value problems which include frequency dependent materials by FETD methods.

There are some approaches to employing the Debye model in the FETD method since it is the simplest model for the description of electromagnetic fields in dispersive materials. The Debye model is predominantly suitable for liquids.

Approaches to employing other dispersive models in the FETD method have not been investigated sufficiently yet. Namely, the Lorentz model, which is widely used for solids, and the commonly used Drude model wait for further investigation. All these mentioned models can describe fields in a wide spectrum of real materials. Various approaches for analyzing electromagnetic fields in dispersive media by using these models in FETD methods are necessary for modern electromagnetics.

4 FINITE ELEMENT TIME DOMAIN METHOD

This chapter concentrates on a general description of the finite element time domain (FETD) method. The main advantages and disadvantages of the FETD method are discussed. Here, we describe the most important aspects of the FETD method, which are necessary for understanding following chapters.

The largest part of this chapter is devoted to the derivation of a general algorithm for time schemes which will result in the improved final equation. A comparison of suitable time schemes for FETD methods is provided.

A general overview and a detailed description of the FETD method can be found in [16]. Advanced techniques for the FETD method are described in [4].

4.1 Time domain versus frequency domain

Maxwell's equations can be formulated in the time domain or the frequency domain. Numerical solvers for both the domains have their advantages and disadvantages. A robust implementation and a fast solution of a system of linear equations are the most important aspects usually [4]. Basically, we solve Maxwell's equations in one domain only because the solution for another domain can be obtained by using the Fourier transform. In reality, the choice of the domain depends on the nature of solved problems, computational time, experiences etc. [15].

Disadvantages of the time domain

- Many measurements are defined in the frequency domain.

- The frequency domain solver has to solve a system of linear equations for each frequency which is independent on the excitation. It is trivial to find a solution for a new excitation.

- In the frequency domain, the density of the mesh varies with different frequency. The recommendations for the mesh generation are related to the wavelength. Generation of an appropriate mesh for the time domain is more complicated.

- The mathematical model in the time domain is more complicated compared to the frequency domain.

- Modeling of an appropriate excitation is difficult in the time domain.

- Modeling dispersive media in the time domain is rather complicated.

- There are not many papers and books on time domain electromagnetics.

Advantages of the time domain

- Formulation of problems in the time domain can provide the solutions over a wide band of frequencies using the Fourier transform.

- All processes in the real world are a function of time.

- Time-domain algorithms are better suited for parallel processing.

- Better visual representations for understanding the field interactions can be implemented in the time domain.

- Time domain methods are capable to model nonlinear components, devices and media effectively [56].

4.2 General aspects of time domain modeling

The formulation and the numerical implementation of time domain models involve several basic steps in general. In this paragraph, we will briefly describe the main steps and potential complications. In later chapters, we will provide a detailed description of the implementation of the FETD method.

Model development

The major problem always consists in creating a proper mathematical model which sufficiently describes physical phenomena. The creation of a model is especially difficult for complex problems such as a structure with various materials or even a whole aircraft [2]. In order to reduce the computational time efficiently, we have to find an appropriate physical approximation of a real problem and an appropriate mathematical model of this physical approximation [13]. In many cases, the metal is modeled as a *Perfect Electric Conductor* (PEC), vacuum coefficients are used instead of air coefficients etc. These approximations mostly depend on used methods, a computational domain and required accuracy of the results.

Numerical method

Another major step consists in applying the finite element method on the approximation of the mathematical model. FEM is suitable for a specific class of electromagnetic problems. Often, FEM has to be necessarily extended or combined FEM with other numerical methods [4]. For example:

- Absorbing boundary conditions have to be introduced so that open electromagnetic problems can be modeled;

- Models of dispersive materials have to be introduced so that fields in frequency-dependent structures can be analyzed [54].

Approach for solving a problem

We consider the time-dependent Maxwell curl equations or their equivalents. These equations are sampled in space and time utilizing an appropriate geometrical space grid and suitable basis functions and testing functions [20]. In order to save computational resources, it is always useful to use the simplest approximation which ensures sufficient results.

Excitation requirements

Results of the analysis of time domain problems are highly dependent on a way of the excitation. In many cases, an incident plane wave is used. There are more methods of modeling the excitation [57]. Boundary conditions belong to the most useful ones [28].

4.3   Finite elements

The finite element method (FEM) is a powerful and versatile tool for the analysis of various electromagnetic problems. Together with Finite Differences (FD), Finite Volumes (FV), Integral Equations (IE) and various hybrid techniques, FEM is a part of computational electromagnetic (CEM) techniques [18]. These techniques have been successfully implemented in many commercial software packages for analyzing real-life electromagnetic problems [2]. CEM techniques have improved over the years. Nowadays, CEM are able to analyze various complex problems. But there are still many problems that have to be solved.

Every method from CEM has specific advantages and areas of applicability. Comparison of different CEM methods can be found in many papers [58].

The finite element method is a general numerical method for solving boundary-value problems, which are described by partial differential equations and boundary conditions [59]. In the case of time domain, boundary conditions have to be completed by initial conditions also.

The standard application of FEM for the analysis of EM problems is described in detail in many texts [1]. FEM provides an approximation of an unknown field quantity over the whole analyzed structure.

Generally, a boundary-value problem can be defined in the domain denoted Ω:

$$\Im\phi = f \tag{4.1}$$

where $\Im$ is a differential operator, f is the excitation or the forcing function and ϕ denotes the unknown quantity. Solution of this problem is defined in the Hilbert space [13]. Equation (4.1) together with specific boundary conditions can build a problem to be solved by FEM.

FEM comprises many parts of numerical mathematics such as meshing, approximation, solving systems of ordinary differential equations, solving systems of linear equations etc. [20].

The crucial part of FEM includes assembling finite-element matrices. Various methods have been developed for this purpose. The Ritz method, known as a variational finite-element method and the Galerkin method have been used most widely [1].

The Ritz method obtains solutions by minimizing a functional. Definition of a functional is the most difficult part of this approach.

The Galerkin method is a special case of the weighted residual method where the residuum has to be orthogonal to the basis functions. Basis functions are used for the approximation of an unknown quantity [11]. If the differential operator in equation (4.1)

is self-adjoint, positive definite etc., then the Galerkin method results in the same finite-element matrices as the Ritz approach [13].

We use the Galerkin approach in later chapters.

Mathematical model

As mentioned above, the finite element method is a numerical method for obtaining approximate solutions of boundary value problems. In the electromagnetism, FEM solves boundary value problems including Maxwell's equations or wave equations and boundary conditions.

In the time domain, an initial-boundary value problem (IBVP) in the volume Ω includes the wave equation, and can be defined as follows:

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) + \sigma \frac{\partial \mathbf{E}}{\partial t} + \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \ \text{ in } \Omega \tag{4.2}$$

Here $\mathbf{E}$ is the vector of electric field intensity, σ is the electric conductivity, ε and μ are permittivity and permeability. The typical boundary conditions are:

$$\mathbf{n} \times \mathbf{E} = 0 \ \text{ on } \partial\Omega_e \tag{4.3a}$$

$$\mathbf{n} \times \left(\nabla \times \mathbf{E} \right) = 0 \ \text{ on } \partial\Omega_m \tag{4.3b}$$

where $\partial\Omega_e$ and $\partial\Omega_m$ denotes perfect electric and perfect magnetic surfaces respectively, $\mathbf{n}$ is the unit normal vector of the surface.

The condition (4.3a) implies that the tangential component of the electric field equals zero over the surface of a perfectly conductive wall, which is often called an electric wall. The second condition (4.3b) is the boundary coincident with its symmetrical lines. The equation implies the same for the tangential component of a magnetic field. The surface is called a magnetic wall [4].

The following initial conditions are given to obtain a unique solution. Usually, initial conditions are assumed to be zero:

$$\mathbf{E}\left(\mathbf{r},0\right) = 0 \quad \frac{\partial \mathbf{E}\left(\mathbf{r},0\right)}{\partial t} = 0 \tag{4.3b}$$

The electromagnetic problem defined by (4.2) to (4.4) can be solved analytically for few cases only. For most problems, we can find an approximate solution by numerical methods such as finite elements.

Many electromagnetic problems are defined in an open area. Since the FEM a discretization of a whole computational domain, we have to truncate the unbounded space into a finite space. Figure 4.1 shows this concept.
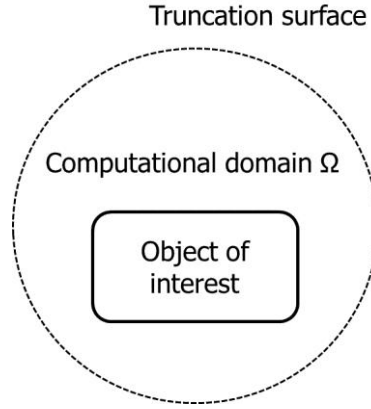
Fig. 4.1: Initial boundary-value problem:
computational domain truncated by artificial surface.

The ideal boundary condition causes that the radiated field passes the boundary without any distortion or reflection. The mathematical expression for the first-order absorbing boundary condition is

$$\mathbf{n} \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{E} \right) + Y_0 \mathbf{n} \times \left(\mathbf{n} \times \frac{1}{\partial t} \mathbf{E} \right) \approx 0 \tag{4.5}$$

Here, $\mathbf{E}$ is electric field intensity, $\mathbf{n}$ is the normal to the boundary, and Y_0 is admittance of free space.

The absorbing boundary condition (4.5) has to be placed in a sufficient distance away from the analyzed object for achieving a reasonable accuracy [4].

The expressions (4.2) to (4.5) are an example of possible mathematical models. Generally, (4.2) to (4.5) is the most frequently used form of the wave equation with possible boundary conditions. This mathematical model will be used to demonstrate our setup goals sufficiently.

An appropriate model needs to be developed for a particular electromagnetic problem [13].

Space discretization of finite element method

We start the space discretization with the formulation of a weak form of the wave equation (4.2) [1]. As mentioned above, we will choose the Galerkin method for computing the approximation of electromagnetic fields. We apply the divergence theorem and the vector identity on the equation (4.2). Then, boundary conditions (4.3) and a proper choice of N testing functions $\mathbf{V}_i(\mathbf{r})$ yields:

$$\iiint_{\Omega} \left\{ [\nabla \times \mathbf{V}_i] \cdot \frac{1}{\mu} [\nabla \times \mathbf{E}(\mathbf{r},t)] + \sigma \mathbf{V}_i \cdot \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \mathbf{V}_i \cdot \varepsilon \frac{\partial^2 \mathbf{E}(\mathbf{r},t)}{\partial t^2} \right\} d\Omega = 0 \tag{4.6}$$

where $\mathbf{V}_i$ is the vector weighting function, $\mathbf{E}$ is the electric field intensity, μ is the permeability and ε is the permittivity.

The electric field can be expanded in any time t and any position $\mathbf{r}$ as follows:

$$\mathbf{E}(\mathbf{r},t) = \sum_{i=1}^{N} e^i(t) \mathbf{W}_i(\mathbf{r}) \tag{4.7}$$

Here, $\mathbf{W}_i(\mathbf{r})$ are vector basis functions, and $e^i(t)$ denote time-dependent approximation coefficients. There are lots of books and papers discussing a proper choice of basis functions [60].

Defining $\mathbf{V}_i(\mathbf{r}) = \mathbf{W}_i(\mathbf{r})$ and integrating (4.6) over the whole computational domain Ω results in a system of ordinary differential equations [61]:

$$\mathbf{T}\frac{d^2 e(t)}{dt^2} + \mathbf{B}\frac{de(t)}{dt} + \mathbf{S}e(t) + \mathbf{f} = 0 \tag{4.8}$$

Here, $\mathbf{f}$ stands for the excitation vector, and the individual entries of the finite element matrices $\mathbf{S}$, $\mathbf{B}$ and $\mathbf{T}$ are given by:

$$S_{ij} = \int_{\Omega} \left(\nabla \times \mathbf{W}_i(\mathbf{r}) \right) \cdot \frac{1}{\mu} \left(\nabla \times \mathbf{W}_j(\mathbf{r}) \right) d\Omega \tag{4.9}$$

$$T_{ij} = \int_{\Omega} \mathbf{W}_i(\mathbf{r}) \cdot \varepsilon \mathbf{W}_j(\mathbf{r}) d\Omega \tag{4.10}$$

$$T_{ij} = \sigma \int_{\Omega} \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{W}_j(\mathbf{r}) d\Omega \tag{4.11}$$

Lots of books have been published about space discretization. One of the best sources with various examples is in [1]. In the rest of the work we use symbol W for weighting (testing) functions and basis functions.

Time domain discretization

The equation (4.8) is usually discretized by time schemes such as a direct integration or a finite difference method [62]. There are just a few simple recommendations which scheme is suitable for which kind of a problem [26]. Equation (4.8) is a second-order ordinary differential equation, which can be solved by various approaches. The most popular technique is the Newmark method. The Newmark method includes two coefficients which define a specific time scheme. Generally, the Newmark method is unconditionally stable and exhibits the best truncation error [63].

For each time scheme, the time variable t is discretized as $t = n\Delta t$, where Δt denotes the time step and n is a natural number. The unknown coefficient $e(t)$ in the equation (4.8) is approximated by the following expression:

$$e(t) = \sum_{i=1}^{M} e^i(t) N_i(t) \tag{4.12}$$

Here, M is the number of time steps and $N_i(t)$ denotes shape functions varied in time. The result of the Newmark method is the final equation which has to be solved for each time step [64]:

$$\left\{\frac{1}{\Delta t^2}\mathbf{T} + \frac{\gamma}{\Delta t}\mathbf{B} + \beta\mathbf{S}\right\}e^{n+1} = \left\{\frac{2}{\Delta t^2}\mathbf{T} - \frac{1-2\gamma}{\Delta t}\mathbf{B} + \left(\frac{1}{2} + \gamma - 2\beta\right)\mathbf{S}\right\}e^{n}$$

$$-\left\{\frac{1}{\Delta t^2}\mathbf{T} - \frac{1-\gamma}{\Delta t}\mathbf{B} + \left(\frac{1}{2} - \gamma + \beta\right)\mathbf{S}\right\}e^{n-1} \qquad (4.13)$$

$$-\left[\beta f^{n+1} + \left(\frac{1}{2} + \gamma - 2\beta\right)f^{n} + \left(\frac{1}{2} - \gamma + \beta\right)f^{n-1}\right]$$

Here, γ and β are coefficients to be properly chosen, $\mathbf{T}$, $\mathbf{B}$ and $\mathbf{S}$ are finite-element matrices, Δt is the time step, e^n is the temporal sample of field intensity and f^n is the temporal sample of an excitation quantity.

The stability and the accuracy belong to very important issues of all numerical techniques. The scheme (4.13) is unconditionally stable for $\gamma \geq 1/2$ and $\beta \geq 1/4$ [65]. If we set $\gamma = 1/2$ and $\beta = 1/4$, the Newmark method is reduced to the trapezoidal rule:

$$\left\{\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}\mathbf{B} + \frac{1}{4}\mathbf{S}\right\}e^{n+1} = \left\{\frac{2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\mathbf{S}\right\}e^{n}$$

$$-\left\{\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}\mathbf{B} + \frac{1}{4}\mathbf{S}\right\}e^{n-1} - \left[\frac{1}{4}f^{n+1} + \frac{1}{2}f^{n} + \frac{1}{4}f^{n-1}\right] \qquad (4.14)$$

The paper [31] gives an overview of the stability of time schemes for FETD methods. The recommendation for the optimal length of the time step which ensures a sufficient accuracy can be found in [66]. This time step is defined as

$$\Delta t = \frac{\Delta x}{c\sqrt{m}} \qquad (4.15)$$

where Δx is the minimal length of an edge in the spatial discretization, c is the speed of light and m is the dimension of the problem.

Another useful algorithm is the difference scheme due to its simplicity to derive and implement [20]. For some advanced approaches for solving complicated electromagnetic structures, we have to use a combination of presented algorithms [67].

4.4   Time domain approximation – improved equation

Deriving the Newmark scheme from the beginning is a complicated task, and it is hard to see what is behind this approximation [25]. In many papers, authors use this scheme without any deep explanation of behavior.

All time stepping algorithms including the Newmark method and the finite difference method can be derived with less effort by applying a weighted residual algorithm [27]. This approach gives us a deeper understanding of the time stepping processes, and can be effectively used for solving time dependent problems.

A detailed look at a general two-step algorithm

The derivation starts from the differential equation (4.8). The time variable t is discretized in the same manner as mentioned above. The unknown coefficient $e(t)$ is approximated in every $2\Delta t$ interval by the expression

$$e(t) = \sum_{i=-1}^{1} e^i N_i(t) \tag{4.1ž}$$

where $N_i(t)$ denotes a second-order polynomial expansion called the shape function (4.17). This expansion can be derived by using the Lagrange polynomial

$$N_{-1} = \frac{t^2}{2\Delta t^2} - \frac{t\Delta t}{2\Delta t^2} \qquad N_0 = -\frac{t^2 - \Delta t^2}{\Delta t^2} \qquad N_1 = \frac{t^2}{2\Delta t^2} + \frac{t\Delta t}{2\Delta t^2} \tag{4.17}$$

The temporal shape functions (4.17) are depicted in Fig 4.2.
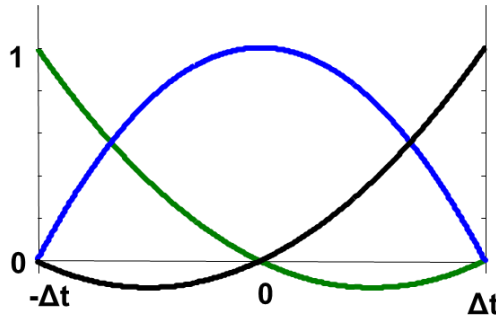
Fig. 4.2: Temporal shape functions.

We substitute the coefficient $e(t)$ given by (4.16) into the equation (4.8). Multiplying $e(t)$ by a weighting function W and integrating over the time interval $2\Delta t$ gives us

$$\int_{-\Delta t}^{\Delta t} W \left\{ \mathbf{T} \sum \frac{\partial^2 N_i}{\partial t^2} e^i + \mathbf{B} \sum \frac{\partial N_i}{\partial t} e^i + \mathbf{S} \sum N_i e^i + \sum N_i \mathbf{f} \right\} dt = 0 \tag{4.18}$$

The equation (4.18) shows us that we need to compute the first derivative of shape functions

$$\frac{\partial N_{-1}}{\partial t} = \frac{t}{\Delta t^2} - \frac{\Delta t}{2\Delta t^2} \qquad \frac{\partial N_0}{\partial t} = -\frac{2t}{\Delta t^2} \qquad \frac{\partial N_1}{\partial t} = \frac{t}{\Delta t^2} + \frac{\Delta t}{2\Delta t^2} \tag{4.19}$$

and the second derivative of the shape functions

$$\frac{\partial^2 N_{-1}}{\partial t^2} = \frac{1}{\Delta t^2} \qquad \frac{\partial^2 N_0}{\partial t^2} = -\frac{2}{\Delta t^2} \qquad \frac{\partial^2 N_1}{\partial t^2} = \frac{1}{\Delta t^2} \tag{4.20}$$

This treatment gives us an equation in the form

$$\int_{-\Delta t}^{\Delta t} W \left\{ \mathbf{T} \left[e^{-1} - 2e^0 + e^1 \right] + \mathbf{B} \left[\left(t - \frac{\Delta t}{2} \right) e^{-1} - 2te^0 + \left(t + \frac{\Delta t}{2} \right) e^1 \right] \right.$$
$$\left. + \mathbf{S} \left[\left(\frac{t^2}{2} - \frac{t\Delta t}{2} \right) e^{-1} - \left(t^2 - \Delta t^2 \right) e^0 + \left(\frac{t^2}{2} + \frac{t\Delta t}{2} \right) e^1 \right] + \Delta t^2 \mathbf{f} \right\} dt = 0 \tag{4.21}$$

Introducing coefficients γ and β as weighted parameters given by

$$\gamma = \frac{\int\limits_{-\Delta t}^{\Delta t} W \cdot \left(\frac{t}{\Delta t} + \frac{1}{2} \right) dt}{\int\limits_{-\Delta t}^{\Delta t} W dt} \tag{4.22}$$

$$\beta = \frac{\frac{1}{2} \int\limits_{-\Delta t}^{\Delta t} W \cdot \left(\frac{t^2}{\Delta t^2} + \frac{t}{\Delta t} \right) dt}{\int\limits_{-\Delta t}^{\Delta t} W dt} \tag{4.23}$$

we can rewrite the equation (4.21) to the same equation as (4.13).

In this approach, the approximation behind coefficients γ and β is more obvious. The most useful weighting functions W are shown in Fig 4.3.
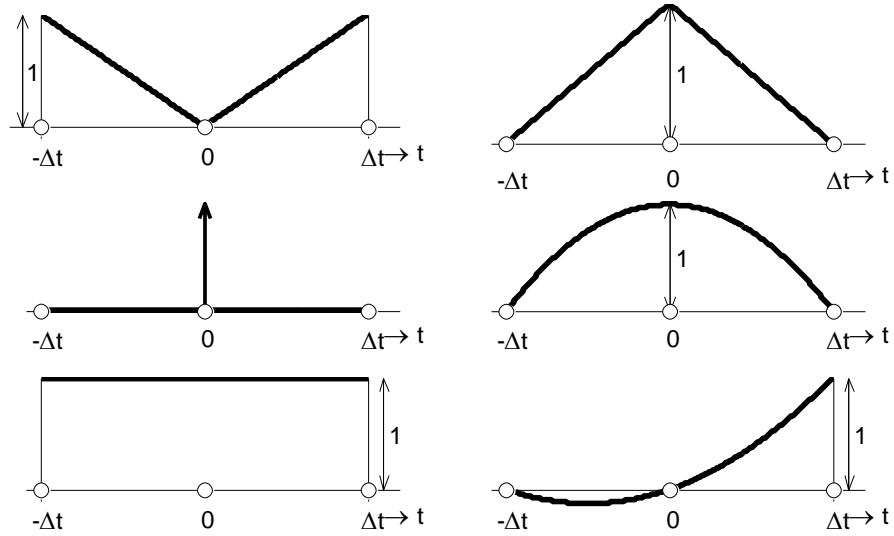
Fig. 4.3: The most useful weighting functions. **Left** (from the top): average acceleration, central difference (Dirac impulse), linear acceleration. **Right** (from the top): Fox-Goodwin method, ($\beta = 1/2$, $\gamma = 1/10$), Galerkin method.

In order to achieve the same equation as (4.14), we need to use a weighting function defined on the interval $\langle -\Delta t, \Delta t \rangle$ as

$$W = \left| \frac{t}{\Delta t} \right| \tag{4.24}$$

Then, the coefficients (4.22) and (4.23) will be $\gamma = 1/2$ and $\beta = 1/4$. In Figure 4.3, the expression (4.24) corresponds with the function on the top left.

The same approach can be employed for general multi-step algorithms. The difference is in a choice of shape and weighting functions and the integration over a longer time discretized domain. This brings higher requirements on computational resources since the higher number of time coefficients is necessary to be stored. Generally, this two-step algorithm is sufficient enough for solving majority of electromagnetic problems.

4.5 Comparison of temporal schemes

There are many temporal schemes possibly used in FETD methods due to the generality of the algorithm. We published a comparison of the most appropriate schemes for FETD methods with the analytical method in [68].

Table 4.1: Results for temporal schemes.

	γ	β	*Method*	*Comment*
1	-1/2	0	Forward difference	Unstable
2	1/2	0	Central difference	Oscillation, stable for small Δt
3	3/2	1	Backward difference	Stable, worse accuracy
4	1/2	1/6	Linear acceleration	Stable, for optimal Δt excellent result
5	1/2	1/10		Worse accuracy, stable for small Δt
6	3/2	4/5	Galerkin	Unconditionally stable, worse accuracy
7	1/2	1/12	Fox-Goodwin	Worse accuracy, stable for small Δt
8	1/2	1/4	Average acceleration	Unconditionally stable, for optimal Δt excellent result

Our testing model involves the propagation of the electromagnetic wave with boundary conditions set to a perfect electric conductor to excite reflected waves. The comparison was aimed to find an appropriate time scheme for the FETD method. The result is used for the analysis of other problems including dispersive materials.

As an excitation pulse, we have chosen the power exponential pulse [69]

$$V_0\left(t\right)=V_{\max}\left(\frac{t}{t_r}\right)^{v}\exp\left[-v\left(\frac{t}{t_r}-1\right)\right]H\left(t\right) \tag{4.25}$$

Here, $V_{\max}$ is pulse amplitude, v is the rising exponent of the pulse, t_r is the pulse rise time and $H(t)$ is the Heaviside unit step. This pulse has two important advantages : the pulse is causal and has a finite number of derivations. More detailed information about this comparison can be found in [68].
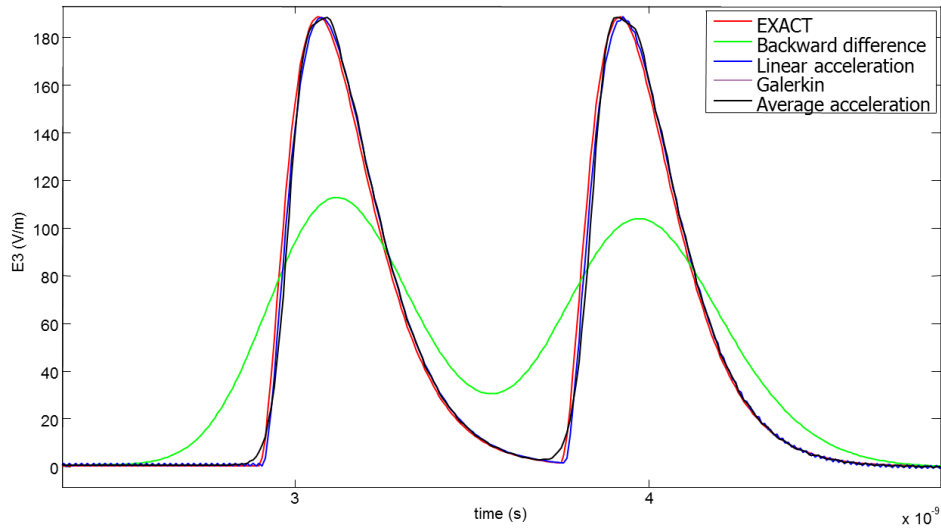
Fig. 4.4: Comparison of temporal schemes. Result after the first reflection:
an non-sharp excitation pulse
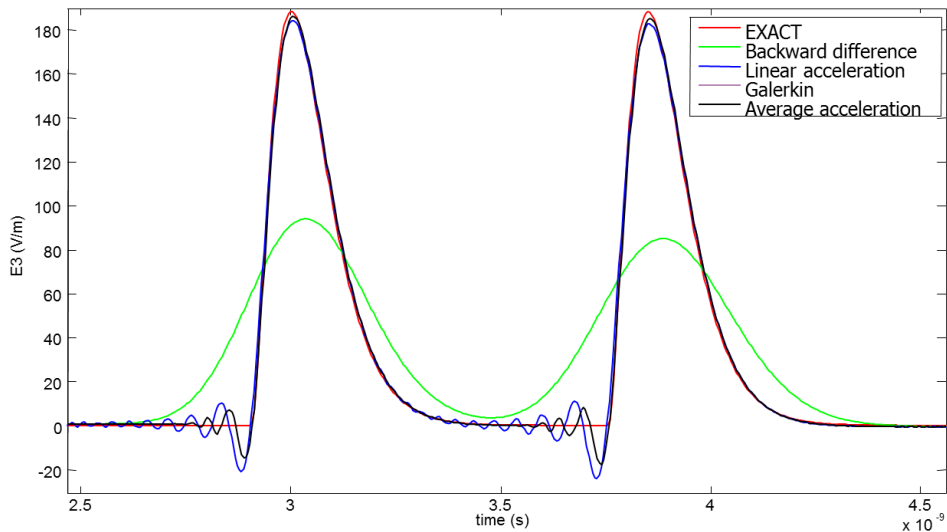
Fig. 4.5: Comparison of temporal schemes. Result after the first reflection:
a sharper excitation pulse was considered.

In Table 4.1, we can find results of the most suitable time schemes for the finite element time domain method with comments about their applicability. The scheme called *Average acceleration* provides the best results.

In Figure 4.4, we can see the comparison of some schemes from Table 4.1. Schemes are compared with the exact solution. The same kind of schemes is compared in Fig. 4.5 with a sharper excitation pulse. In this figure, each scheme has a problem to copy results of the exact solution. Again, the Average acceleration provides the best result even though oscillations are visible. This comparison shows how FETD solutions depend on an excitation pulse.

4.6 Modelling of materials

We can face some difficulties in the finite element approach if we want to analyze fields in environments comprising specific materials such as dispersive ones, anisotropic ones or others [4]. Analysis of electromagnetic fields in complex media is reviewed in [5].

A standard finite element approach using node-based elements could produce nonphysical solutions in case of different materials inside the analyzed structure. Edge-based basis functions were developed to overcome these difficulties [70]. The edge approximation exploits vectors and is able to solve the vector wave equation. Many papers have been published about this approach and the improvement of this type of approximation is still in progress [72].

It is also possible to analyze structures with anisotropic materials by the edge elements [9]. An anisotropic material is described by a tensor. The approach of the FETD method is almost the same as described in the previous chapter.

Let us suppose that we analyze fields in an environment where permeability and permittivity are considered to be anisotropic. In this case, permittivity and permeability are described by tensors $\boldsymbol{\mu}$ and $\boldsymbol{\varepsilon}$:

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{bmatrix}^{-1} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \tag{4.26}$$

Now, we need to change matrices (4.9) and (4.10):

$$S_{ij} = \int_{\Omega} \left(\nabla \times \mathbf{W}_i(\mathbf{r}) \right) \cdot \boldsymbol{\mu} \left(\nabla \times \mathbf{W}_j(\mathbf{r}) \right) d\Omega \tag{4.27}$$

$$T_{ij} = \int_{\Omega} \mathbf{W}_i(\mathbf{r}) \cdot \boldsymbol{\varepsilon} \mathbf{W}_j(\mathbf{r}) d\Omega \tag{4.28}$$

The most serious complication is caused by a dispersive material. We are concentrating on this problem in the rest of the thesis.

4.7 Conclusion

Finite element method is a powerful tool for solving electromagnetic problems. The main advantages of formulating and analyzing electromagnetic problems in the time domain are a deeper understanding of real physical processes, even though there is an additional variable which has to be dealt with.

The main problem consists in creating a mathematical model which sufficiently describes physical phenomena. An appropriate application of the finite element method on the analysis of this problem is another important step.

In this chapter, we prepared the FETD approach for a later analysis of fields in dispersive media. Space discretization is described in many publications and does not need any special treatment due to dispersive model effects time discretization. An improved final equation allows a detailed look at the algorithm for time schemes.

We compared the most suitable approaches for FETD. We described ways of dealing with problems comprising various types of materials.

All these steps can be understood as a necessary preparation for defining the complex model comprising dispersive media to be solved by the FETD method in future chapters.

5 TECHNIQUES FOR ANALYZING FIELDS IN DISPERSIVE MEDIA

In this chapter, we will briefly introduce the theory behind the dispersive medium and will discuss the most frequently used mathematical models of dispersive media. We will discuss the methods for analyzing electromagnetic fields interacting with dispersive materials. Later, we will develop methods for analyzing electromagnetic problems including these dispersive models to be suitable for the FETD method.

5.1 Dispersive material

Material parameters can be assumed to be constant to obtain acceptably accurate results for some problems. The process of employing constant parameters is an approximation of real materials, because all materials exhibit dispersion to some extent in general [71].

To achieve more precise models of the interaction between electromagnetic fields and materials, we have to to define material as dispersive ones.

If the speed of a wave is constant and depends on the physical properties of the medium only, then the parameters of the medium do not depend on frequency. This medium is called a non-dispersive medium and waves traveling through this medium have a constant shape [73]. This is an idealized situation, of course.

In reality, the wave speed depends on the frequency of the wave. In this case, higher frequencies travel faster than lower frequencies. As a result, the wave pulse spreads out and changes its shape [74]. A deeper theory of dispersive media can be found in books about electromagnetic fields [75].

5.2 Dispersive model in time domain

The electromagnetic field is described by Maxwell's equations. The differential form of these equations is

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t}, \tag{5.1}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial \mathbf{D}(\mathbf{r},t)}{\partial t}, \tag{5.2}$$

where, $\mathbf{E}$ is the electric field, $\mathbf{D}$ is the displacement field, $\mathbf{H}$ is the magnetic field and $\mathbf{B}$ is the magnetic induction.

The constitutive relations are completely independent on the Maxwell equations. The traditional description of constitutive relations is

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} \tag{5.3}$$

$$\mathbf{B} = \mu_0 \mu_r \mathbf{H} \tag{5.4}$$

where ε_r and μ_r are the relative permittivity and relative permeability, respectively. The relations (5.3) and (5.4) do not include any frequency dependence and are suitable for materials with constant parameters.

Several different models for the constitutive relations can be found in the literature [76]. The useful constitutive relation in the time domain is given by

$$\mathbf{D}(\mathbf{r},t) = \varepsilon_0 \left\{ \varepsilon_1(r)\mathbf{E}(\mathbf{r},t) + \left(\chi(\mathbf{r},.) * \mathbf{E}(\mathbf{r},.) \right)(t) \right\} \tag{5.5}$$

$$\mathbf{B} = \mu_0 \mu_r \mathbf{H}, \tag{5.6}$$

Here χ is the susceptibility kernel of the medium. The time convolution integral is defined as

$$\left(\chi(\mathbf{r},.) * \mathbf{E}(\mathbf{r},.) \right)(t) = \int_{-\infty}^{t} \chi(\mathbf{r},t-t')\mathbf{E}(\mathbf{r},t')dt' \tag{5.7}$$

The finite element method mostly solves problems described by the wave equation instead of Maxwell equations. We can derive the wave equation without any complications from (5.1), (5.2) and (5.5), (5.6):

$$\nabla \times (\nabla \times \mathbf{E}) + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} (\varepsilon_r \mathbf{E} + \chi * \mathbf{E}) = 0, \tag{5.8}$$

In a linear classical electrodynamics, most materials can be characterized as the Debye type material, the Lorentz type material or the Drude type material [48].

5.3   Dispersive models

Solving the equation (5.8) brings the problem with the time convolution. There are methods that use (5.8) directly. Defining the same problem in the frequency domain allows us to solve the time convolution in other ways. During the process, we use the Fourier transform to invert the problem into the time domain. This seems to be a useful process for avoiding a direct solving of the time convolution. For these reasons, we introduce each dispersive model in the frequency domain and the time domain suitable for our purposes. A useful source of dispersive models is [66]. A deep theoretical description of dispersive models can be found in [77].

5.3.1   Debye model

The Debye model also known as the *Relaxation model* is an appropriate model for polar liquids such as water. The susceptibility kernel in the time domain is defined as [43]:

$$\chi(t) = \left(\frac{\varepsilon_s - \varepsilon_\infty}{\tau} \right) e^{-t/\tau} U(t) \tag{5.9}$$

where ε_s is the static permittivity, ε_∞ is the permittivity for $\omega \to \infty$, τ is the relaxation time and $U(t)$ is the unit step.

The susceptibility kernel corresponding to (5.9) in frequency domain is

$$\chi(\omega) = \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau} \tag{5.10}$$

where ω is an angular frequency and j is the imaginary unit.

5.3.2 Lorentz model

Lorentz model or the *Resonance model* is used as a model for electromagnetic behavior in solids. The susceptibility kernel in the time domain is defined as [76]:

$$\chi(t) = \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\sqrt{\omega_0^2 - \delta^2}} e^{-\delta t} \sin\left(\sqrt{\omega_0^2 - \delta^2}\, t\right) U(t) \tag{5.11}$$

Here, ε_s is the static permittivity, ε_∞ is the permittivity for $\omega \to \infty$, ω_0 is the resonant frequency, δ is the damping constant and $U(t)$ is the unit step.

The susceptibility kernel corresponding to (5.11) in frequency domain is

$$\chi(t) = \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 + j\omega\delta - \omega^2} \tag{5.12}$$

where ω is an angular frequency and j is the imaginary unit. Note that the relation between the damping constant and the relaxation time is $\delta = 1/\tau$.

5.3.3 Drude model

The susceptibility kernel for the Drude model in the time domain is defined as [78]:

$$\chi(t) = \frac{\omega_p^2}{\delta}\left(1 - e^{-\delta t}\right) U(t) \tag{5.13}$$

Here, ω_p is the pole angular frequency, δ is the damping constant and $U(t)$ is the unit step.

The susceptibility kernel corresponding to (5.13) in frequency domain is

$$\chi(\omega) = \frac{\omega_p^2}{j\omega\delta - \omega^2} \tag{5.14}$$

where ω is an angular frequency and j is the imaginary unit. This model is a special case of the Lorentz model [79]. Note that the relation between the damping constant and the relaxation time is $\delta = 1/\tau$.

5.4   Methods for analyzing fields in dispersive media

Lots of methods have been developed and successfully applied for the finite difference time domain analysis of electromagnetic fields in dispersive media [80]. Not many of them have been used for finite element time domain methods. In many

approaches, the authors usually directly solve the time convolution which brings additional requirements for the memory storage. Algorithms are often difficult to apply and some of them do not have a clear physical background. Another reason for developing new algorithms is a complicated mathematical background of the existing ones and the an attempt of a relatively easier implementation [79].

As mentioned in the first chapter, the presented development was motivated by the HIRF-SE project and was aimed to improve or develop methods for the analysis of fields in environments comprising various dispersive models. We developed a new technique called the *Digital filter based method* which can be also employed by other numerical methods such as FDTD [81]. Further development has been concentrating on improving and applying existing techniques for the finite element time domain method. We worked on two other methods:

- The first method is based on the *Recursive Convolution*. This method was implemented for analyzing fields in environments with the Debye model of dispersive media only.

- The second method is based on the *Direct Time Integration* technique [51].

5.5   Recursive convolution method

This method is based on [49]. We use this method for the Debye model only. For other models, it is difficult to deal with the susceptibility kernel.

In this method, the displacement field is substituted into the wave equation before the implementation of the FETD method. The wave equation contains time convolution in the second time derivative. This method deals with problems including the formulation (5.8). In the system of ordinary differential equations, we have to solve the time convolution. We can use more ways to discretize this convolution in this system. Our approach uses the technique where the time convolution is discretized by the following time scheme which is obtained from a two-step algorithm:

$$\frac{\partial^2 (\chi * e)}{\partial t^2} = \frac{C^{n+1} - 2C^n + C^{n-1}}{\Delta t^2} \tag{5.15}$$

where C denotes a discrete form of the time convolution

$$C^k = (e * \chi)^k \tag{5.16}$$

for $k = n + 1, n, n - 1$.

The term C^{n+1} is then evaluated recursively

$$C^{n+1} = \alpha C^n + \int_{n\Delta t}^{(n+1)\Delta t} \chi((n+1)\Delta t - \tau) e(\tau) d\tau \tag{5.17}$$

Here, α can represent the past development of the time convolution, which has a usual form of an exponential function. The coefficient α can be relatively easily obtained for the Debye model. For other models, the evaluation of the coefficient α causes additional problems.

The temporarily variable coefficient $e(t)$ for electric field is discretized by an approach such as

$$e(t) = e^n + \frac{e^{n+1} - e^n}{\Delta t}(t - n\Delta t)$$

(5.18)

Then the integral in (5.17) is solved. The result depends on the kernel χ.

In other methods based on the *Recursive Convolution*, the second derivative of the time convolution is separated and the kernel or the coefficient for electric field is expressed without the second time derivative [48].

5.6   Direct Time Integration (DTI)

The DTI technique has been successfully employed by the FDTD method. DTI can be used for all the investigated dispersive models without additional complications. The method is based on the transformation of the electric field and the displacement field into the time domain by the Inverse Fourier transform. This equation is discretized by a numerical technique. As a result, a coefficient for the displacement field d in the time step $n+1$ is obtained. The wave equation is discretized for both the field variables e and d. The term d in the discrete form of the wave equation for the time step $n+1$ is then substituted from the result of d in the time step $n+1$ from the previously mentioned equation.

There are various models of dispersive media suitable for this method. We firstly will describe the general approach for the DTI technique [51]. This method is based on [53] where authors concentrate on 1-D problems only.

For dispersive media, we can define the macroscopic electric polarization P. The relation between D, E and P is

$$D = \varepsilon_0 \varepsilon_r E + P$$

(5.19)

To include frequency dependence into the TDFE model, we will use the relation between D and P. Let us compute the Inverse Fourier transform of the complex permittivity expression

$$\varepsilon(\omega) = \frac{D(\omega)}{P(\omega)}$$

(5.20)

At any time step n, this method requires the storage of M previous values of D and $M-1$ previous values of E beyond the current field values. The final formula has a form

$$E^i = f\left(D^i, ..., D^{i-M}; E^{i-1}, ..., E^{i-M}\right)$$

(5.21)

where M is the order of the time scheme.

5.6.1   Debye model
We show how this method works for the first-order Debye dispersion model. This model is described in the frequency domain by

$$P = \varepsilon_0 \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau} E \tag{5.22}$$

We rewrite this equation

$$(1 + j\omega\tau)P = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)E \tag{5.23}$$

Applying Inverse Fourier transform on (5.23) brings a first-order differential equation in time

$$P + \tau \frac{dP}{dt} = \varepsilon_0(\varepsilon_\infty - \varepsilon_s)E \tag{5.24}$$

This equation is then discretized by appropriate numerical methods to obtain a final discrete scheme.

5.6.2 Lorentz model

The Lorentz model is described in the frequency domain by

$$P = \varepsilon_0 \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 + j\omega\delta - \omega^2} E \tag{5.25}$$

We rewrite this equation

$$(\omega_0^2 + j\omega\delta - \omega^2)P = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_0^2 E \tag{5.26}$$

Applying Inverse Fourier transform on (5.23) brings a first-order differential equation in time

$$\omega_0^2 P + \delta \frac{dP}{dt} + \frac{d^2 P}{dt^2} = \varepsilon_0(\varepsilon_\infty - \varepsilon_s)\omega_0^2 E \tag{5.27}$$

This equation is then discretized by appropriate numerical methods to obtain a final discrete scheme.

5.6.3 Drude model

The Drude model is described in the frequency domain by

$$P = \varepsilon_0 \frac{\omega_p^2}{j\omega\delta - \omega^2} E \tag{5.28}$$

We rewrite this equation

$$(j\omega\delta - \omega^2)P = \varepsilon_0 \omega_p^2 E \tag{5.29}$$

Applying Inverse Fourier transform on (5.23) brings a first-order differential equation in time

$$\delta \frac{dP}{dt} + \frac{d^2 P}{dt^2} = \varepsilon_0 \omega_p^2 E \tag{5.30}$$

This equation is then discretized by appropriate numerical methods to obtain a final discrete scheme.

5.7 Digital filter based technique

We have developed an approach for dispersive models based on a digital filtering [81]. This approach is also suitable for other numerical methods. The method is based on the bilinear transformation.

The concept of expressing the time domain simulation in terms of the z variable, used in discrete time systems, is applied. The frequency characteristics of chosen dispersive models are transformed into the z plane using the so called bilinear transformation, which maps the imaginary axis of the s plane into the unit circle on the z plane. The resulting digital filter gives the relation between the electric field and the electric displacement vectors. This approach can be easily implemented with an appropriate accuracy into the finite element time domain method.

As a starting point of further considerations, we use the formulas (5.10), (5.12) and (5.14) defined by the s variable on a complex plane. Since we concentrate on the time discretization only, the symbols D and E used in the rest of the thesis stand for continuous vector fields, and the symbols d^n and e^n stand for vectors of samples taken in finite element nodes in the time step $n\Delta t$, where n is a natural number and Δt is the time step.

Our approach uses the bilinear transformation, described in [83]

$$s = \frac{2}{\Delta t} \frac{1 - z^{-1}}{1 + z^{-1}} \tag{5.31}$$

This transformation is used to map the complex variable s into the z plane so that the imaginary axis on the s plane is the unit circle on the z plane.

All the models (5.10), (5.12) and (5.14) can be expressed as a transfer function in the space of the Z transform:

$$H\left(z^{-1}\right) = \frac{D\left(z^{-1}\right)}{E\left(z^{-1}\right)} \tag{5.32}$$

From this expression, we can obtain discrete time schemes.

5.7.1 Debye model

The relation for the Debye model (5.10) between the s transforms of D and E is

$$D(s) = \frac{\Delta\varepsilon}{1 + s\tau} E(s) \tag{5.33}$$

Substituting (5.31) into (5.33) yields the transfer function

$$\frac{D\left(z^{-1}\right)}{E\left(z^{-1}\right)} = \frac{\Delta\varepsilon\left(1+z^{-1}\right)}{1+z^{-1}+\dfrac{2\tau}{\Delta t}\left(1-z^{-1}\right)} E(s) \tag{5.34}$$

From (5.34), we can directly write the corresponding difference formula

$$\left(1+\frac{2\tau}{\Delta t}\right)d^{n+1} + \left(1-\frac{2\tau}{\Delta t}\right)d^{n} = \Delta\varepsilon e^{n+1} + \Delta\varepsilon e^{n} \tag{5.35}$$

which finally yields the direct update scheme

$$d^{n+1} = -\frac{C_2}{C_1}d^n + \frac{\Delta\varepsilon}{C_1}e^{n+1} + \frac{\Delta\varepsilon}{C_1}e^n \tag{5.36}$$

where

$$C_1 = 1 + \frac{2\tau}{\Delta t} \tag{5.37}$$

$$C_2 = 1 - \frac{2\tau}{\Delta t} \tag{5.38}$$

5.7.2   Lorentz model

The relation for the Lorentz model (5.12) between the s transforms of D and E is

$$D(s) = \frac{\Delta\varepsilon\omega_0^2}{\omega_0^2 + s\delta + s^2} E(s) \tag{5.39}$$

Substituting (5.31) into (5.39) yields the transfer function

$$\frac{D\left(z^{-1}\right)}{E\left(z^{-1}\right)} = \frac{\Delta\varepsilon\omega_0^2 + 2\Delta\varepsilon\omega_0^2 z^{-1} + \Delta\varepsilon\omega_0^2 z^{-2}}{C_1 + C_2 z^{-1} + C_3 z^{-2}} \tag{5.40}$$

where

$$C_1 = \omega_0^2 + \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{5.41}$$

$$C_2 = 2\omega_0^2 - \frac{8}{\Delta t^2} \tag{5.42}$$

$$C_3 = \omega_0^2 - \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{5.43}$$

From (5.40) we can directly write the direct update scheme:

$$d^{n+1} = -\frac{C_2}{C_1}d^n - \frac{C_3}{C_1}d^{n-1} + \frac{\Delta\varepsilon\omega_0^2}{C_1}e^{n+1} + \frac{2\Delta\varepsilon\omega_0^2}{C_1}e^n + \frac{\Delta\varepsilon\omega_0^2}{C_1}e^{n-1} \tag{5.44}$$

5.7.3   Drude model

The relation for the Drude model (5.14) between the s transforms of D and E is

$$D(s) = \frac{\omega_p^2}{s\delta + s^2} E(s) \tag{5.45}$$

Substituting (5.31) into (5.45) yields the transfer function

$$\frac{D(z^{-1})}{E(z^{-1})} = \frac{\omega_p^2 + 2\omega_p^2 z^{-1} + \omega_p^2 z^{-2}}{C_1 + C_2 z^{-1} + C_3 z^{-2}} \tag{5.46}$$

where

$$C_1 = \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{5.47}$$

$$C_2 = -\frac{8}{\Delta t^2} \tag{5.48}$$

$$C_3 = -\frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{5.49}$$

From (5.46), we can directly write the direct update scheme:

$$d^{n+1} = -\frac{C_2}{C_1}d^n - \frac{C_3}{C_1}d^{n-1} + \frac{\omega_p^2}{C_1}e^{n+1} + \frac{2\omega_p^2}{C_1}e^n + \frac{\Delta\varepsilon\omega_p^2}{C_1}e^{n-1} \tag{5.50}$$

5.7.4 Discrete scheme

The corresponding wave equation, discretized in space, is of the following form:

$$\mathbf{L}E = -\frac{\partial^2}{\partial t^2}D \tag{5.51}$$

Here, the symbol $\mathbf{L}$ acts as the differential operator discretized in space. The operator is defined according to the finite element method. Application of the time scheme for the discretization in time yields

$$\mathbf{L}\left(\frac{e^{n+1}}{4} + \frac{e^n}{2} + \frac{e^{n-1}}{4}\right) = \frac{1}{\Delta t^2}\left(d^{n+1} - 2d^n + d^{n-1}\right) \tag{5.52}$$

Substitution of expressions (5.36), (5.44) or (5.50) into (5.52) yields the final formulas.

5.8 Conclusion

In this chapter, we briefly presented the theory of the dispersive medium and the most frequently used dispersive models of dispersive media. We described three methods for analyzing electromagnetic fields in environments with objects described by these dispersive models:

- The first method of field analysis in dispersive environments is based on the *Recursive convolution*. We can use this method for the Debye model of dispersive media only due to its difficulty.

- The second method of field analysis in dispersive environments is based on the *Direct Time Integration* technique.

Both these approaches and their employing in the FETD method can improve the process of analyzing electromagnetic fields in dispersive media.

The last method is a newly developed method which exploits principles of digital filtering techniques [84]. This method can be used for all the three developed models of dispersive media.

6 TIME DOMAIN FINITE ELEMENT MODELING OF DISPERSIVE MEDIA

In this chapter, we will discuss the exploitation of the finite element time domain (FETD) method for analyzing electromagnetic fields in dispersive media. We will use all the FETD approaches discussed in Chapter 4 (Ritz approach, Galerkin approach, different temporal schemes). We will investigate all the FETD methods for fields in dispersive media described in Chapter 5 (the recursive convolution, the direct time integration, the digital filtering technique).

The chapter concentrates on the FETD analysis of fields in free-space containing a dispersive material which is represented by a specific dispersive model (the Drude one, the Lorentz one, the Debye one). The free-space is defined as a vacuum. Absorbing boundary conditions are employed to truncate the free-space.

First, we will introduce the mathematical formulation of fields in free space containing general dispersive models of 1-D and 3-D objects. Then, we will discuss methods for analyzing fields. Mathematical models for both the dimensions of interest are discretized in space according to an appropriate FEM. Developed dispersive models do not depend on space; models affect the time discretization only.

Finally, FETD methods for analyzing fields in dispersive media are compared.

6.1 Mathematical models and space discretization

6.1.1 Model development for 1-D problem

We start the description of the mathematical model with an initial-boundary value problem which includes wave equation for the electric field in the computational domain defined on the interval z:

$$\frac{1}{\mu_0} \frac{\partial^2 E(x,t)}{\partial z^2} = \frac{\partial^2 D(x,t)}{\partial t^2} + \sigma \frac{\partial E(x,t)}{\partial t} \quad z \in \langle a,b \rangle \tag{6.1}$$

Here, E is the electric field intensity, D is the displacement vector, μ_0 stands for free-space permeability, μ_r stands for relative permeability, and σ is electric conductivity.

In order to truncate the finite computational domain, we introduce absorbing boundary conditions which describe the behavior of electric field in boundary points. This can be defined as

$$\left| \frac{\partial E(x,t)}{\partial t} - c \frac{\partial E(x,t)}{\partial z} \right|_{z=a} = 0 \tag{6.2a}$$

$$\left| \frac{\partial E(x,t)}{\partial t} + c \frac{\partial E(x,t)}{\partial z} \right|_{z=b} = 0 \tag{6.2b}$$

where c denotes the speed of light in vacuum.

For simplicity, we omit parentheses after each variable but still assume that all the variables are functions of space and time.

Our models use an electric field as an excitation pulse. Source of the electric field is based on a technique called the total field decomposition. The total field in equation (6.1) can be defined as

$$E = E^{inc} + E^{sc} \tag{6.3}$$

where E represents the total field, E^{inc} is the incident field and E^{sc} denotes the scattered field. We expect no reflection on the boundary from the scattered field. We consider the source in the boundary point a. This can be defined as

$$\left| \frac{1}{c} \frac{\partial E^{sc}}{\partial t} - \frac{\partial E^{sc}}{\partial z} \right|_{z=a} = 0 \tag{6.4}$$

Substituting (6.3) into (6.4), we obtain:

$$\left| \frac{1}{c} \frac{\partial E}{\partial t} - \frac{\partial E}{\partial z} \right|_{z=a} = \left| \frac{1}{c} \frac{\partial E^{inc}}{\partial t} - \frac{\partial E^{inc}}{\partial z} \right|_{z=a} \tag{6.5}$$

The expression to be used for describing the total electric field on the boundary, which defines the absorbing boundary condition and the source, is given by

$$\left| \frac{\partial E}{\partial z} \right|_{z=a} = \left| \frac{1}{c} \frac{\partial E}{\partial t} - \frac{1}{c} \frac{\partial E^{inc}}{\partial t} + \frac{\partial E^{inc}}{\partial z} \right|_{z=a} \tag{6.6}$$

The homogeneous initial conditions to be used later are defined as

$$E(x,0) = 0 \tag{6.7a}$$

$$\frac{\partial E(x,0)}{\partial t} = 0 \tag{6.7b}$$

6.1.2   Spatial discretization in 1-D

Assuming the existence of a unique solution, we can formulate the weak form of the solution by using weighted residual method. In this approach, we multiply the wave equation (6.1) by testing functions W, and integrate the product over the whole interval $\langle a,b \rangle$. Note that the testing function W is a function of space only:

$$\int_a^b W \left(\frac{1}{\mu_0} \frac{\partial^2 E}{\partial z^2} - \frac{\partial^2 D}{\partial t^2} - \sigma \frac{\partial E}{\partial t} \right) dz = 0 \tag{6.8}$$

The equation (6.8) can be rewritten:

$$\int_a^b W \frac{\partial^2 D}{\partial t^2} dz + \sigma \int_a^b W \frac{\partial E}{\partial t} dz - \frac{1}{\mu_0} \int_a^b W \frac{\partial^2 E}{\partial z^2} dz = 0 \tag{6.9}$$

The last part of the left-hand side term of (6.9) can be modified using integration by parts

$$-\frac{1}{\mu_0}\int_a^b W\frac{\partial^2 E}{\partial z^2}dz = \begin{vmatrix} u=W & u'=W' \\ v'=\dfrac{\partial^2 E}{\partial z^2} & v=\dfrac{\partial E}{\partial z} \end{vmatrix} = -\frac{1}{\mu_0}\left|W\frac{\partial E}{\partial z}\right|_a^b + \frac{1}{\mu_0}\left(\int_a^b\frac{\partial W}{\partial z}\frac{\partial E}{\partial z}dz\right) \quad (6.10)$$

Equation (6.10) equals to

$$-\frac{1}{\mu_0}\left(W(b)\frac{\partial E(b)}{\partial z}-W(a)\frac{\partial E(a)}{\partial z}\right)+\frac{1}{\mu_0}\left(\int_a^b\frac{\partial W}{\partial z}\frac{\partial E}{\partial z}dz\right) \quad (6.11)$$

We replace the last part of equation (6.9) by (6.11):

$$\int_a^b W\frac{\partial^2 D}{\partial t^2}dz + \sigma\int_a^b W\frac{\partial E}{\partial t}dz - \frac{1}{\mu_0}\left(W(b)\frac{\partial E(b)}{\partial z}-W(a)\frac{\partial E(a)}{\partial z}\right)$$
$$+\frac{1}{\mu_0}\left(\int_a^b\frac{\partial W}{\partial z}\frac{\partial E}{\partial z}dz\right)=0$$

$$(6.12)$$

The weak form of the wave equation (6.1), which includes absorbing boundary conditions (ABC; 6.2b) and source (6.6), looks like:

$$\int_a^b W\frac{\partial^2 D}{\partial t^2}dz + \sigma\int_a^b W\frac{\partial E}{\partial t}dz$$
$$+\frac{1}{\mu_0}\left(W(b)\left|\frac{1}{c}\frac{\partial E}{\partial t}\right|_{z=b}+W(a)\left|\frac{1}{c}\frac{\partial E}{\partial t}-\frac{1}{c}\frac{\partial E^{inc}}{\partial t}+\frac{\partial E^{inc}}{\partial z}\right|_{z=a}\right)+\frac{1}{\mu_0}\left(\int_a^b\frac{\partial W}{\partial z}\frac{\partial E}{\partial z}dz\right)=0$$

$$(6.13)$$

In order to solve the equation (6.13), we need to approximate the electric field E. The approximation of the electric field E is given by

$$E(t,z)=\sum_{i=0}^M W_i(z)e_i(t) \quad (6.14)$$

where basis functions W are the same as testing functions used above (the Galerkin approach). We substitute the electric field in (6.13) by (6.14) and obtain the equation

$$\mathbf{T}\frac{\partial^2 D}{\partial t^2}+(\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t}+\mathbf{S}e+\mathbf{g}=0 \quad (6.15)$$

where matrices are defined as

$$S_{ij}=\frac{1}{\mu_0}\int_a^b\frac{\partial W_i}{\partial z}\frac{\partial W_j}{\partial z}dz \quad (6.16)$$

$$Q_{ij}=\sigma\int_a^b W_i W_j dz \quad (6.17)$$

$$B_{ij}=\frac{1}{\mu_0}\frac{1}{c}\left[W_i(a)W_j(a)+W_i(b)W_j(b)\right] \quad (6.18)$$

The source vector is

$$g_i = \frac{1}{\mu_0}\left[W_i(a)\left(-\frac{1}{c}\frac{\partial E^{inc}(a)}{\partial t} + \frac{\partial E^{inc}(a)}{\partial z}\right)\right] \tag{6.19}$$

The first term on the left-hand side in the equation (6.15) is not defined yet. Approximation of the displacement vector D depends on a technique to be used and a model of the dispersive material.

6.1.3   Model development for 3-D problem

The wave equation for electric field in the computational domain V is

$$\nabla\times\left[\frac{1}{\mu_0\mu_r}\nabla\times\mathbf{E}(\mathbf{r},t)\right] + \frac{\partial^2\mathbf{D}(\mathbf{r},t)}{\partial t^2} + \sigma\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t} = 0 \quad \mathbf{r}\in V \tag{6.20}$$

where $\mathbf{E}$ is electric field, $\mathbf{D}$ is displacement vector, μ_0 stands for free-space permeability, μ_r stands for relative permeability, and σ is electric conductivity.

An absorbing boundary condition for the simulation of electric field in free space is given on the surface S_{ABC} by

$$\mathbf{n}\times\left[\frac{1}{\mu_0\mu_r}\nabla\times\mathbf{E}(\mathbf{r},t)\right] + Y_0\frac{\partial}{\partial t}\left[\mathbf{n}\times\mathbf{n}\times\mathbf{E}(\mathbf{r},t)\right] = 0 \quad \mathbf{r}\in S_{ABC} \tag{6.21}$$

where $\mathbf{n}$ is the outward unit vector normal to the surface, Y_0 is the free-space admittance.

The source of electric field is based on a total field decomposition:

$$\mathbf{E} = \mathbf{E}^{inc} + \mathbf{E}^{sc} \tag{6.22}$$

where $\mathbf{E}$ represents the total field, $\mathbf{E}^{inc}$ is the incident field and $\mathbf{E}^{sc}$ is the scattered field. The surface, where the source is supposed, is denoted as S_{inc}. We expect no reflections on the boundary from scattered fields. After certain modifications, this can be defined as

$$\begin{aligned}
&\mathbf{n}\times\left[\frac{1}{\mu_0\mu_r}\nabla\times\mathbf{E}(\mathbf{r},t)\right] + Y_0\frac{\partial}{\partial t}\left[\mathbf{n}\times\mathbf{n}\times\mathbf{E}(\mathbf{r},t)\right] = \\
&\mathbf{n}\times\left[\frac{1}{\mu_0\mu_r}\nabla\times\mathbf{E}^{inc}(\mathbf{r},t)\right] + Y_0\frac{\partial}{\partial t}\left[\mathbf{n}\times\mathbf{n}\times\mathbf{E}^{inc}(\mathbf{r},t)\right]
\end{aligned} \tag{6.23}$$

The homogeneous initial conditions to be used later are defined as

$$\mathbf{E}(\mathbf{r},t) = 0 \tag{6.24a}$$

$$\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t} = 0 \tag{6.24b}$$

6.1.4   Spatial discretization in 3-D

Assuming the existence of a unique solution, we can formulate the weak form of the solution using the Galerkin approach. In this approach, we multiply the wave

equation (6.20) by testing functions **N** and integrate the product over the whole volume *V*. Note that **N** is the function of space only:

$$\iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\nabla \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] + \frac{\partial^2 \mathbf{D}(\mathbf{r},t)}{\partial t^2} + \sigma \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} \right) dV = 0 \qquad (6.25)$$

The equation (6.25) can be rewritten to

$$\iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\nabla \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] \right) dV + \iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\frac{\partial^2 \mathbf{D}(\mathbf{r},t)}{\partial t^2} \right) dV$$

$$+ \iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\sigma \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} \right) dV = 0 \qquad (6.26)$$

The first part on the left-hand side of the equation (6.26) can be modified using the vector identity

$$\mathbf{a} \cdot (\nabla \times \mathbf{b}) = (\nabla \times \mathbf{a}) \cdot \mathbf{b} - \nabla \cdot (\mathbf{a} \times \mathbf{b})$$

as

$$\iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\nabla \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] \right) dV =$$

$$\iiint_V [\nabla \times \mathbf{W}(\mathbf{r})] \cdot \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] dV - \iiint_V \nabla \cdot \left(\mathbf{W}(\mathbf{r}) \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] \right) dV \qquad (6.27)$$

The last term on the right-hand side of the equation (6.27) can be rewritten using the divergence theorem

$$\iiint_V \nabla \cdot \mathbf{f} dV = \oiint_S \mathbf{n} \cdot \mathbf{f} dS \qquad (6.28)$$

which yields

$$\iiint_V \nabla \cdot \left(\mathbf{W}(\mathbf{r}) \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] \right) dV = \oiint_S \mathbf{n} \cdot \left[\mathbf{W}(\mathbf{r}) \times \left(\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right) \right] dS \qquad (6.29)$$

Applying the vector identity

$$(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = -\mathbf{a}(\mathbf{c} \times \mathbf{b})$$

we can obtain from (6.29) the expression

$$\oiint_S \mathbf{n} \cdot \left[\mathbf{W}(\mathbf{r}) \times \left(\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right) \right] dS = -\oiint_S \mathbf{W}(\mathbf{r}) \cdot \left[\mathbf{n} \times \left(\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right) \right] dS \qquad (6.30)$$

The final form of the first part on the left-hand side of equation (6.26) is

$$\iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\nabla \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] \right) dV =$$

$$\iiint_V \left[\nabla \times \mathbf{W}(\mathbf{r}) \right] \cdot \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] dV + \oiint_S \mathbf{W}(\mathbf{r}) \cdot \left[\mathbf{n} \times \left(\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right) \right] dS \quad (6.31)$$

The last term on the left-hand side of (6.31) enables us to implement the ABC and the excitation.

The weak form of the wave equation (6.20) including the ABC (6.21) and the excitation (6.23) is

$$\iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\frac{\partial^2 \mathbf{D}(\mathbf{r},t)}{\partial t^2} \right) dV + \iiint_V \mathbf{W}(\mathbf{r}) \cdot \left(\sigma \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} \right) dV$$

$$+ \iiint_V \left[\nabla \times \mathbf{W}(\mathbf{r}) \right] \cdot \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}(\mathbf{r},t) \right] dV - \oiint_{S_{ABC}} \mathbf{W}(\mathbf{r}) \cdot \left[Y_0 \frac{\partial}{\partial t} \left[\mathbf{n} \times \mathbf{n} \times \mathbf{E}(\mathbf{r},t) \right] \right] dS$$

$$- \oiint_{S_{inc}} \mathbf{W}(\mathbf{r}) \cdot \left[Y_0 \frac{\partial}{\partial t} \left[\mathbf{n} \times \mathbf{n} \times \mathbf{E}(\mathbf{r},t) \right] \right] dS + \quad (6.32)$$

$$\oiint_{S_{inc}} \mathbf{W}(\mathbf{r}) \cdot \left[\mathbf{n} \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}^{inc}(\mathbf{r},t) \right] + Y_0 \frac{\partial}{\partial t} \left[\mathbf{n} \times \mathbf{n} \times \mathbf{E}^{inc}(\mathbf{r},t) \right] \right] dS = 0$$

In order to solve the equation (6.32), we need to approximate the electric field $\mathbf{E}$:

$$\mathbf{E}(\mathbf{r},t) = \sum_{i=0}^{M} \mathbf{W}_i(\mathbf{r}) e_i(t) \quad (6.33)$$

Here, the approximation (basis) functions $\mathbf{N}$ are the same as testing functions used above. We substitute the electric field in (6.32) by (6.33) and obtain the equation

$$\mathbf{T} \frac{\partial^2 D}{\partial t^2} + (\mathbf{Q} + \mathbf{B}) \frac{\partial e}{\partial t} + \mathbf{S} e + \mathbf{g} = 0 \quad (6.34)$$

Here, the matrices are defined as

$$S_{ij} = \frac{1}{\mu_0 \mu_r} \iiint_V \nabla \times \mathbf{W}_i \cdot \nabla \times \mathbf{W}_j dV \quad (6.35)$$

$$Q_{ij} = \sigma \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \quad (6.36)$$

$$B_{ij} = -Y_0 \oiint_{S_{ABC}} \mathbf{W}_i \cdot \left[\mathbf{n} \times \mathbf{n} \times \mathbf{W}_j \right] dS - Y_0 \oiint_{S_{inc}} \mathbf{W}_i \cdot \left[\mathbf{n} \times \mathbf{n} \times \mathbf{W}_j \right] dS \quad (6.37)$$

The source vector is given by the expression:

$$g_i = \oiint_{S_{inc}} \mathbf{W}_i \cdot \left[\mathbf{n} \times \left[\frac{1}{\mu_0 \mu_r} \nabla \times \mathbf{E}^{inc}(\mathbf{r},t) \right] + Y_0 \frac{\partial}{\partial t} \left[\mathbf{n} \times \mathbf{n} \times \mathbf{E}^{inc}(\mathbf{r},t) \right] \right] dS \quad (6.38)$$

The first term on the left-hand side in the equation (6.34) is not defined yet. The approximation of the displacement vector **D** depends on the technique used and the model of the dispersive material.

Obviously, equations (6.15) and (6.34) are of the same form. Thanks to this reason, we can provide an approach for solving this form of the equation.

6.2 Debye model

In this paragraph, we will investigate the Debye model.

6.2.1 Direct Time Integration

The relation between E and D for 1-D problem is given by the expression

$$D = \varepsilon_0 \varepsilon_\infty E + P \tag{6.39}$$

The first part in the equation (6.13) then becomes

$$\int_a^b W \frac{\partial^2 D}{\partial t^2} dz = \varepsilon_0 \varepsilon_\infty \int_a^b W \frac{\partial^2 E}{\partial t^2} dz + \int_a^b W \frac{\partial^2 P}{\partial t^2} dz \tag{6.40}$$

For the approximation of **E**, we use the same expression as in (6.14), and **P** is given by

$$P(x,t) = \sum_{i=0}^{M} W_i(x) p_i(t) \tag{6.41}$$

The equation (6.15) is now transformed into

$$\mathbf{T} \frac{\partial^2 e}{\partial t^2} + (\mathbf{Q} + \mathbf{B}) \frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^p \frac{\partial^2 p}{\partial t^2} + \mathbf{g} = 0 \tag{6.42}$$

Here, coefficients e and p are functions of time and new matrices **T** and $\mathbf{T}^p$ are defined as

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \int_a^b W_i W_j dz \tag{6.43}$$

$$T_{ij}^p = \int_a^b W_i W_j dz \tag{6.44}$$

In the case of a 3-D problem, the first part of the equation (6.32) becomes

$$\iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{D}}{\partial t^2} \right) dV = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{E}}{\partial t^2} \right) dV + \iiint_V \mathbf{W} \cdot \frac{\partial^2 \mathbf{P}}{\partial t^2} dV \tag{6.45}$$

For the approximation of **E** we use the same expression as in (6.33) and **P** is given by

$$\mathbf{P}(\mathbf{r},t) = \sum_{i=0}^{M} \mathbf{W}_i(\mathbf{r}) p_i(t) \tag{6.46}$$

The equation (6.34) is now transformed into (6.42). Only the matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{N}_i \cdot \mathbf{N}_j dV \tag{6.47}$$

$$T_{ij}^p = \iiint_V \mathbf{N}_i \cdot \mathbf{N}_j dV \tag{6.48}$$

The initial conditions can be defined for 1-D as

$$P(x,0) = 0 \quad \frac{\partial P(x,0)}{\partial t} = 0 \tag{6.49a}$$

and for 3-D as

$$\mathbf{P}(\mathbf{r},0) = 0 \quad \frac{\partial \mathbf{P}(\mathbf{r},0)}{\partial t} = 0 \tag{6.49b}$$

Now we can treat the equation (6.42) in the same manner for both the dimensions.

The description of the Debye model is given by the differential equation of the form

$$\tau \frac{\partial p}{\partial t} + p = \varepsilon_0 \left(\varepsilon_s - \varepsilon_\infty \right) e \tag{6.50}$$

We need the second derivative of the equation (6.50) since there is the second derivative of p in the equation (6.42):

$$\frac{\partial^2 p}{\partial t^2} = -\frac{1}{\tau} \frac{\partial p}{\partial t} + \frac{\varepsilon_0}{\tau} \left(\varepsilon_s - \varepsilon_\infty \right) \frac{\partial e}{\partial t} \tag{6.51}$$

Substituting (6.51) and t (6.50) into the equation (6.42), we obtain:

$$\mathbf{T} \frac{\partial^2 e}{\partial t^2} + \left(\mathbf{Q} + \mathbf{B} + \mathbf{T}^e \right) \frac{\partial e}{\partial t} + \left(\mathbf{S} + \mathbf{T}^m \right) e + \mathbf{T}^k p + \mathbf{g} = 0 \tag{6.52}$$

where

$$\mathbf{T}^e = \frac{\varepsilon_0}{\tau} \left(\varepsilon_s - \varepsilon_\infty \right) \mathbf{T}^p \tag{6.53}$$

$$\mathbf{T}^m = -\frac{\varepsilon_0}{\tau^2} \left(\varepsilon_s - \varepsilon_\infty \right) \mathbf{T}^p \tag{6.54}$$

$$\mathbf{T}^k = \frac{1}{\tau^2} \mathbf{T}^p \tag{6.55}$$

Now, we have a system of ordinary differential equations (6.52) which can be solved by an appropriate time scheme.

Applying a two-step algorithm described in Chapter 4.4, we can rewrite (6.52) to the system

$$\mathbf{T}\left(\frac{e^{n+1}-2e^n+e^{n-1}}{\Delta t^2}\right)+\left(\mathbf{Q}+\mathbf{B}+\mathbf{T}^e\right)\left(\frac{e^{n+1}-e^{n-1}}{2\Delta t}\right)$$

$$+\left(\mathbf{S}+\mathbf{T}^m\right)\left(\frac{e^{n+1}+2e^n+e^{n-1}}{4}\right)+\mathbf{T}^k p^n+\mathbf{g}^n=0 \tag{6.56}$$

The final equation is of the form:

$$\left(\frac{1}{\Delta t^2}\mathbf{T}+\frac{1}{2\Delta t}\left(\mathbf{Q}+\mathbf{B}+\mathbf{T}^e\right)+\frac{1}{4}\left(\mathbf{S}+\mathbf{T}^m\right)\right)e^{n+1}=-\left(\frac{-2}{\Delta t^2}\mathbf{T}+\frac{1}{2}\left(\mathbf{S}+\mathbf{T}^m\right)\right)e^n$$

$$-\left(\frac{1}{\Delta t^2}\mathbf{T}-\frac{1}{2\Delta t}\left(\mathbf{Q}+\mathbf{B}+\mathbf{T}^e\right)+\frac{1}{4}\left(\mathbf{S}+\mathbf{T}^m\right)\right)e^{n-1}-\mathbf{T}^k p^n-\mathbf{g}^n \tag{6.57}$$

The equation (6.57) has only the variable e in the time step $n+1$. This means that we can solve this system of linear equations. To obtain proper coefficients for the term p^n in (6.57), we again use the equation (6.50). For this purpose, we will apply the θ-method on (6.50):

$$\tau\frac{p^n-p^{n-1}}{\Delta t}=-p^{n+\theta}+\varepsilon_0\left(\varepsilon_s-\varepsilon_\infty\right)e^{n+\theta} \tag{6.58}$$

Generally:

$$v^{n+\theta}=\theta v^n+\left(1-\theta\right)v^{n-1} \tag{6.59}$$

Then:

$$p^n\left(1+\theta\frac{\Delta t}{\tau}\right)=\left[1-\frac{\Delta t}{\tau}\left(1-\theta\right)\right]p^{n-1}+\varepsilon_0\left(\varepsilon_s-\varepsilon_\infty\right)\frac{\Delta t}{\tau}\left(\theta e^n+\left(1-\theta\right)e^{n-1}\right) \tag{6.60}$$

The equation (6.57) has to be solved in each time step. The optimum value of the coefficient θ is 1/2.

6.2.2 Recursive convolution technique

The relation between E and D for 1-D problem is given by

$$D=\varepsilon_0\hat{\varepsilon}_r E \tag{6.61}$$

where

$$\hat{\varepsilon}_r=\varepsilon_\infty+\frac{\left(\varepsilon_s-\varepsilon_\infty\right)}{\tau}\exp\left(\frac{-t}{\tau}\right)=\varepsilon_\infty+\chi \tag{6.62}$$

Implying the relation (6.61) into the first part of the equation (6.13), we obtain

$$\int_a^b W\frac{\partial^2 D}{\partial t^2}dz=\varepsilon_0\varepsilon_\infty\int_a^b W\frac{\partial^2 E}{\partial t^2}dz+\varepsilon_0\int_a^b W\frac{\partial^2\left(E*\chi\right)}{\partial t^2}dz \tag{6.63}$$

The equation (6.15) is of the form now

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2}+(\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t}+\mathbf{S}e+\mathbf{T}^c\frac{\partial^2\left(e*\chi\right)}{\partial t^2}+\mathbf{g}=0 \qquad (6.64)$$

where

$$T_{ij}=\varepsilon_0\varepsilon_\infty\int_a^b W_iW_j\,dz \qquad (6.65)$$

$$T_{ij}^c=\varepsilon_0\int_a^b W_iW_j\,dz \qquad (6.66)$$

In the case of a 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W}\cdot\left(\frac{\partial^2\mathbf{D}}{\partial t^2}\right)dV=\varepsilon_0\varepsilon_\infty\iiint_V \mathbf{W}\cdot\left(\frac{\partial^2\mathbf{E}}{\partial t^2}\right)dV+\varepsilon_0\iiint_V \mathbf{W}\cdot\frac{\partial^2\left(\mathbf{E}*\chi\right)}{\partial t^2}dV \qquad (6.67)$$

The equation (6.34) is now of the same form as (6.64). Only the matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as

$$T_{ij}=\varepsilon_0\varepsilon_\infty\iiint_V \mathbf{W}_i\cdot\mathbf{W}_j\,dV \qquad (6.68)$$

$$T_{ij}^c=\varepsilon_0\iiint_V \mathbf{W}_i\cdot\mathbf{W}_j\,dV \qquad (6.69)$$

Now we have the system of ordinary differential equations (6.64) which can be solved by an appropriate time scheme.

Applying two-step algorithm described in the Chapter 4.4, we obtain from (6.64) the system:

$$\mathbf{T}\left(\frac{e^{n+1}-2e^n+e^{n-1}}{\Delta t^2}\right)+(\mathbf{Q}+\mathbf{B})\left(\frac{e^{n+1}-e^{n-1}}{2\Delta t}\right)+\mathbf{S}\left(\frac{e^n+2e^n+e^n}{4}\right)$$
$$+\mathbf{T}^c\left(\frac{C^{n+1}-2C^n+C^{n-1}}{\Delta t^2}\right)+\mathbf{g}^n=0 \qquad (6.70)$$

where

$$C^k=\left(E*\chi\right)^k \qquad (6.71)$$

for $k=n+1,\,n,\,n-1$.

We can write the expression

$$C^{n+1}=\exp\left(-\frac{\Delta t}{\tau}\right)C^n+\int_{n\Delta t}^{(n+1)\Delta t}\chi\left((n+1)\Delta t-\tau\right)e(\tau)\,d\tau \qquad (6.72)$$

which is the recursive form of (5.9).

We approximate e as follows:

$$e(t)=e^n+\frac{e^{n+1}-e^n}{\Delta t}(t-n\Delta t) \qquad (6.73)$$

The expression for C^{n+1} is then

$$C^{n+1} = \exp\left(-\frac{\Delta t}{\tau}\right)C^n + \psi_1 e^{n+1} + \psi_2 e^n \tag{6.74}$$

where

$$\psi_1 = \tau\left(\chi(0)\left(1 - \frac{\tau}{\Delta t}\right) + \chi(\Delta t)\frac{\tau}{\Delta t}\right)e^{n+1} \tag{6.75a}$$

$$\psi_2 = \tau\left(\chi(0)\frac{\tau}{\Delta t} - \chi(\Delta t)\left(1 + \frac{\tau}{\Delta t}\right)\right)e^n \tag{6.75b}$$

Substituting (6.74) into (6.70), we obtain the final equation

$$\mathbf{T}\left(\frac{e^{n+1} - 2e^n + e^{n-1}}{\Delta t^2}\right) + (\mathbf{Q} + \mathbf{B})\left(\frac{e^{n+1} - e^{n-1}}{2\Delta t}\right) + \mathbf{S}\left(\frac{e^n + 2e^n + e^n}{4}\right)$$

$$+ \mathbf{T}^c\left(\frac{\exp\left(-\frac{\Delta t}{\tau}\right)C^n + \psi_1 e^{n+1} + \psi_2 e^n - 2C^n + C^{n-1}}{\Delta t^2}\right) + \mathbf{g}^n = 0 \tag{6.76}$$

which can be rewritten into

$$\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}(\mathbf{Q} + \mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{\psi_1}{\Delta t^2}\mathbf{T}^c\right)e^{n+1} = -\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\mathbf{S} + \frac{\psi_2}{\Delta t^2}\mathbf{T}^c\right)e^n$$

$$-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}(\mathbf{Q} + \mathbf{B}) + \frac{1}{4}\mathbf{S}\right)e^{n-1} \tag{6.77}$$

$$-\frac{\left[\exp\left(-\frac{\Delta t}{\tau}\right) - 2\right]}{\Delta t^2}\mathbf{T}^c C^n - \frac{1}{\Delta t^2}\mathbf{T}^c C^{n-1} - \mathbf{g}^n$$

This equation is solved in each time step. For obtaining C^n and C^{n-1}, we use the equation (6.74).

6.2.3   Digital filter based technique

The relation between E and D for 1-D problem in the frequency domain is given by

$$D(\omega) = \varepsilon_0 \hat{\varepsilon}_r(\omega) E(\omega) \tag{6.78}$$

where

$$\hat{\varepsilon}_r = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)}{1 + j\omega\tau} = \varepsilon_\infty + \chi(\omega) \tag{6.79}$$

Without the loss of generality, we can rewrite the first part of the equation (6.13) into

$$\int_a^b W \frac{\partial^2 D}{\partial t^2} dz = \varepsilon_0 \varepsilon_\infty \int_a^b W \frac{\partial^2 E}{\partial t^2} dz + \varepsilon_0 \int_a^b W \frac{\partial^2 D_\chi}{\partial t^2} dz \tag{6.80}$$

because the first term on the right-hand side in (6.79) is frequency-independent .

The expression for D_χ in the frequency domain is

$$D(\omega) = \chi(\omega) E(\omega) \tag{6.81}$$

For the approximation of **E** we use the same expression as in (6.14):

$$D_\chi(x,t) = \sum_{i=0}^M W_i(z) d_{\chi i}(t) \tag{6.41}$$

The equation (6.15) is of the form now

$$\mathbf{T} \frac{\partial^2 e}{\partial t^2} + (\mathbf{Q} + \mathbf{B}) \frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^d \frac{\partial^2 d_\chi}{\partial t^2} + \mathbf{g} = 0 \tag{6.82}$$

where

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \int_a^b W_i W_j dz \tag{6.83}$$

$$T_{ij}^d = \varepsilon_0 \int_a^b W_i W_j dz \tag{6.84}$$

In the case of the 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{D}}{\partial t^2} \right) dV = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{E}}{\partial t^2} \right) dV + \varepsilon_0 \iiint_V \mathbf{W} \cdot \frac{\partial^2 \mathbf{D}_\chi}{\partial t^2} dV \tag{6.85}$$

The equation (6.34) is now of the same form as (6.82). Only matrices $\mathbf{T}$ and $\mathbf{T}^d$ are defined as follows:

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.86}$$

$$T_{ij}^c = \varepsilon_0 \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.87}$$

Now, we have the system of ordinary differential equations (6.64) which can be solved by an appropriate time scheme.

Applying the two-step algorithm described in the Chapter 4.4, we obtain from (6.82) the system

$$\mathbf{T} \left(\frac{e^{n+1} - 2e^n + e^{n-1}}{\Delta t^2} \right) + (\mathbf{Q} + \mathbf{B}) \left(\frac{e^{n+1} - e^{n-1}}{2\Delta t} \right) + \mathbf{S} \left(\frac{e^n + 2e^n + e^n}{4} \right)$$
$$+ \mathbf{T}^d \left(\frac{d_\chi^{n+1} - 2d_\chi^n + d_\chi^{n-1}}{\Delta t^2} \right) + \mathbf{g}^n = 0 \tag{6.88}$$

As mentioned in the Chapter 5.7.1, we use the expression

$$d_\chi^{n+1} = -\frac{C1}{C2}d_\chi^n + \frac{\Delta\varepsilon}{C1}e^{n+1} + \frac{\Delta\varepsilon}{C1}e^n \qquad (6.89)$$

where

$$C_1 = 1 + \frac{2\tau}{\Delta t} \qquad (6.90)$$

$$C_2 = 1 - \frac{2\tau}{\Delta t} \qquad (6.91)$$

The equation (6.88) becomes

$$\mathbf{T}\left(\frac{e^{n+1} - 2e^n + e^{n-1}}{\Delta t^2}\right) + (\mathbf{Q}+\mathbf{B})\left(\frac{e^{n+1} - e^{n-1}}{2\Delta t}\right) + \mathbf{S}\left(\frac{e^n + 2e^n + e^n}{4}\right)$$

$$+ \mathbf{T}^d\left(\frac{-\frac{C1}{C2}d_\chi^n + \frac{\Delta\varepsilon}{C1}e^{n+1} + \frac{\Delta\varepsilon}{C1}e^n - 2d_\chi^n + d_\chi^{n-1}}{\Delta t^2}\right) + \mathbf{g}^n = 0 \qquad (6.92)$$

The equation (6.92) can be rewritten into the final system of linear equations

$$\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{1}{\Delta t^2}\frac{\Delta\varepsilon}{C1}\mathbf{T}^d\right)e^{n+1} = -\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\mathbf{S} + \frac{1}{\Delta t^2}\frac{\Delta\varepsilon}{C1}\mathbf{T}^d\right)e^n$$

$$-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S}\right)e^{n-1} + \frac{1}{\Delta t^2}\left(\frac{C1}{C2} + 2\right)\mathbf{T}^d d^n - \frac{1}{\Delta t^2}\mathbf{T}^d d^{n-1} - \mathbf{g}^n \qquad (6.93)$$

This equation is solved in each time step. In order to obtain d_χ^n and d_χ^{n-1}, we use the equation (6.89).

6.2.4 Comparison and verification of methods

The first two test cases verify the digital filter based technique. As an example test, the value of S_{11} for a dielectric obstacle filling the WR90 waveguide has been calculated. Since the reference values are difficult to obtain in literature, the time domain results have been compared with the results of the frequency domain finite difference analysis.

In the first test, the parameters of the obstacle corresponding to the breast tissue [5] have been chosen, specifically: $\varepsilon_\infty = 7.81$, $\Delta\varepsilon = 40.14$, $\tau = 10.62ps$ and $\sigma = 0.71S/m$. The dielectric obstacle was loaded into the WR90 waveguide, which was 6 mm long. The mesh was discretized with the spatial step $\Delta z = 0.3$ mm and the corresponding time step was equal to 0.8 ps. The frequency characteristics are shown in Figure 6.1, together with the reference plot. Good agreement between these two methods is visible.
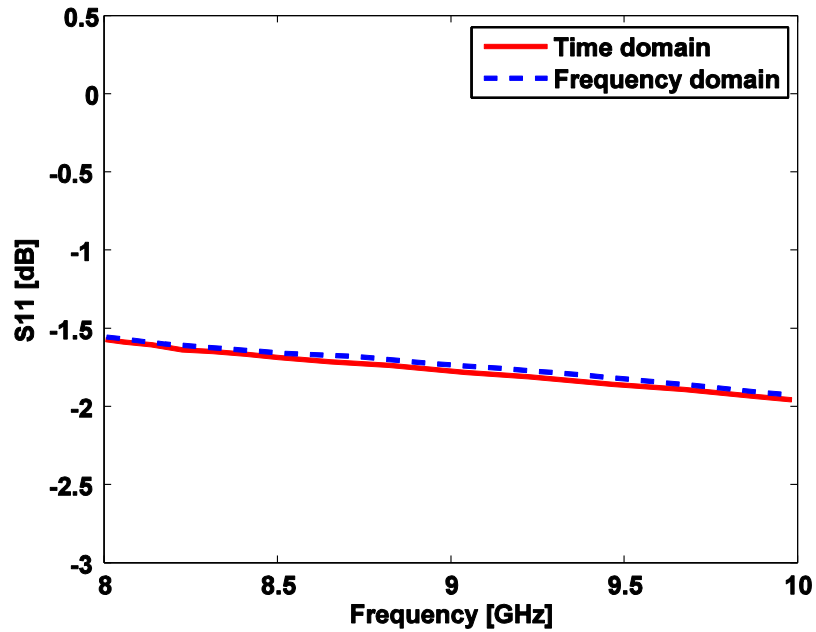
Fig. 6.1: Frequency response of the reflection coefficient at the input
of the waveguide WR90 loaded by the obstacle with parameters of breast tissue.
Time domain (red, solid) versus frequency domain (blue, dashed).

As another example test, the value of S_{11} for a dielectric obstacle filling W90 waveguide has been calculated. The parameters of the obstacles are $\varepsilon_\infty = 7.81$, $\Delta\varepsilon = 20.14$, $\tau = 1.62$ ps and $\sigma = 0.71$ S/m. Parameters of the obstacle do not correspond to any physical material.

Shorter relaxation time, however, implicitly resulted in smaller losses and finally a smaller reflection. Finally, the resonant characteristics could be obtained. Resonant characteristics are better for validating the algorithm. The results are presented in Figure 6.2. Obviously, a good agreement between the two methods is achieved.
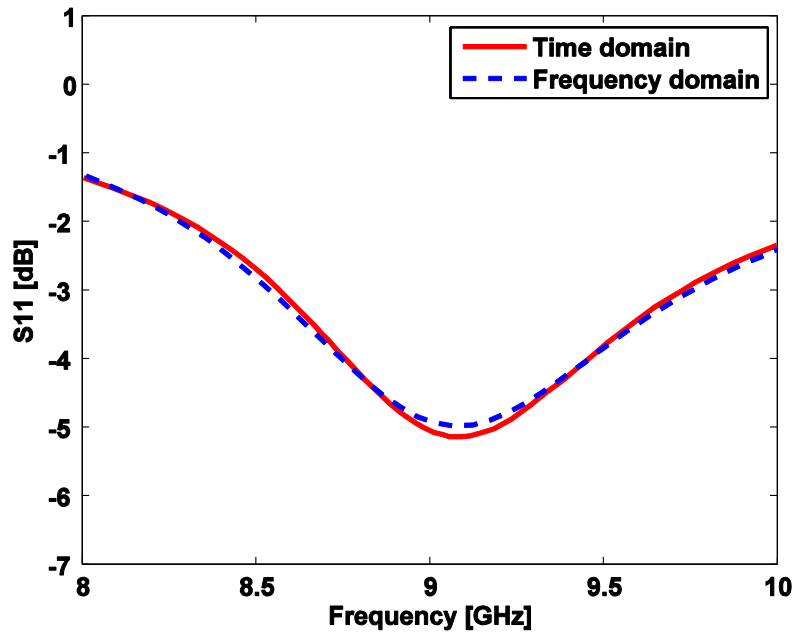
Fig. 6.2: Frequency response of the reflection coefficient at the input of the waveguide loaded by the obstacle with non-physical parameters. Time domain (red, solid) versus frequency domain (blue, dashed).
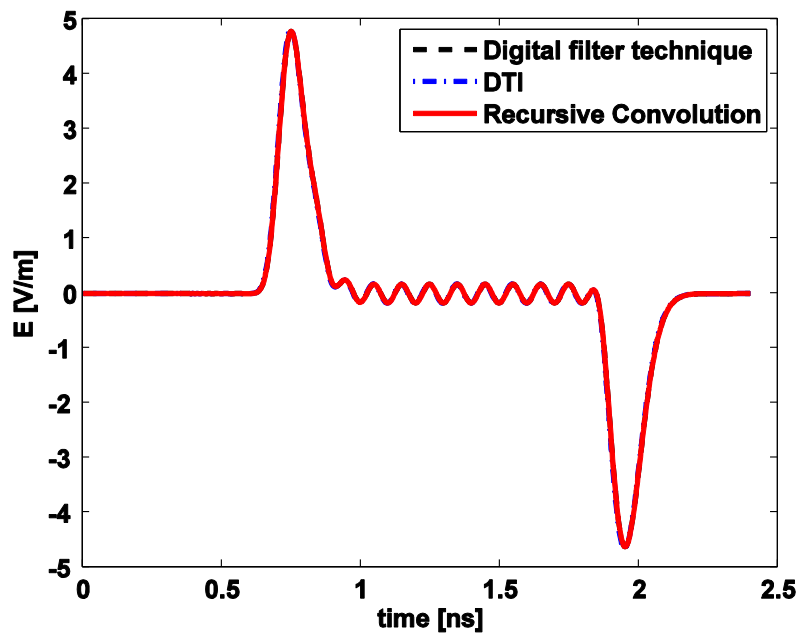

Fig. 6.3: Time response of the electric field intensity at a depth of 15 mm in the Debye medium.
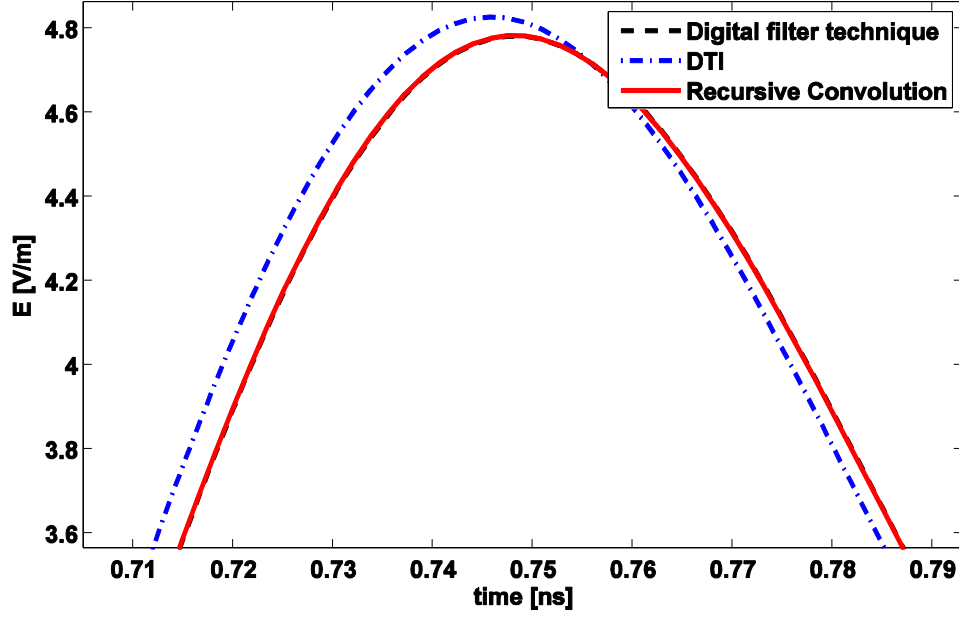
Fig. 6.4: Time response of the electric field intensity at a depth of 15 mm in the Debye medium: a detail.

In order to verify all the developed methods for the Debye model, we consider the following example inspired by [52]. The medium is defined with the following parameters: $\varepsilon_\infty = 1$, $\varepsilon_s = 78.2$, $\tau = 8.1ps$. The excitation pulse is a sine wave with 12 cycles. The frequency of this pulse is 10 GHz. A time trace of the electric field at a depth of 15 mm into Debye medium was recorded. In Figure 6.3, we can see comparison of all three methods, the Digital filter based technique, the Direct Time Integration technique and the Recursive Convolution. Good agreement between these three methods is visible.

In Figure 6.4, a detail of the same result is depicted. Obviously, results from the digital filter technique and the recursive convolution closely copy each other.

6.3 Lorentz model

In this paragraph, we will investigate methods for analysing electromagnetic fields in dispersive media described by the Lorentz model.

6.3.1 Direct Time Integration

The relation between E and D for 1-D problem is given by the expression

$$D = \varepsilon_0 \varepsilon_\infty E + P \tag{6.94}$$

The first term in the equation (6.13) becomes then

$$\int_a^b W \frac{\partial^2 D}{\partial t^2} dz = \varepsilon_0 \varepsilon_\infty \int_a^b W \frac{\partial^2 E}{\partial t^2} dz + \int_a^b W \frac{\partial^2 P}{\partial t^2} dz \tag{6.95}$$

For the approximation of E, we use the same expression as in (6.14). For P, we define

$$P(\mathrm{x},t) = \sum_{i=0}^{M} W_i(x) p_i(t) \tag{6.96}$$

The equation (6.15) is now of the form:

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2} + (\mathbf{Q} + \mathbf{B})\frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^p \frac{\partial^2 p}{\partial t^2} + \mathbf{g} = 0 \tag{6.97}$$

Here, coefficients e and p are functions of time. New matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as follows:

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \int_a^b W_i W_j dz \tag{6.98}$$

$$T_{ij}^p = \int_a^b W_i W_j dz \tag{6.99}$$

In the case of the 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{D}}{\partial t^2}\right) dV = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{E}}{\partial t^2}\right) dV + \iiint_V \mathbf{W} \cdot \frac{\partial^2 \mathbf{P}}{\partial t^2} dV \tag{6.100}$$

For the approximation of $\mathbf{E}$, we use the same expression as in (6.33). For $\mathbf{P}$, we define:

$$\mathbf{P}(\mathbf{r},t) = \sum_{i=0}^{M} \mathbf{W}_i(\mathbf{r}) p_i(t) \tag{6.101}$$

The equation (6.34) is now of the same form as (6.42). Only the matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as follows:

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.102}$$

$$T_{ij}^p = \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.103}$$

The initial conditions can be defined for 1-D as

$$P(x,0) = 0 \quad \frac{\partial P(x,0)}{\partial t} = 0 \tag{6.104}$$

and for 3-D as

$$\mathbf{P}(\mathbf{r},0) = 0 \quad \frac{\partial \mathbf{P}(\mathbf{r},0)}{\partial t} = 0 \tag{6.105}$$

Now, we can treat the equation (6.97) in the same manner for both the dimensions.

The description of the Lorentz model is given by the differential equation which is of the form:

$$\frac{\partial^2 p}{\partial t^2} + \frac{1}{\tau}\frac{\partial p}{\partial t} + \omega_0^2 p = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_0^2 e \tag{6.106}$$

We need the second derivative of the equation (6.106) because in the equation (6.97), the second derivative of p has to be substituted:

$$\frac{\partial^2 p}{\partial t^2} = -\frac{1}{\tau}\frac{\partial p}{\partial t} - \omega_0^2 p + \varepsilon_0 \left(\varepsilon_s - \varepsilon_\infty\right)\omega_0^2 e \tag{6.107}$$

Substituting (6.107) into the equation (6.97), we obtain:

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2} + \left(\mathbf{Q}+\mathbf{B}\right)\frac{\partial e}{\partial t} + \left(\mathbf{S}+\mathbf{T}^e\right)e + \mathbf{T}^m\frac{\partial p}{\partial t} + \mathbf{T}^k p + \mathbf{g} = 0 \tag{6.108}$$

where

$$\mathbf{T}^e = \varepsilon_0 \left(\varepsilon_s - \varepsilon_\infty\right)\omega_0^2 \mathbf{T}^p \tag{6.109}$$

$$\mathbf{T}^m = -\frac{1}{\tau}\mathbf{T}^p \tag{6.110}$$

$$\mathbf{T}^k = -\omega_0^2 \mathbf{T}^p \tag{6.111}$$

Now, we have the system of ordinary differential equations (6.108) which can be solved by an appropriate time scheme.

Applying the two-step algorithm described in the Chapter 4.4, we obtain from (6.108) the following system:

$$\mathbf{T}\left(\frac{e^{n+1} - 2e^n + e^{n-1}}{\Delta t^2}\right) + \left(\mathbf{Q}+\mathbf{B}\right)\left(\frac{e^{n+1} - e^{n-1}}{2\Delta t}\right)$$
$$+ \left(\mathbf{S}+\mathbf{T}^e\right)\left(\frac{e^{n+1} + 2e^n + e^{n-1}}{4}\right) + \mathbf{T}^m\left(\frac{p^{n+1} - p^{n-1}}{2\Delta t}\right) + \mathbf{T}^k p^n + \mathbf{g}^n = 0 \tag{6.112}$$

From (6.112), we can obtain

$$\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}\left(\mathbf{Q}+\mathbf{B}\right) + \frac{1}{4}\left(\mathbf{S}+\mathbf{T}^e\right)\right)e^{n+1} = -\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\left(\mathbf{S}+\mathbf{T}^e\right)\right)e^n$$
$$-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}\left(\mathbf{Q}+\mathbf{B}\right) + \frac{1}{4}\left(\mathbf{S}+\mathbf{T}^e\right)\right)e^{n-1} \tag{6.113}$$
$$-\frac{1}{2\Delta t}\mathbf{T}^m p^{n+1} + \frac{1}{2\Delta t}\mathbf{T}^m p^{n-1} - \mathbf{T}^k p^n - \mathbf{g}^n$$

The equation (6.113) has two variables for the time step $n+1$. We substitute the coefficient p^{n+1} into (6.113) with the following expression. We use the difference method on the expression (6.106):

$$\frac{p^{n+1} - 2p^n + p^{n-1}}{\Delta t^2} = -\frac{1}{\tau}\frac{p^{n+1} - p^{n-1}}{2\Delta t} - \omega_0^2 p^n + \varepsilon_0 \left(\varepsilon_s - \varepsilon_\infty\right)\omega_0^2 e^n \tag{6.114}$$

Finally, we obtain from (6.114):

$$\left(\frac{1}{\Delta t^2}+\frac{1}{2\Delta t\tau}\right)p^{n+1}=\left[\frac{2}{\Delta t^2}-\omega_0^2\right]p^n+\left(-\frac{1}{\Delta t^2}+\frac{1}{2\Delta t\tau}\right)p^{n-1}$$
$$+\varepsilon_0\left(\varepsilon_s-\varepsilon_\infty\right)\omega_0^2 e^n$$

(6.115)

The final system of linear equations is of the form:

$$\left(\frac{1}{\Delta t^2}\mathbf{T}+\frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B})+\frac{1}{4}\left(\mathbf{S}+\mathbf{T}^e\right)\right)e^{n+1}=$$
$$-\left(\frac{-2}{\Delta t^2}\mathbf{T}+\frac{1}{2}\left(\mathbf{S}+\mathbf{T}^e\right)-\frac{C_3}{2\Delta t}\mathbf{T}^m\right)e^n$$
$$-\left(\frac{1}{\Delta t^2}\mathbf{T}-\frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B})+\frac{1}{4}\left(\mathbf{S}+\mathbf{T}^e\right)\right)e^{n-1}$$
$$+\left(\frac{1}{2\Delta t}\mathbf{T}^m-\frac{C_2}{2\Delta t}\mathbf{T}^m\right)p^{n-1}+\left(-\mathbf{T}^k-\frac{C_1}{2\Delta t}\mathbf{T}^m\right)p^n-\mathbf{g}^n$$

(6.116)

where

$$C_1=\frac{\left[\dfrac{2}{\Delta t^2}-\omega_0^2\right]}{\left(\dfrac{1}{\Delta t^2}+\dfrac{1}{2\Delta t\tau}\right)}\quad C_2=\frac{\left(-\dfrac{1}{\Delta t^2}+\dfrac{1}{2\Delta t\tau}\right)}{\left(\dfrac{1}{\Delta t^2}+\dfrac{1}{2\Delta t\tau}\right)}\quad C_3=\frac{\varepsilon_0\left(\varepsilon_s-\varepsilon_\infty\right)\omega_0^2}{\left(\dfrac{1}{\Delta t^2}+\dfrac{1}{2\Delta t\tau}\right)}$$

(6.117)

The equation (6.116) is solved in each time step. For solving p^n, we use the equation (6.115).

6.3.2 Digital filter based technique

The relation between E and D for 1-D problem in the frequency domain is given by

$$D(\omega)=\varepsilon_0\hat{\varepsilon}_r(\omega)E(\omega)$$

(6.118)

where

$$\hat{\varepsilon}_r=\varepsilon_\infty+\frac{\left(\varepsilon_s-\varepsilon_\infty\right)\omega_0^2}{\omega_0^2+j\omega\delta-\omega^2}=\varepsilon_\infty+\chi(\omega)$$

(6.119)

Without the loss of generality, we can rewrite the first part of the equation (6.13) into (6.120) because the first term on the right-hand side in (6.119) does not depend on frequency:

$$\int_a^b W\frac{\partial^2 D}{\partial t^2}dz=\varepsilon_0\varepsilon_\infty\int_a^b W\frac{\partial^2 E}{\partial t^2}dz+\varepsilon_0\int_a^b W\frac{\partial^2 D_\chi}{\partial t^2}dz$$

(6.120)

The expression for D_χ in the frequency domain is

$$D(\omega)=\chi(\omega)E(\omega)$$

(6. 121)

For the approximation of $\mathbf{E}$, we use the same expression as in (6.14). For D_χ, we define:

$$D_\chi(x,t) = \sum_{i=0}^{M} W_i(x) d_{\chi i}(t) \tag{6.122}$$

The equation (6.15) is of the form now

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2} + (\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^d\frac{\partial^2 d_\chi}{\partial t^2} + \mathbf{g} = 0 \tag{6.123}$$

where

$$T_{ij} = \varepsilon_0\varepsilon_\infty \int_a^b W_i W_j dz \tag{6.124}$$

$$T_{ij}^d = \varepsilon_0 \int_a^b W_i W_j dz \tag{6.125}$$

In the case of the 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W}\cdot\left(\frac{\partial^2 \mathbf{D}}{\partial t^2}\right)dV = \varepsilon_0\varepsilon_\infty \iiint_V \mathbf{W}\cdot\left(\frac{\partial^2 \mathbf{E}}{\partial t^2}\right)dV + \varepsilon_0 \iiint_V \mathbf{W}\cdot\frac{\partial^2 \mathbf{D}_\chi}{\partial t^2}dV \tag{6.126}$$

The equation (6.34) is now of the same form as (6.82). Only the matrices $\mathbf{T}$ and $\mathbf{T}^d$ are defined as

$$T_{ij} = \varepsilon_0\varepsilon_\infty \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.127}$$

$$T_{ij}^c = \varepsilon_0 \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.128}$$

Now, we have the system of ordinary differential equations (6.64) which can be solved by an appropriate time scheme.

Applying the two-step algorithm described in the Chapter 4.4, we obtain from (6.82) the system

$$\mathbf{T}\left(\frac{e^{n+1}-2e^n+e^{n-1}}{\Delta t^2}\right) + (\mathbf{Q}+\mathbf{B})\left(\frac{e^{n+1}-e^{n-1}}{2\Delta t}\right) + \mathbf{S}\left(\frac{e^n+2e^n+e^n}{4}\right)$$
$$+\mathbf{T}^d\left(\frac{d_\chi^{n+1}-2d_\chi^n+d_\chi^{n-1}}{\Delta t^2}\right) + \mathbf{g}^n = 0 \tag{6.129}$$

As mentioned in the Chapter 5.7.2, we use the expression

$$d_\chi^{n+1} = -\frac{C_2}{C_1}d_\chi^n - \frac{C_3}{C_1}d_\chi^{n-1} + \frac{\Delta\varepsilon\omega_0^2}{C_1}e^{n+1} + \frac{2\Delta\varepsilon\omega_0^2}{C_1}e^n + \frac{\Delta\varepsilon\omega_0^2}{C_1}e^{n-1} \tag{6.130}$$

where

$$C_1 = \omega_0^2 + \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{6. 131}$$

$$C_2 = 2\omega_0^2 - \frac{8}{\Delta t^2} \tag{6. 132}$$

$$C_3 = \omega_0^2 - \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \tag{6. 133}$$

The equation (6.129) can be rewritten into the final system of linear equations after using the substitution (6.130):

$$
\begin{aligned}
\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{\Delta\varepsilon\omega_0^2}{\Delta t^2 C_1}\mathbf{T}^d \right)e^{n+1} = \\
-\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\mathbf{S} + \frac{2\Delta\varepsilon\omega_0^2}{\Delta t^2 C_1}\mathbf{T}^d \right)e^{n} \\
-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{\Delta\varepsilon\omega_0^2}{\Delta t^2 C_1}\mathbf{T}^d \right)e^{n-1} \\
+\left(\frac{C_2}{C_1} + 2 \right)\frac{1}{\Delta t^2}\mathbf{T}^d d_\chi^n - \left(1 - \frac{C_3}{C_1} \right)\frac{1}{\Delta t^2}\mathbf{T}^d d_\chi^{n-1} - \mathbf{g}^n
\end{aligned}
\tag{6.134}
$$

This equation is solved in each time step. For obtaining d_χ^n and d_χ^{n-1}, we use the equation (6.130).

6.3.3 Comparison and verification of methods

In order to verify our methods for the Lorentz model, we consider a problem including the following medium with parameters $\varepsilon_s = 2.25$, $\varepsilon_\infty = 1.0$, $\delta = 5.599 \times 10^{15}$ rad/s and $\omega_0 = 4 \times 10^{16}$ [52]. The medium is irradiated from vacuum by 12 cycles of a sine wave with the carrier frequency at 1.5 PHz. A time trace of the electric field at a depth of 0.01 mm was recorded. We compare both two developed methods. We investigated the Direct Time Integration technique and the method based on digital filtering. Figure 6.5 shows results from both methods. Obviously, the calculated results agree very well with each other.

In another simulation, we consider a metallic sphere coated with the Lorentz medium with parameters $\varepsilon_s = 4.0$, $\varepsilon_\infty = 1.0$, $\omega_0 = 2\delta = 50$ Mrad/s. The metallic sphere has a radius of 0.8 m and the coating has a thickness of 0.2 m [48]. Figure 6.6 shows results for the electric field as a function of time. The results of the Direct Time Integration technique and the method based on digital filtering are compared with the exact solution from [48]. Good agreement between these three methods is visible.
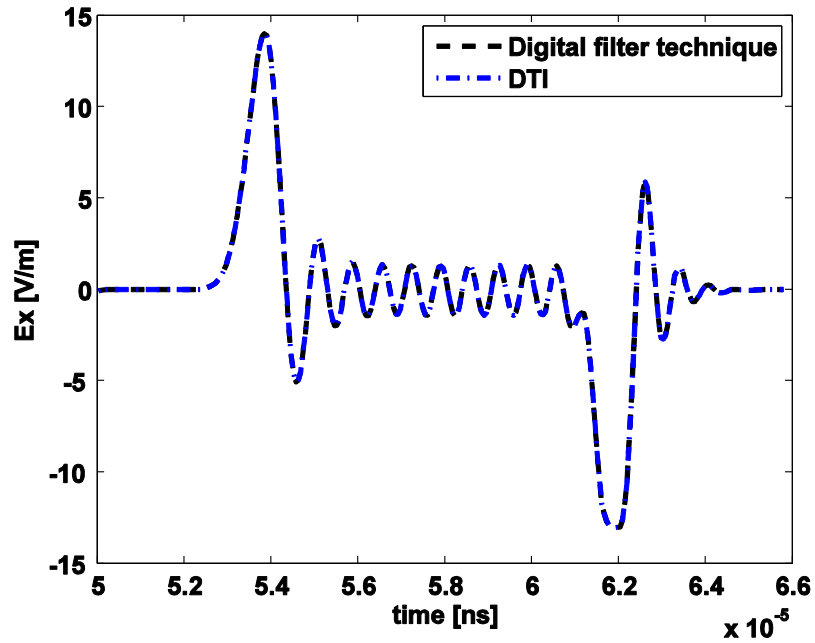
Fig. 6.5: Time response of the electric field intensity at the depth of 0.01 mm in the Lorentz model of the dispersive medium irradiated from free space.

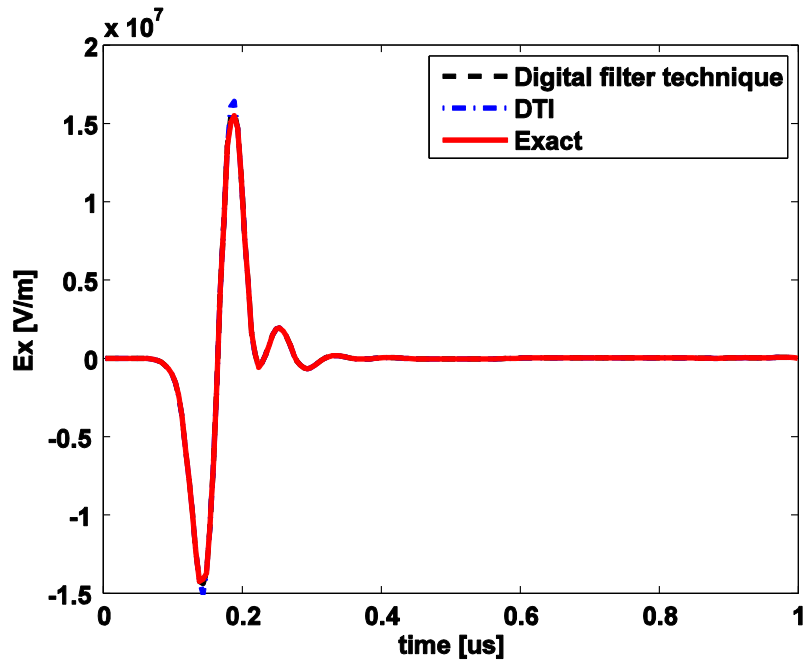**Fig. 6.6:** Time response of the electric field intensity in a Lorentz model of the dispersive coat of a metallic sphere irradiated from free space.

6.4 Drude model

In this paragraph, we investigate methods for the analysis of electromagnetic waves in a dispersive medium described by the Drude model.

6.4.1 Direct Time Integration

The relation between E and D for 1-D problem is given by the expression:

$$D = \varepsilon_0 \varepsilon_\infty E + P \tag{6.135}$$

The first part in the equation (6.13) then becomes

$$\int_a^b W \frac{\partial^2 D}{\partial t^2} dz = \varepsilon_0 \varepsilon_\infty \int_a^b W \frac{\partial^2 E}{\partial t^2} dz + \int_a^b W \frac{\partial^2 P}{\partial t^2} dz \tag{6.136}$$

For the approximation of E, we use the same expression as in (6.14). For P, we define:

$$P(x,t) = \sum_{i=0}^{M} W_i(x) p_i(t) \tag{6.137}$$

The equation (6.15) is now of the form

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2} + (\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^p \frac{\partial^2 p}{\partial t^2} + \mathbf{g} = 0 \tag{6.138}$$

Here, coefficients e and p are functions of time. New matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \int_a^b W_i W_j dz \tag{6.139}$$

$$T_{ij}^p = \int_a^b W_i W_j dz \tag{6.140}$$

In the case of the 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{D}}{\partial t^2} \right) dV = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{E}}{\partial t^2} \right) dV + \iiint_V \mathbf{W} \cdot \frac{\partial^2 \mathbf{P}}{\partial t^2} dV \tag{6.141}$$

For the approximation of $\mathbf{E}$, we use the same expression as in (6.33). For $\mathbf{P}$, we define:

$$\mathbf{P}(\mathbf{r},t) = \sum_{i=0}^{M} \mathbf{W}_i(\mathbf{r}) p_i(t) \tag{6.142}$$

The equation (6.34) is now of the same form as (6.138). Only matrices $\mathbf{T}$ and $\mathbf{T}^p$ are defined as

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.143}$$

$$T_{ij}^p = \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.144}$$

The initial conditions can be defined for 1-D as

$$P(x,0) = 0 \quad \frac{\partial P(x,0)}{\partial t} = 0 \tag{6.145}$$

and for 3-D as

$$\mathbf{P}(\mathbf{r},0)=0 \qquad \frac{\partial \mathbf{P}(\mathbf{r},0)}{\partial t}=0 \qquad (6.146)$$

Now we can treat the equation (6.138) in the same manner for both dimensions.

The description of the Drude model is given by the differential equation which is of the form:

$$\frac{\partial^2 p}{\partial t^2}+\frac{1}{\tau}\frac{\partial p}{\partial t}=\varepsilon_0\omega_p^2 e \qquad (6.147)$$

We need the second derivative of the equation (6.106) since the equation (6.138) contains the second derivative of p:

$$\frac{\partial^2 p}{\partial t^2}=-\frac{1}{\tau}\frac{\partial p}{\partial t}+\varepsilon_0\omega_p^2 e \qquad (6.148)$$

After substitution of (6.148) into the equation (6.138), we obtain:

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2}+(\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t}+(\mathbf{S}+\mathbf{T}^e)e+\mathbf{T}^m\frac{\partial p}{\partial t}+\mathbf{g}=0 \qquad (6.149)$$

where

$$\mathbf{T}^e=\varepsilon_0\omega_0^2\mathbf{T}^p \qquad (6.150)$$

$$\mathbf{T}^m=-\frac{1}{\tau}\mathbf{T}^p \qquad (6.151)$$

Now, we have the system of ordinary differential equations (6.149) which can be solved by an appropriate time scheme.

Applying the two-step algorithm described in the Chapter 4.4, we obtain from (6.149) the system

$$\mathbf{T}\left(\frac{e^{n+1}-2e^n+e^{n-1}}{\Delta t^2}\right)+(\mathbf{Q}+\mathbf{B})\left(\frac{e^{n+1}-e^{n-1}}{2\Delta t}\right)$$
$$+(\mathbf{S}+\mathbf{T}^e)\left(\frac{e^{n+1}+2e^n+e^{n-1}}{4}\right)+\mathbf{T}^m\left(\frac{p^{n+1}-p^{n-1}}{2\Delta t}\right)+\mathbf{g}^n=0 \qquad (6.152)$$

From (6.152), we can obtain

$$\left(\frac{1}{\Delta t^2}\mathbf{T}+\frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B})+\frac{1}{4}(\mathbf{S}+\mathbf{T}^e)\right)e^{n+1}=-\left(\frac{-2}{\Delta t^2}\mathbf{T}+\frac{1}{2}(\mathbf{S}+\mathbf{T}^e)\right)e^n$$
$$-\left(\frac{1}{\Delta t^2}\mathbf{T}-\frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B})+\frac{1}{4}(\mathbf{S}+\mathbf{T}^e)\right)e^{n-1} \qquad (6.153)$$
$$-\frac{1}{2\Delta t}\mathbf{T}^m p^{n+1}+\frac{1}{2\Delta t}\mathbf{T}^m p^{n-1}-\mathbf{g}^n$$

The equation (6.153) has two variables for the time step $n+1$. We substitute the coefficient p^{n+1} into (6.153) with the following expression. We apply the difference method on the expression (6.148):

$$\frac{p^{n+1} - 2p^n + p^{n-1}}{\Delta t^2} = -\frac{1}{\tau}\frac{p^{n+1} - p^{n-1}}{2\Delta t} + \omega_0^2 e^n \tag{6.154}$$

We obtain from (6.154)

$$\left(\frac{1}{\Delta t^2} + \frac{1}{2\Delta t\tau}\right)p^{n+1} = \frac{2}{\Delta t^2}p^n + \left(-\frac{1}{\Delta t^2} + \frac{1}{2\Delta t\tau}\right)p^{n-1} + \omega_0^2 e^n \tag{6.155}$$

The final system of linear equations is of the form

$$\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}(\mathbf{S}+\mathbf{T}^e)\right)e^{n+1} =$$

$$-\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}(\mathbf{S}+\mathbf{T}^e) - \frac{C_3}{2\Delta t}\mathbf{T}^m\right)e^n$$

$$-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}(\mathbf{S}+\mathbf{T}^e)\right)e^{n-1}$$

$$+\left(\frac{1}{2\Delta t}\mathbf{T}^m - \frac{C_2}{2\Delta t}\mathbf{T}^m\right)p^{n-1} - \frac{C_1}{2\Delta t}\mathbf{T}^m p^n - \mathbf{g}^n \tag{6.156}$$

where

$$C_1 = \frac{\dfrac{2}{\Delta t^2}}{\left(\dfrac{1}{\Delta t^2} + \dfrac{1}{2\Delta t\tau}\right)} \quad C_2 = \frac{\left(-\dfrac{1}{\Delta t^2} + \dfrac{1}{2\Delta t\tau}\right)}{\left(\dfrac{1}{\Delta t^2} + \dfrac{1}{2\Delta t\tau}\right)} \quad C_3 = \frac{\omega_0^2}{\left(\dfrac{1}{\Delta t^2} + \dfrac{1}{2\Delta t\tau}\right)} \tag{6.157}$$

This equation (6.156) is solved in each time step. For solving p^n, we use the equation (6.155).

6.4.2 Digital filter based technique

The relation between E and D for 1-D problem in the frequency domain is given by

$$D(\omega) = \varepsilon_0 \hat{\varepsilon}_r(\omega)E(\omega) \tag{6.158}$$

where

$$\hat{\varepsilon}_r = \varepsilon_\infty + \frac{\omega_p^2}{j\omega\delta - \omega^2} = \varepsilon_\infty + \chi(\omega) \tag{6.159}$$

Without losing the generality, we can rewrite the first part of the equation (6.13) into (6.160) because the first term on the right-hand side in (6.159) does not depend on frequency:

$$\int_a^b W\frac{\partial^2 D}{\partial t^2}dz = \varepsilon_0\varepsilon_\infty\int_a^b W\frac{\partial^2 E}{\partial t^2}dz + \varepsilon_0\int_a^b W\frac{\partial^2 D_\chi}{\partial t^2}dz \tag{6.160}$$

The expression for D_χ in the frequency domain is

$$D(\omega) = \chi(\omega) E(\omega) \tag{6.161}$$

Approximating E, we use the same expression as in (6.14). For D_χ, we define:

$$D_\chi(x,t) = \sum_{i=0}^{M} W_i(x) d_{\chi i}(t) \tag{6.162}$$

The equation (6.15) is now of the form

$$\mathbf{T}\frac{\partial^2 e}{\partial t^2} + (\mathbf{Q}+\mathbf{B})\frac{\partial e}{\partial t} + \mathbf{S}e + \mathbf{T}^d \frac{\partial^2 d_\chi}{\partial t^2} + \mathbf{g} = 0 \tag{6.163}$$

where

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \int_a^b W_i W_j dz \tag{6.164}$$

$$T_{ij}^d = \varepsilon_0 \int_a^b W_i W_j dz \tag{6.165}$$

In the case of the 3-D problem, the first part in the equation (6.32) becomes

$$\iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{D}}{\partial t^2}\right) dV = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W} \cdot \left(\frac{\partial^2 \mathbf{E}}{\partial t^2}\right) dV + \varepsilon_0 \iiint_V \mathbf{W} \cdot \frac{\partial^2 \mathbf{D}_\chi}{\partial t^2} dV \tag{6.166}$$

The equation (6.34) is now of the same form as (6.163). Only matrices $\mathbf{T}$ and $\mathbf{T}^d$ are defined as

$$T_{ij} = \varepsilon_0 \varepsilon_\infty \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.167}$$

$$T_{ij}^c = \varepsilon_0 \iiint_V \mathbf{W}_i \cdot \mathbf{W}_j dV \tag{6.168}$$

Now we have the system of ordinary differential equations (6.163) which can be solved by an appropriate time scheme.

Applying the two-step algorithm described in the Chapter 4.4, we obtain from (6.163) the system

$$\mathbf{T}\left(\frac{e^{n+1} - 2e^n + e^{n-1}}{\Delta t^2}\right) + (\mathbf{Q}+\mathbf{B})\left(\frac{e^{n+1} - e^{n-1}}{2\Delta t}\right) + \mathbf{S}\left(\frac{e^n + 2e^n + e^n}{4}\right)$$
$$+ \mathbf{T}^d\left(\frac{d_\chi^{n+1} - 2d_\chi^n + d_\chi^{n-1}}{\Delta t^2}\right) + \mathbf{g}^n = 0 \tag{6.169}$$

As mentioned in the Chapter 5.7.3, we use the expression

$$d_\chi^{n+1} = -\frac{C_2}{C_1} d_\chi^n - \frac{C_3}{C_1} d_\chi^{n-1} + \frac{\omega_p^2}{C_1} e^{n+1} + \frac{2\omega_p^2}{C_1} e^n + \frac{\omega_p^2}{C_1} e^{n-1} \tag{6.170}$$

where

$$C_1 = \frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \qquad (6.\,171)$$

$$C_2 = -\frac{8}{\Delta t^2} \qquad (6.\,172)$$

$$C_3 = -\frac{2}{\Delta t}\delta + \frac{4}{\Delta t^2} \qquad (6.\,173)$$

The equation (6.169) can be rewritten into the final system of linear equations after using the substitution (6.170)

$$
\begin{aligned}
\left(\frac{1}{\Delta t^2}\mathbf{T} + \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{\omega_p^2}{\Delta t^2 C_1}\mathbf{T}^d \right) e^{n+1} = \\
-\left(\frac{-2}{\Delta t^2}\mathbf{T} + \frac{1}{2}\mathbf{S} + \frac{2\omega_p^2}{\Delta t^2 C_1}\mathbf{T}^d \right) e^{n} \\
-\left(\frac{1}{\Delta t^2}\mathbf{T} - \frac{1}{2\Delta t}(\mathbf{Q}+\mathbf{B}) + \frac{1}{4}\mathbf{S} + \frac{\omega_p^2}{\Delta t^2 C_1}\mathbf{T}^d \right) e^{n-1} \\
+\left(\frac{C_2}{C_1}+2 \right)\frac{1}{\Delta t^2}\mathbf{T}^d d_\chi^n - \left(1 - \frac{C_3}{C_1} \right)\frac{1}{\Delta t^2}\mathbf{T}^d d_\chi^{n-1} - \mathbf{g}^n
\end{aligned}
\qquad (6.174)
$$

This equation is solved in each time step. For obtaining d_χ^n and d_χ^{n-1}, we use the equation (6.170).

6.4.3 Comparison of methods

In order to verify the developed methods for the Drude model, we consider an example described in [48]. The model has a metallic sphere coated with the layer of following parameters $\omega_p = \delta = 50\,\mathrm{Mrad/s}$. The metallic sphere has a radius of 0.8 m and the coating has a thickness of 0.2 m. This coated sphere is illuminated by an *x*-polarized incident plane wave propagating along the *z*-direction. The results of the Direct Time Integration technique and the Digital filter technique are compared with the exact solution [48]. Figure 6.7 shows the comparison of results. A good agreement between the developed methods and methods from the referenced paper is visible.
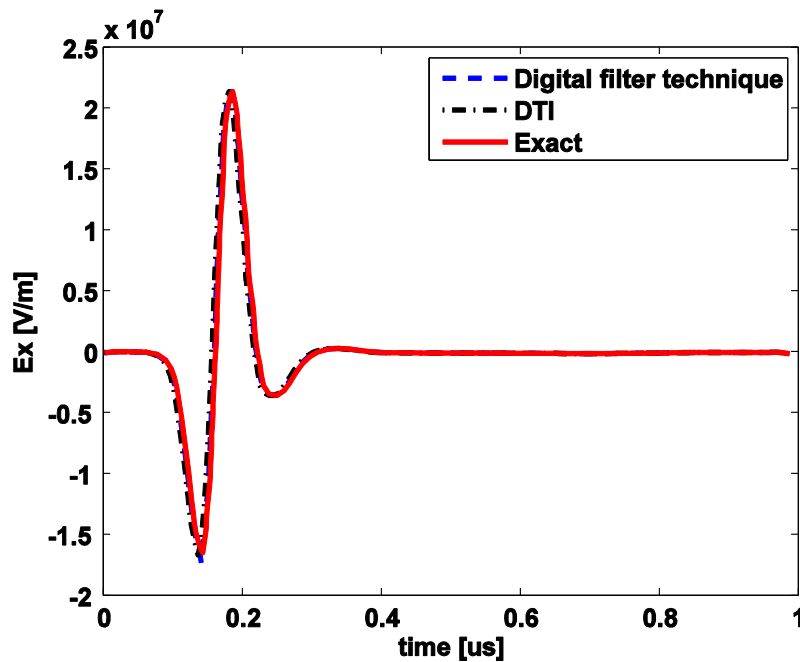
Fig. 6.7: Time response of the electric field intensity in the Drude model of the dispersive coating of the metallic sphere illuminated in the free space.

6.5 Conclusion

We employed finite element time domain method for solving initial-boundary value problems including dispersive models. We investigated all methods proposed in Chapter 5. Since the Debye model is the simplest dispersive model, we analyzed electromagnetic fields in this model with all the methods. For the Lorentz model and the Drude model, we employed Direct time integration technique and Digital filter based method. The obtained results verify the ability of these developed and improved methods. These methods are suitable to be employed for solving electromagnetic problems. Another improvement of these methods is possible.

The new method based on the digital filtering seems to work perfectly. Investigation of the behavior with a higher order of time approximation can improve results. The methods can be used for the solution of other dispersive models or multi-pole problems.

A possible method for analyzing fields in dispersive media can be created by the combination of transformation techniques and the generalized two-step method. Inverse problems including a dispersive material with the combination of optimization techniques can be investigated.

Other recommendation is dealing with an anisotropic material and a dispersive medium. The developed method based on the digital filtering can be used for employing Perfectly Matched Layer (PML) into the FETD method due to dispersive layers.

7 CONCLUSIONS

In the thesis, we developed and improved methods for analyzing electromagnetic field in dispersive media by the finite element time domain method (FETD).

We briefly introduced the project HIRF-SE and the tool BUTFE which gave us the motivation for analyzing fields in dispersive models by FETD method since this issue has not been sufficiently investigated yet.

We developed an approach for the FETD method which is suitable for employing dispersive models for analyzing fields in dispersive media. We introduced a general two-step approach for the time scheme and compared the most appropriate schemes for FETD. We published the results of this comparison at the conference [68].

In the main part, we described three methods for solving fields in dispersive models such as the Debye model, the Lorentz model and the Drude model. The first method of field analysis in Debye dispersive environments is based on the *Recursive convolution*. The second method of the field analysis for all three models in dispersive environments is based on the *Direct Time Integration* technique. A novel approach which exploits principles of digital filtering techniques was presented. This method was published at the conference [81].

We employed the finite element time domain method for solving initial-boundary value problems including dispersive models. We developed mathematical models for 1-D and 3-D problems. We employed all proposed methods on these models and described in detail to the way of analysis. The obtained results verified the functionality of these developed and improved methods. These methods are suitable to be employed for solving electromagnetic problems. We described the approach for dealing with this problem for our newly developed method in article [84]. We compared all the methods and discussed the results. Another improvement of these methods was discussed.

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