

ON THE FINITE-DIFFERENCE MODELLING OF ELECTROMAGNETIC PROBLEMS IN STRUCTURED LATTICES

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Abstract

The thesis concentrates on the numerical analysis of electromagnetic fields with the finite difference method. Simple and fast approximative techniques are studied and developed for the estimation of the electromagnetic properties of various structures. Especially, techniques which preserve the simplicity of a structured lattice are explored. The emphasis in the thesis is put more into the rapid estimations than into the absolute accuracy of the studied parameters. Another goal is to give information about the characteristics of the studied structures: filters, dielectric mixtures and frequency selective surfaces.

Filter structures are analysed with the finite-difference time-domain method. A simple trick is introduced to transform the curved shapes in a certain practical filter configuration into rectangular shapes to conform to the finite-difference computation lattice.

Procedures which use finite difference methods to analyse dielectric mixtures are introduced. They are applied to calculate effective permittivities of two-phase random mixtures. The results are compared with theoretical mixing models with a conclusion that none of them agrees with the numerical results in the whole range of volume fraction. Therefore, a new empirical mixing model is created based on the numerical results.

Polarisation transformation properties of frequency selective surfaces are also studied and some wide-band polariser structures are presented. It is shown how one-dimensional array models can give a good starting point for a two-dimensional array design.

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Alkusanat

Tämän väitöskirjan tutkimustyö tehtiin Sähkömagnetiikan laboratoriossa Teknillisessä korkeakoulussa vuodesta 1998 vuoteen 2002. Kiitän Sovelletun sähkömagnetiikan tutkijakoulua, Elektroniikkainsinöörien säätiötä, Tekniikan edistämissäätiötä, Jenny ja Antti Wihurin rahastoa ja Emil Aaltosen säätiötä jatko-opintojeni rahoituksesta.

Kaikki opettajani ansaitsevat suuren kiitoksen. Erityisesti haluan kiittää Prof. Keijo Nikoskista ja Prof. Ari Sihvolaa, jotka ovat tarjonneet minulle mahdollisuuden tehdä kiinnostavaksi kokemaani tutkimusta. Suuret kiitokset Juha Juntuselle ja Sami Ilvoselle jakamastaan tietoteknisestä osaamisesta. Kiitokset koko Sähkömagnetiikan laboratorion henkilökunnalle.

Syksystä 2000 syksyyn 2001 työskentelin Sovelletun sähkömagnetiikan ryhmässä Victorian yliopistossa Kanadassa vierailevana tutkijana. Lämpimät kiitokset Prof. Maria Stuchlylle tästä hienosta kokemuksesta.

Kiitos perheelleni tuesta ja avusta.

Kiitos Tuija, kun olet rinnallani kulkenut.

Foreword

The research for this thesis was made at the Electromagnetics Laboratory of the Helsinki University of Technology from 1998 to 2002. I wish to thank The Graduate School of Applied Electromagnetics, The Finnish Society of Electronics Engineers, Tekniikan edistämissäätiö, Jenny ja Antti Wihurin rahasto and Emil Aaltosen Säätiö for the funding.

I would like to thank all the teachers I have had. Special thanks to Prof. Keijo Nikoskinen and Prof. Ari Sihvola who offered the opportunity to do the research I was interested in. Thanks to Juha Juntunen and Sami Ilvonen for the computer support. Thanks to coauthors and all the people in the Electromagnetics Laboratory .

From the fall of 2000 I worked one year as a visiting scientist in the Applied Electromagnetics Group of the University of Victoria, Canada. Warm thanks to Prof. Maria Stuchly who gave the chance to the great experience.

Thanks to my family for the loving support.

Thank you Tuija for meeting the adventures of life with me.

List of Publications

- [P1] K. Kärkkäinen, K. Nikoskinen, “Rapid FDTD simulation of filter structures involving cylindrical shapes”, *1998 Asia-Pacific Microwave Conference Proceedings*, Yokohama, Japan, Vol. 2, pp. 797–800, 1998.
- [P2] O. Pekonen, K. Kärkkäinen, A. Sihvola, K. Nikoskinen, “Numerical testing of dielectric mixing rules by FDTD method”, *Journal of Electromagnetic Waves and Applications*, Vol. 13, pp. 67–87, 1999.
- [P3] K. Kärkkäinen, A. Sihvola, K. Nikoskinen, “Effective permittivity of mixtures: numerical validation by the FDTD method”, *IEEE Transactions on Geoscience and Remote Sensing*, Vol. 38, No. 3, pp. 1303–1308, May 2000.
- [P4] K. Kärkkäinen, A. Sihvola, K. Nikoskinen, “Analysis of a three-dimensional mixture with finite difference method”, *IEEE Transactions on Geoscience and Remote Sensing*, Vol. 39, No. 5, pp. 1013–1018, May 2001.
- [P5] K. Kärkkäinen, M. Stuchly, “Frequency selective surface as a polarisation transformer”, *accepted for publication in IEE Proceedings - Microwaves, Antennas and Propagation*
- [P6] K. Kärkkäinen, “Field dependent local effective permittivity for the finite difference analysis of arbitrary dielectric interfaces”, *Electromagnetics Laboratory Report Series*, Report 398, Espoo, Sep. 2002, also submitted for publication in *IEEE Transactions on Antennas and Propagation*.

The papers [P1, P3, P4, P5] were mainly done by the author. All the required computer codes for the finite-difference modelling were implemented and the simulations were carried out by the author. Professors Ari Sihvola, Keijo Nikoskinen and Maria Stuchly contributed as advisors during the research.

In [P2] Professors Ari Sihvola and Keijo Nikoskinen presented the original idea of calculating effective permittivities with the FDTD method. The first and the second author prepared the simulation program and calculated the results in co-operation.

[P6] was done by the author.

In all the papers the first author was mainly responsible for the manuscript.

1 Introduction

In electromagnetics, like in many fields of physics, the behaviour of nature is predicted using partial differential equations. In 1864 James Clerk Maxwell introduced the equations that are applied still today. In fact, electromagnetics means the science of Maxwell's equations in many contexts. The equations are¹

$$\nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B} \quad (1)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial}{\partial t}\mathbf{D} \quad (2)$$

$$\nabla \cdot \mathbf{D} = \rho \quad (3)$$

$$\nabla \cdot \mathbf{B} = 0. \quad (4)$$

The electric flux \mathbf{D} , the electric field \mathbf{E} , the magnetic flux \mathbf{B} , the magnetic field \mathbf{H} and the current density \mathbf{J} are dependent on place and time and they are connected through the constitutive equations

$$\mathbf{D} = \epsilon\mathbf{E} \quad (5)$$

$$\mathbf{B} = \mu\mathbf{H} \quad (6)$$

$$\mathbf{J} = \sigma\mathbf{E} \quad (7)$$

where μ , ϵ and σ stand for the material permeability, permittivity and conductivity, respectively. Equations (5)–(7) hold for an isotropic material. More general relations are also possible to describe anisotropic and chiral materials [1].

The equations (1)–(7) can be combined to get a system of equations for the Cartesian field components as

$$\mu \frac{\partial}{\partial t} H_x = \frac{\partial}{\partial z} E_y - \frac{\partial}{\partial y} E_z \quad (8)$$

$$\mu \frac{\partial}{\partial t} H_y = \frac{\partial}{\partial x} E_z - \frac{\partial}{\partial z} E_x \quad (9)$$

$$\mu \frac{\partial}{\partial t} H_z = \frac{\partial}{\partial y} E_x - \frac{\partial}{\partial x} E_y \quad (10)$$

$$\epsilon \frac{\partial}{\partial t} E_x = \frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y - \sigma E_x \quad (11)$$

$$\epsilon \frac{\partial}{\partial t} E_y = \frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z - \sigma E_y \quad (12)$$

$$\epsilon \frac{\partial}{\partial t} E_z = \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x - \sigma E_z. \quad (13)$$

The equations connect the components of the electric (E) and the magnetic (H) fields. The time derivative of the magnetic field depends on the spatial

¹The original system of 20 equations was simplified to this modern notation by Oliver Heaviside.

derivative of the electric field, and vice versa. Generally a closed-form solution of these equations for a complex geometry is impossible to find. Therefore, many approximative techniques have been developed to analyse the structures of interest. Especially, the birth of computers gave scientists new means to model partial differential equations. Among the simplest numerical techniques is the finite difference method (FD). In this thesis, the effort was made for trying to understand the characteristics of the finite difference method when applied in electromagnetics. Another target was to determine various characteristics of certain simulated structures (filters, mixtures and frequency selective surfaces). The geometries of the studied structures enforced to explore new algorithms to describe arbitrary material interfaces. The goal was to develop techniques which on the one hand can be easily implemented in numerical algorithms and which on the other hand preserve the simplicity of the FD method.

The structure of this overview of the thesis is as follows: The next section gives an overview of the most frequently applied numerical methods in electromagnetics. The basics of finite differences in static field problems are revisited and the fundamental problem of modelling the material interface is considered through a one-dimensional example in Section 3. Section 4 gives a short review to the finite differences in time domain (FDTD). Finally, the application area of material mixtures is introduced in Section 5.

2 Brief overview of numerical electromagnetics

The most popular methods in electromagnetic field analysis include the method of moments (MOM), the finite element method (FEM), the boundary element method (BEM) and the finite difference method (FD) [2, 3, 4, 5]. MOM can be considered as a very general concept which includes both FEM and BEM [5, 6], and it can be used to solve both differential and integral equations. However, generally in electromagnetics literature the MOM is referred as a method to solve an integral equation formulation of the field problem and thus it can be understood as a means to numerically solve induced sources on the structure. For example, in electrostatics the charge distribution could be approximated as a sum of point charges whose amplitudes can be obtained by the MOM algorithm.

MOM, FEM and BEM are projection methods in which an approximate solution for the studied problem is sought as a sum of basis functions i.e. the exact solution is projected to the chosen function space. This leads to a matrix equation and to the problem of finding the inverse of the matrix. As an integral equation method the MOM is powerful especially in the open field problems because the surroundings of the structure do not have to be discretised. It means that the inverted matrix is typically small. The BEM was developed to offer a procedure for the discretisation of boundary-integral equations. Boundaries of the problem are divided into finite elements in a FEM fashion.

FEM is used to solve differential equations and hence it requires the discretisation of the entire problem domain. Therefore, the matrix that has to be inverted is big. On the other hand, because the basis functions are functions

differing from zero only in chosen subdomains, the matrix is also sparse. The strength of the FEM is the ability to model complex-shaped and inhomogeneous structures. Subdomains or elements can be chosen to closely conform the original geometry of material boundaries.

The FD method differs clearly from the above mentioned methods. It is based on the straight discretisation of differential equations. The differentials are replaced by finite differences. Usually the difference approximations are determined using Taylor series. In the simplest form the solution is approximated in a uniform rectangular lattice of discrete points. The advantage of the FD method is the simplicity to model complex materials. Additionally, it can be easily applied for the time-domain analysis (FDTD) as contrary to FEM, MOM and BEM which are essentially frequency-domain methods. The drawback of the FD method is the difficulty to model geometries of arbitrary shapes. For example curved surfaces cannot be accurately described in the rectangular lattice. In this thesis attention is paid to deal with this problem especially in case of dielectric interfaces.

3 Finite differences

The derivative of a function $f(x)$ at point x_0 is

$$\frac{\partial}{\partial x} f(x)|_{x=x_0} = \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h}. \quad (14)$$

Hence, the derivative means the change of a function value with relation to its argument. In the FD method the derivatives are approximated locally by finite difference quotients ($h > 0$) instead of a limit. For example,

$$\frac{\partial}{\partial x} f(x)|_{x=x_0} \approx \frac{f(x_0 + h) - f(x_0)}{h} \quad (15)$$

is called the forward difference. The backward difference would read

$$\frac{\partial}{\partial x} f(x)|_{x=x_0} \approx \frac{f(x_0) - f(x_0 - h)}{h}. \quad (16)$$

In other words, the finite differences estimate the local derivative by calculating the total change of a function value within the interval h . Figure 1 illustrates the approximations.

At a glance we can find the forward and backward difference approximations not to be very accurate i.e. dashed lines are not parallel with the tangential of the curve. In this example case the value of h should be reduced in order to get better accuracy. While looking at Figure 1 imagine the situation in which h becomes smaller and the dashed line approaches the solid line and finally they coincide as h goes to zero. The smaller the distance h the better the accuracy. If we take the average of the forward and backward differences we get the central

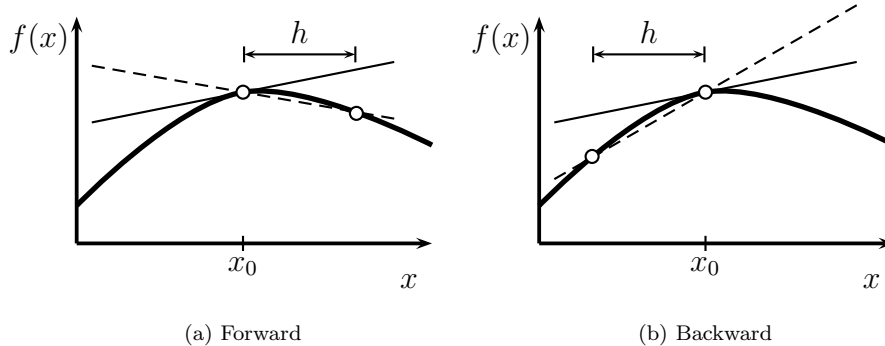


Figure 1: Difference approximations

difference formula

$$\frac{\partial}{\partial x} f(x)|_{x=x_0} \approx \frac{1}{2} \left[\frac{f(x_0+h) - f(x_0)}{h} + \frac{f(x_0) - f(x_0-h)}{h} \right] \quad (17)$$

$$= \frac{f(x_0+h) - f(x_0-h)}{2h} \quad (18)$$

Figure 2 shows the geometrical illustration of the central difference. The dashed line is almost parallel with the solid line i.e. the approximation is very accurate even with the twice bigger lattice constant ($2h$) than in case of forward and backward differences.

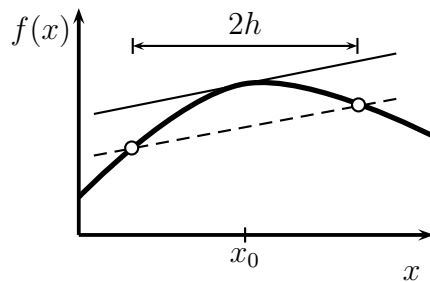


Figure 2: The central difference

The central difference is said to be second order accurate. In other words, it can calculate exactly the derivatives of polynomials up to second degree. This can be proved by analysing an arbitrary third order polynomial

$$f(x) = ax^3 + bx^2 + cx + d \quad (19)$$

The derivative of the polynomial in an arbitrary point x_0 is

$$f'(x_0) = 3ax_0^2 + 2bx_0 + c \quad (20)$$

The central difference approximation at the same point is

$$\begin{aligned} f'(x_0) &\approx \frac{f(x_0 + h) - f(x_0 - h)}{2h} \\ &= \frac{a(x_0 + h)^3 + b(x_0 + h)^2 + c(x_0 + h) + d}{2h} \\ &\quad - \frac{a(x_0 - h)^3 + b(x_0 - h)^2 + c(x_0 - h) + d}{2h} \\ &= 3ax_0^2 + 2bx_0 + c + ah^2 \end{aligned} \quad (21)$$

The approximation approaches the exact value when h becomes smaller. However, we can notice that if $a = 0$ the difference approximation is exact for all values of h . This corresponds to the quadratic polynomial.

It is also possible to approximate higher derivatives with the finite differences [7, 8]. For example the central difference approximation of the second derivative is

$$\frac{\partial^2}{\partial x^2} f(x)|_{x=x_0} \approx \frac{\frac{f(x_0+h)-f(x_0)}{h} - \frac{f(x_0)-f(x_0-h)}{h}}{h} \quad (22)$$

$$= \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} \quad (23)$$

3.1 1D example

Let us consider a parallel plate condenser which has infinite size of plates. One of the plates is set to the potential of 0 volts and the other plate to the potential of 1 volt. The insulator consists of two different dielectrics as shown in Figure 3 and the total thickness is one meter. Material interface is parallel with the plates.

In electrostatics the governing equation is the Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi) = \rho \quad (24)$$

in which ϕ is the electric potential and ρ is the charge density. Equation (24) is written in rectangular coordinate system as

$$\frac{\partial}{\partial x} \left(\epsilon \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon \frac{\partial \phi}{\partial z} \right) = \rho. \quad (25)$$

In this example the geometry varies only in one coordinate direction. Let us choose it to be the x -direction. Therefore, the differentials in y - and z - directions are zero. In insulator medium there are no free charges and (25) becomes

$$\frac{\partial}{\partial x} \left(\epsilon \frac{\partial \phi}{\partial x} \right) = 0 \quad (26)$$

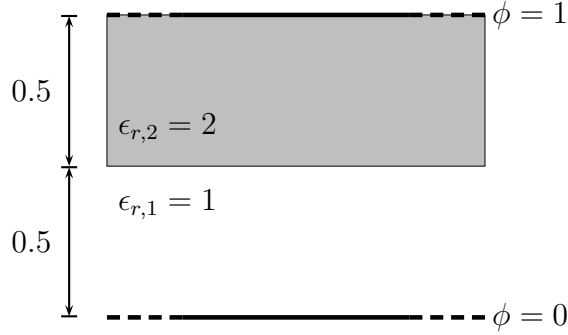


Figure 3: Parallel plate condensor

The solution is simple and it can be calculated analytically to get

$$\phi(x) = \begin{cases} \frac{4}{3}x & , x \leq 0.5 \\ \frac{2}{3}x + \frac{1}{3} & , x > 0.5 \end{cases} \quad (27)$$

which satisfies the interface conditions i.e. ϕ is continuous and the normal electric flux $\epsilon \frac{\partial}{\partial x} \phi$ is continuous through the interface. However, as an introduction to FD methods we calculate the problem numerically. Equation (26) can be approximated with the central differences as follows

$$\frac{\partial}{\partial x} \left(\epsilon \frac{\partial}{\partial x} \phi \right) \Big|_{x=x_0} \approx \frac{\epsilon(x_0 + h/2) \frac{\partial}{\partial x} \phi|_{x=x_0+h/2} - \epsilon(x_0 - h/2) \frac{\partial}{\partial x} \phi|_{x=x_0-h/2}}{h} \quad (28)$$

$$\approx \frac{\epsilon(x_0 + h/2) \frac{\phi(x_0+h) - \phi(x_0)}{h} - \epsilon(x_0 - h/2) \frac{\phi(x_0) - \phi(x_0-h)}{h}}{h} \quad (29)$$

$$= \frac{1}{h^2} \left\{ \epsilon(x_0 - h/2) \phi(x_0 - h) - \left[\epsilon(x_0 - h/2) + \epsilon(x_0 + h/2) \right] \phi(x_0) + \epsilon(x_0 + h/2) \phi(x_0 + h) \right\} = 0. \quad (30)$$

$$\phi(x_0) = \frac{\epsilon(x_0 - h/2) \phi(x_0 - h) + \epsilon(x_0 + h/2) \phi(x_0 + h)}{\epsilon(x_0 - h/2) + \epsilon(x_0 + h/2)} \quad (31)$$

Next, we divide the solution space into the five domains equal in size i.e. $h = 1/5$. Figure 4 illustrates the computation lattice. The notations

$$\phi_i = \phi(ih) \quad (32)$$

$$\epsilon_i = \epsilon(ih) \quad (33)$$

are used onwards.

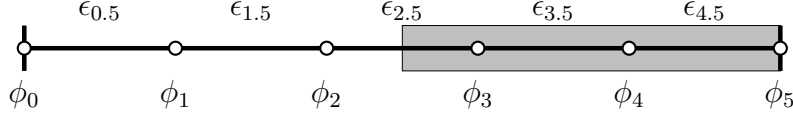


Figure 4: Computation lattice

While looking at Figure 4 the question arises: What is the permittivity value $\epsilon_{2.5}$ in the vicinity of dielectric interface? Is it $\epsilon_{r,1}$, $\epsilon_{r,2}$ or something else? To deal with this problem let us try different values.

a) $\epsilon_{2.5} = \epsilon_{r,1} = 1$:

Applying the equation (31) in every potential node inside the capacitor we obtain the system of equations

$$\phi_1 = \frac{\phi_0 + \phi_2}{2} \quad (34)$$

$$\phi_2 = \frac{\phi_1 + \phi_3}{2} \quad (35)$$

$$\phi_3 = \frac{\phi_2 + 2\phi_4}{3} \quad (36)$$

$$\phi_4 = \frac{2\phi_3 + 2\phi_5}{4} \quad (37)$$

$$(38)$$

In addition, the boundary conditions for the potential are

$$\phi_0 = 0 \quad (39)$$

$$\phi_5 = 1. \quad (40)$$

The same in matrix form is

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -3 & 2 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (41)$$

The potential is the average of the neighbouring potential values everywhere except in the vicinity of the material interface. There, the weighted average is

applied. The solution of the system of linear equations is

$$\begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 2/8 \\ 4/8 \\ 6/8 \\ 7/8 \\ 1 \end{pmatrix} \quad (42)$$

The solution is plotted with the exact solution in Figure 5. The numerical solution deviates clearly from the exact solution. It appears that the material interface in the numerical solution is shifted by $h/2$. Indeed, a more thorough analytical study would reveal the numerical solution to be exact for the geometry in which material interface lies in position $x = 0.6$.

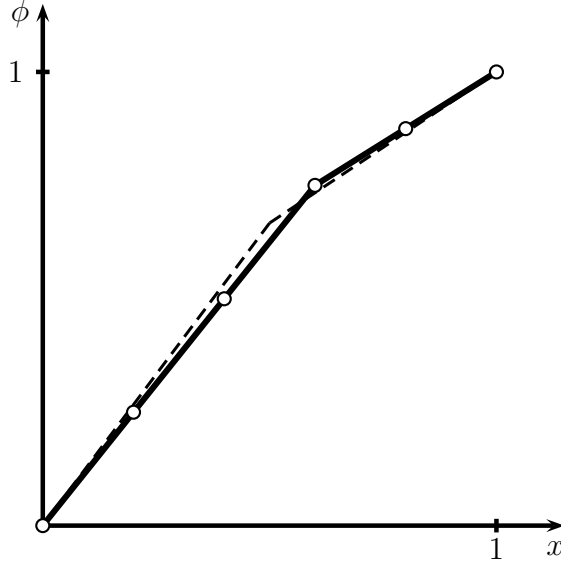


Figure 5: Numerical solution of case $\epsilon_{2.5} = 1$ (solid line) plotted against the exact solution (dashed line)

b) $\epsilon_{2.5} = \epsilon_{r,2} = 2$:

The system of equations is now

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -3 & 2 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (43)$$

and its solution is

$$\begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 2/7 \\ 4/7 \\ 5/7 \\ 6/7 \\ 1 \end{pmatrix}. \quad (44)$$

The solution is plotted in Figure 6. As we might have guessed the interface is shifted to other direction in this case. The solution is exact for the geometry in which material interface is located at $x = 0.4$.

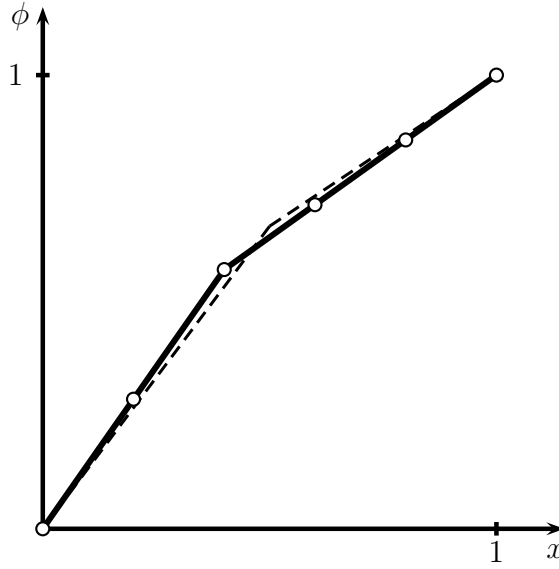


Figure 6: Numerical solution of case $\epsilon_{2.5} = 2$ (solid line) plotted against the exact solution (dashed line)

Neither one of the cases gave us the right result. The question remains: How to get more accurate solution? Previous cases taught us that it is possible to get the exact solution if a computational node is located at the material interface. Hence, the computation lattice could be rearranged as shown in Figure 7. Now, the lattice constant h is $1/6$. The matrix equation for this lattice is

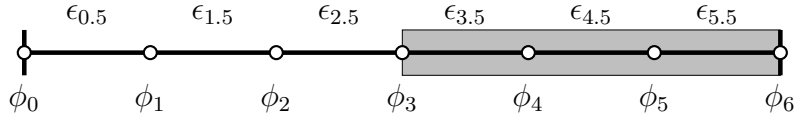


Figure 7: Rearranged computation lattice

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -3 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (45)$$

The solution of the equation is

$$\begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 2/9 \\ 4/9 \\ 6/9 \\ 7/9 \\ 8/9 \\ 1 \end{pmatrix} \quad (46)$$

which is exact. The technique of choosing a suitable lattice seems to be outstanding. With a proximal analysis we can obtain the exact solution. The bad news is that this is not the case in 2D or 3D problems. The reason is that 2D and 3D objects can produce potential fields which are not piecewise linear or not even quadratic. Maybe these kind of observations gave start to the development of finite element methods (FEM)[9]. FEM is based on a reasonable choice of computation lattice. The geometry is divided into small domains and the strategy is to find the solution as a sum of basis functions. The basis functions can be high-order polynomials to enable approximate solutions having derivatives of high-order. However, the purpose of this thesis is to study the application of FD methods with structured lattices. Here, the word structured means that the lattice is regular and it does not have to be adapted to conform to the geometry of the analysed structure. The advantage is fastness because the generation of 2D or 3D mesh for an arbitrary geometry is difficult and time consuming. Therefore, we go back to the original problem of finding the permittivity $\epsilon_{2.5}$ in Figure 4.

Obviously, if we liked to model an interface lying anywhere between potential nodes ϕ_2 and ϕ_3 the permittivity $\epsilon_{2.5}$ would have to be a function of interface location. Next, we try to find a formula for this local effective permittivity.

The constitutive equation in 1D is

$$D = \epsilon E \quad (47)$$

It connects the electric flux D and the electric field E together. Therefore, let us define the effective permittivity between two points to be

$$\epsilon_{\text{eff}} = \frac{D_{\text{ave}}}{E_{\text{ave}}} \quad (48)$$

in which D_{ave} is the average electric flux and E_{ave} the average electric field between the points. The normal electric flux through the material interface is continuous i.e.

$$\epsilon_{r,1}E_1 = \epsilon_{r,2}E_2 \quad (49)$$

where E_1 and E_2 are the electric fields in the dielectrics 1 and 2 correspondingly. Figure 8 illustrates the situation. Here, f is the volume fraction of dielectric 2 in the interval h between the points.

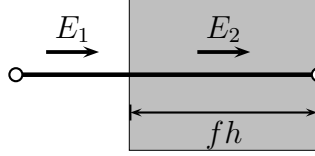


Figure 8: Material interface between two points

Because the electric flux is the same in both materials the equation (48) can be written in form

$$\begin{aligned} \epsilon_{\text{eff}} &= \frac{\epsilon_{r,1}E_1}{E_1(1-f) + E_2f} \\ &= \frac{\epsilon_{r,1}E_1}{E_1(1-f) + \frac{\epsilon_{r,1}}{\epsilon_{r,2}}E_1f} \\ &= \frac{\epsilon_{r,1}\epsilon_{r,2}}{f\epsilon_{r,1} + (1-f)\epsilon_{r,2}} \end{aligned} \quad (50)$$

According to (50) the effective permittivity value $\epsilon_{2.5}$ between the points $x = 0.4$ and $x = 0.6$ is

$$\epsilon_{2.5} = \frac{1 \cdot 2}{1/2 \cdot 1 + (1 - 1/2) \cdot 2} = \frac{4}{3} \quad (51)$$

The matrix equation of the problem is then

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -7/3 & 4/3 & 0 & 0 \\ 0 & 0 & 4/3 & -10/3 & 2 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (52)$$

and the solution is

$$\begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 4/15 \\ 8/15 \\ 11/15 \\ 13/15 \\ 1 \end{pmatrix}. \quad (53)$$

This is the exact solution for the potential. A thorough study would reveal the technique of local effective permittivity to work accurately for arbitrary locations of dielectric interface.

Unfortunately the technique of local effective permittivity does not offer exact solutions for 2D and 3D problems. The reason was mentioned earlier: *2D and 3D objects generate fields that are no longer linear nor quadratic*. However, the local effective permittivities can be applied to find approximate solutions with a structured computational lattice. For example, the papers [12, 13] present techniques to determine the local effective permittivities near dielectric interfaces. The technique introduced in [12] is also used in [P3] which discusses the numerical analysis of dielectric mixtures with the FDTD method. In [P4], a new technique is presented and it is applied in the FD analysis of 3D mixtures. The paper [P6] gives a somewhat different approach to the determination of the local permittivity. While the local effective permittivities in [12, 13, P4] are constants in the technique of the paper [P6] they are dependent on the electric field direction. The performances of the above mentioned techniques are also compared in the estimation of the total electric flux through several different dielectric interface geometries and material contrasts in [P6]. The results indicate a good performance for the field dependent local effective permittivity (FDEP) technique introduced in [P6].

4 Dynamic field solutions

Finite differences are also used to solve dynamic electromagnetic fields. Perhaps, the most popular difference method nowadays is the finite-difference time-domain method (FDTD). It originates from 1966 [10]. The application area of the method is vast [11].

The basic idea of the FDTD is to approximate the Maxwell equations (8)–(13) with central differences. For example the approximation of (8) in point (x_0, y_0, z_0) at time instant t_0 is

$$\begin{aligned} \mu|_{x_0, y_0, z_0} & \frac{H_x|_{x_0, y_0, z_0, t_0 + \frac{\Delta t}{2}} - H_x|_{x_0, y_0, z_0, t_0 - \frac{\Delta t}{2}}}{\Delta t} \\ & = \frac{E_y|_{x_0, y_0, z_0 + \frac{\Delta z}{2}, t_0} - E_y|_{x_0, y_0, z_0 - \frac{\Delta z}{2}, t_0}}{\Delta z} \\ & \quad - \frac{E_z|_{x_0, y_0 + \frac{\Delta y}{2}, z_0, t_0} - E_z|_{x_0, y_0 - \frac{\Delta y}{2}, z_0, t_0}}{\Delta y} \end{aligned} \quad (54)$$

in which Δx , Δy , Δz are the lattice constants in x , y and z directions and Δt is the time step size. The word 'step' refers to the nature of the FDTD algorithm. When all the equations (8)–(13) are transformed into difference equations one can realise that the field values can be calculated explicitly by taking steps in time. From (54) the update equation of the magnetic field component H_x can be solved to get

$$\begin{aligned} H_x|_{x_0, y_0, z_0, t_0 + \frac{\Delta t}{2}} = & H_x|_{x_0, y_0, z_0, t_0 - \frac{\Delta t}{2}} \\ & + \frac{\Delta t}{\mu|_{x_0, y_0, z_0} \Delta z} (E_y|_{x_0, y_0, z_0 + \frac{\Delta z}{2}, t_0} - E_y|_{x_0, y_0, z_0 - \frac{\Delta z}{2}, t_0}) \\ & - \frac{\Delta t}{\mu|_{x_0, y_0, z_0} \Delta y} (E_z|_{x_0, y_0 + \frac{\Delta y}{2}, z_0, t_0} - E_z|_{x_0, y_0 - \frac{\Delta y}{2}, z_0, t_0}) \quad (55) \end{aligned}$$

The difference equations lead to the computation lattice constructed of so-called Yee cells [10]. The field components form a chain-like structure shown in Figure 9. Every electric field component is surrounded by magnetic field components and every magnetic field component is surrounded by electric field components. The choice of the spatial step sizes (Δx , Δy , Δz) affects the possible values of the time step size. To preserve the numerical stability during the simulation the time step has to be

$$\Delta t \leq \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}} \quad (56)$$

everywhere in the computation lattice [39]. The parameter c is the local value for the speed of light.

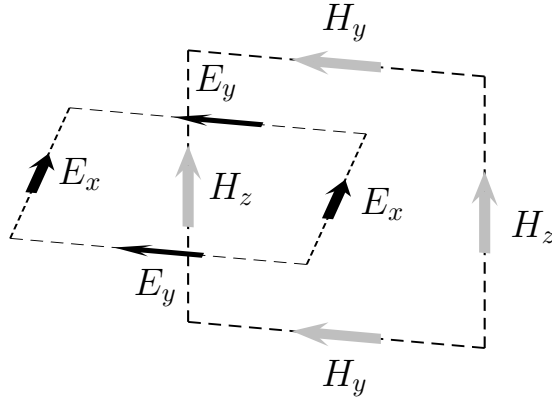


Figure 9: The chain-like lattice of the FDTD method

One of the main issues in the implementation of the FDTD simulation is the treatment of boundary and interface conditions. Even if the problem region

does not have boundaries i.e. the studied structure lies in an open space the computational lattice has to be terminated somewhere because of the limited amount of computing resources. In those cases the absorbing boundary conditions (ABC) have to be applied to simulate the response of an infinite space. ABCs can be divided into analytical [14, 15, 17, 16, 18, 19] and material based conditions [20, 21, 22, 23, 24].

The strength of the FDTD method is the versatility to analyse different materials. However, a problem arises when the material boundaries or interfaces do not match the computational lattice. Several techniques have been proposed for the treatment of arbitrarily located interfaces such as locally conformal lattices [25, 26, 27, 28, 29, 30, 31, 32, 33], effective medium techniques [12, 13, 34] and hybrid techniques [35, 36, 37].

In the previous section the concept of the local effective permittivity was introduced. It was used to solve a static field problem. It is also applicable in dynamic field simulations. Although, for example, the equation (50) was derived for static fields it is reasonable to make use of it also in the FDTD simulations for the electric field components perpendicular to the material interface². The material parameters are defined locally for every field component in the FDTD lattice. The local permittivity is defined for every electric field component and the local permeability for every magnetic field component. To obtain a good approximation for the electromagnetic wave problem the lattice constants have to be small enough compared to the simulated wavelength. The smaller the wavelength (λ) the bigger the values of high-order derivatives. This can be seen in the Taylor series of a sine function:

$$\sin\left(\frac{2\pi}{\lambda}x\right) = \frac{2\pi}{\lambda}x - \frac{1}{3!}\left(\frac{2\pi}{\lambda}\right)^3 x^3 + \frac{1}{5!}\left(\frac{2\pi}{\lambda}\right)^5 x^5 - \dots \quad (57)$$

The amplitudes of high-order terms get bigger when the wavelength λ gets smaller. A generally applied rule of thumb is to have lattice constants Δx , Δy , $\Delta z \leq \lambda/20$. Therefore, it is reasonable to use the concept of effective permittivity for the micro-structure between the lattice nodes.

The FDTD method is applied in the article [P1] which describes the analysis of a certain practical filter structure. The difficulty of modelling the curved surfaces in rectangular mesh is avoided by transforming a circle-shaped tap into a square-shaped one. The idea was to show how the main characteristics of the filter structure can be estimated with the FDTD method rapidly for the wide frequency band.

As mentioned earlier the FDTD method can be applied for numerous different problems in electromagnetics. The papers [P2] and [P3] introduce yet another application area. The FDTD method is used to analyse dielectric mixtures. A mixture sample is put in a parallel plate waveguide and the propagation

²In the FDTD lattice the local electric field components are in many cases parallel to the material interface. Then, the arithmetic average $\epsilon_{\text{eff}} = (1-f)\epsilon_{r,1} + \epsilon_{r,2}f$ for the local effective permittivity has to be used. This is the case for example in one-dimensional FDTD analysis. Notice that the algorithm introduced in [P4] gives these so-called Wiener limit values [38] when the material interface is perpendicular or parallel to the interface.

of a plane wave in the waveguide is simulated. The effective permittivity of the sample is determined by calculating the reflection of a low-frequency wave from the sample.

In paper [P5] the reflection characteristics of frequency selective surfaces are analysed by the FDTD method. In this paper the author applied nonuniform orthogonal meshes [39] to concentrate the computational resources to the locations of fine geometrical details. Also, the technique of the local effective permittivity was used for the lattice cells close to the material interfaces.

5 Numerical analysis of material mixtures

The material parameters in the Maxwell equations (8)–(13) are macroscopic quantities. Therefore, the electromagnetic fields solved from the equations are approximations of the microscopic field distributions. For example, when we are calculating the propagation of radio waves in the air we do not solve the fields acting between the electrons and protons in an atom nor even between the various molecules in air but we calculate the average fields in the size scale of 10^{20} atoms. However, to be able to get good approximations of these macroscopic fields we have to take into account what is happening in the microscopic level. In fact, to model realistically air as a dielectric material, one needs to consider the different scales of microscopic inhomogeneities. Certainly, air consists of many different particles of different sizes. It is a mixture of several gases, liquids and solids. In case of rain, condensed water phase in the form of drops gives a considerable contribution to the susceptibility of air.

Mixing theories are developed in order to predict the effective response of mixtures without having to calculate the microscopic fields. The goal of the theories is to give a method to determine the effective material parameters (permittivity, permeability and conductivity) that can be used in the Maxwell equations.

The constitutive relation connects the electric flux and the electric field in isotropic material locally together as follows

$$\mathbf{D} = \epsilon \mathbf{E}. \quad (58)$$

Hence, the natural way to define the effective permittivity is to define it as a relation between the volume-averaged electric flux and the electric field

$$\epsilon = \frac{\langle \mathbf{D} \rangle}{\langle \mathbf{E} \rangle}. \quad (59)$$

In order to get a good estimation for the effective permittivity the averaging volume V has to be large enough to represent the overall statistics of the mixture. In short, the volume has to contain several inclusion particles as seen in Fig. 10. To obtain a mixing model one has to determine the average electric flux through the mixture for a given exciting electric field.

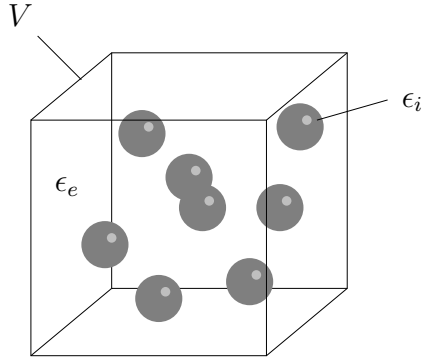


Figure 10: A sample of a material mixture has to be large enough to represent the mixture. ϵ_i and ϵ_e are the inclusion and the environment permittivities, respectively.

Perhaps, the most famous mixing model is the Maxwell Garnett rule [40]

$$\epsilon_{\text{eff}} = \epsilon_e + 3f\epsilon_e \frac{\epsilon_i - \epsilon_e}{\epsilon_i + 2\epsilon_e - f(\epsilon_i - \epsilon_e)} \quad (60)$$

which can be considered also the oldest. It was published in 1904. However, similar approaches were introduced already earlier [41, 42, 43, 44]. The Maxwell Garnett model was created for the mixture in which spheres of permittivity ϵ_i are randomly located in homogeneous environment (ϵ_e) and occupy a volume fraction f (See Fig. 10). Its foundation lies on the analytical solution of one sphere in the infinite space. Therefore, its applicability is restricted to low volume fractions i.e. spheres being far apart. From literature a great number of other theoretical mixing models can be found also for multiphase mixtures [45, 46, 47, 48, 49, 50, 51, 52, 53].

A mixture having arbitrarily shaped inclusion particles close to each other is a difficult problem. Several numerical methods have been proposed to estimate the effective material parameters in such cases [54, 55, 56, 57, 58, 59, 60, 61]. An extensive review of the numerical mixture modeling can be found in [62]. In this thesis, the attention was paid to the approximative determination of the effective permittivity by the finite difference methods. Especially, the papers [P2, P3, P4] are concentrating on this problem. The paper [P2] introduces a technique to model dielectric mixtures with the FDTD method. The mixtures in [P2, P3] were two-dimensional. The inclusion particles were randomly placed circular cylinders and they were allowed to touch each others. For the paper [P3] the author analysed thousands of different mixture samples to get a good picture about the effective permittivity distribution. One has to remember that even the samples having the same inclusion volume fraction can have different effective permittivities because of the different positioning of inclusions. In the paper [P4] the FD method was used to analyse 3D mixtures. The static

electric potential was solved for the periodic structure. One period consisted of several randomly placed spheres. One of the aims of these numerical studies on heterogeneous materials was to test the validity of classical mixing rules, like the Maxwell Garnett [40] and the Bruggeman [46] models. Among the results, one interesting finding was that the Maxwell Garnett is quite acceptable in some cases. The numerical results agreed rather well with the model when the inclusion particles were separate (i.e. the inclusion clusters were not allowed). The simulation results were also used to create a new empirical mixing model.

6 Summary of publications

The common factor of the articles in this thesis is the finite difference method and its application in the modelling of arbitrary geometries. Also, one of the main issues was to study and develop fast approximative techniques for different problems.

The first article [P1] discusses the FDTD analysis of filter structures with cylindrical and rectangular shapes. The main idea in the article is to show how certain cylindrical objects can be replaced by square-shaped ones having same performance in a certain practical filter configuration. The motivation was to develop a fast approximative tool for the design of filters and to avoid the difficult modelling of curved surfaces in the cartesian FDTD lattice.

The second article [P2] proposes a procedure to analyse dielectric mixtures with the FDTD method. A sample of a mixture is put inside a TEM-waveguide. The effective permittivity of the mixture is estimated by determining the reflection of a plane wave from the sample. The numerical results were calculated for randomly placed aligned cylindrical inclusions in a homogeneous background. Therefore, the simulation space was two-dimensional (2D). Various dielectric contrasts were studied and the numerical results were compared with classical mixing rules.

In the third paper [P3] the authors continued the research done in [P2]. Thousands of simulations with random inclusion positionings were run in order to get a good statistical picture about the effective permittivity distribution. The obtained distribution was compared with the theoretical bounds. Results were also set against theoretical mixture models to find that none of the models agree with the numerical results over the whole range of inclusion volume fraction. In this article the authors forgot to mention the diameter of inclusions. It was $0.16d$ in which d is the separation of plates in the waveguide.

The fourth paper [P4] reports the results of a numerical analysis of static electric field in random dielectric materials. The effective permittivity of a 3D mixture was calculated by the finite difference method. Periodic boundary conditions were used to truncate the computation lattice i.e. the mixture was periodic. One period consists of spheres with random positions. In this paper a new technique was developed to model arbitrary dielectric interfaces in rectangular lattice. New empirical mixing rules were created as least squares approximations to fit the collection of numerical results. An interesting discovery for dilute mixtures was that the numerical results agreed rather well with the Maxwell Garnett mixing model [40] when the inclusions were separate. On the other hand, when the inclusions were allowed to touch each others, the results were close to the Bruggeman model [46].

The fifth paper [P5] reports the polarisation transformation properties of frequency selective surfaces. The article presents examples of microstrip structures which transform polarisation from linear to circular. The FDTD method and the waveguide simulator technique were used to analyse the reflection of a plane wave from the structure. The studies showed that a broadband polarisation transformer can be designed for a limited range of angles of incidence. Alter-

natively, a polariser for a wide range of angles of incidence can be designed to operate in a narrow frequency band. Field illustration techniques were applied to design an electronically switchable polariser. The research was done when the author worked as a visiting scientist in the Applied Electromagnetics Group of the University of Victoria, Canada.

The sixth paper [P6] introduces a new technique to model arbitrary dielectric interfaces in a regular finite-difference lattice. The technique is based on the local effective permittivity that is dependent on the field direction in the vicinity of the material interface. The performance of the technique was studied by solving the electrostatic potential of a parallel plate capacitor with several different insulator dielectric geometries. The obtained total electric fluxes are compared to the reference results calculated with the finite element method. The results show that the new technique is a good tool in the estimation of the effective permittivity of a dielectric mixture.

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