FINITE-DIFFERENCE MODELING OF DIELECTRIC INTERFACES IN ELECTROMAGNETICS AND PHOTONICS

MODELOVANJE RAZDVOJNIH DIELEKTRIČNIH POVRŠI U ELEKTROMAGNETICI I FOTONICI METODOM KONAČNIH RAZLIKA

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Sadržaj – Metoda konačnih razlika (FDM) omogućava brzu i efikasnu analizu i simulacije elektromagnetskih polja, što je posebno pogodno za CAD programiranje i dizajn. Mana metode konačnih razlika u frekvencijskom domenu (FDM-FD) je nedovoljno tačna diskretizacija razdvojnih površi dielektrika različitih permitivnosti, a uzrok je neizbežna takozvana stepeničasta aproksimacija. U ovom radu je dat pregled i međusobno poređenje nekih veoma atraktivnih numeričkih koncepata koji omogućavaju efikasan tretman razdvojnih dielektričnih površi. Takozvane poboljšane FD šeme omogućavaju izvođenje FD formula u okolini razdvojnih površi, uz drugi red tačnosti. Metode transformacije koordinata, kao što je strukturno vezana metoda konačnih razlika, omogućavaju da postupak FD diskretizacije prati lokalnu geometriju analizirane strukture. Jedan drugi pristup, koji je predložio autor rada, dovodi do FD formula veće tačnosti od često korišćenih poboljšanih FD formula.

Abstract – The finite difference method (FDM) enables electromagnetic field calculations and simulations at reduced time, what is particularly suitable for CAD software implementations. Frequency domain based FDM (FDM-FD) discretization of structures with the permittivity step at the interface between two dielectric regions suffers from reduced accuracy due to the inevitable staircase approximation. In this paper a few very attractive numerical concepts that allow accurate FD treatment of dielectric interfaces are reviewed and compared. So-called improved FD-schemes enable the derivation of FD formulas providing true accuracy of the second order. In co-ordinate transformation methods, such as the structure related FDM, the discretization procedure exactly matches the local geometry of the structure under analysis. Another approach, proposed by the author, results in the derivation of FD formulas with better accuracy then often-used improved FD formulas.

Keywords – Numerical modeling, Finite difference method, Electromagnetics, Photonics.

1. INTRODUCTION

The finite-difference method (FDM) is widely used numerical method in electromagnetics, [1,2]. FDM has been extensively used in photonics and optoelectronic design in mode solvers, in beam propagation methods (BPMs), [3-5], as a standard method of choice in simulation programs or computer-aided design (CAD) tools where shortened simulation time is mandatory. BPM techniques available include both frequency and time domain approaches for analyzing optical waveguides and waveguide-based optoelectronic devices. CAD applications based on the frequency domain FDM (FD-BPM) have become particularly an attractive approach because of the simplicity of FDM implementation and the sparsity of FDM resultant matrix.

Most conventional implementations of FD-BPM for structures with constant cross-section in a rectangular coordinate system are characterized by low-order truncation errors. Difference equations obtained by standard centered differencing in two dimensions in homogeneous regions are second-order accurate, n = 2, or $O(h^2)$, where h is the FD mesh size. Near the step-index dielectric interfaces, accuracy usually drops to n - 1, and near dielectric corner points difference equations are (n - 2)th-order accurate, resulting with (n - 1)th-order of accuracy of the modal index and modal electromagnetic field. This deficiency of FDM, known as the inevitable staircase approximation of the dielectric boundaries, has pushed most of the researches to concentrate either on the development of the new numerical approaches, or the solution techniques employed to solve the large matrix equation sets that usually result during the FD discretization procedure.

Over the last two decades, certain research efforts have been spent on increasing understanding of the effects of truncation error near the step-index dielectric interfaces and increasing the accuracy of the employed FD discretization procedure, both in semi-vectorial and full-vectorial FD-BPM formulations. The starting point was Stern's work [6] where the concept of a semi-vectorial mode, which neglects minor field components (quasi-TE and quasi-TM cases), has been

introduced, resulting in $O(h^0)$ truncation error. A few years latter, Vassallo [7] proposed an improved three-point FD formulation for the semi-vectorial case providing O(h)accuracy with arbitrary placement of dielectric interfaces between FD grid lines. Yamauchi et al. [8-10] improved Vassallo's approach to give $O(h^2)$ accuracy regardless of interface position. Chiou et al. [11] further improved the accuracy, in the semi-vectorial case, to $O(h^3)$ for arbitrarily positioned interfaces and $O(h^4)$ when interfaces lie on nodes or are centered between them. Chiang et al. [12] generalized Vassallo's and Yamauchi's approach to full-vectorial case to give $O(h^2)$ accuracy for oblique, even curved step-index boundaries. Approaches [11,12] have been followed by others, see for example Wykes et al. [13] where an improvement was proposed for structures containing fine features, such as quantum-well structures and ARROW-C waveguides. Hadley [14,15] derived highly accurate FD formulas, assuming TE polarization, with truncation error in the uniform region $O(h^4)$ to $O(h^6)$ depending on the type of grid employed, and up to the $O(h^5)$ near dielectric interfaces under certain grid-interface conditions. The co-ordinate transformation approaches reformulate FDM in nonorthogonal, so-called structure related (SR) co-ordinate systems, see for example [16-18]. Promising approach has been very recently reported in [19], where the truly twodimensional full-vectorial FDM approach has been proposed for the electromagnetic field discretization near dielectric interfaces featuring with $O(h^4)$, and higher, truncation error.

The aim of this paper is to review and compare those recently developed FDM and FD-BPM methodologies. It is noteworthy to mention that the brief summary given in this introductory section does not cover all approaches proposed in the literature during the last decade. However, in author's opinion, referred approaches have significantly impacted the research and CAD manufacturing in photonics and optoelectronics already, and have made advancements in commercial and in-house tools based on FDM and FD-BPM techniques. Namely, these are: 1) improved formulas FDM approach (Yamauchi, Chiou, Chiang); 2) highly accurate Hadley's approach which can be used for benchmark purposes; 3) structure-related FDM coordinate transformation approach; together with the author's recently proposed twodimensional full-vectorial FD formulas formulation. In the next section these concepts are briefly explained.

2. FDM MODELING OF DIELECTRIC INTERFACES

Let us start from the vector Helmholtz's equation, which in linear and isotropic media, in frequency domain, in terms of transverse electric field \mathbf{E}_t , has a well-known form,

$$\nabla^2 \mathbf{E}_t + k^2 n^2 \mathbf{E}_t = \nabla_t \left[\nabla_t \cdot \mathbf{E}_t - \frac{1}{n^2} \nabla_t (n^2 \mathbf{E}_t) \right], \quad (1)$$

where $k = \omega \sqrt{\varepsilon_0 \mu_0}$, $n = \sqrt{\varepsilon_r}$, we assume that $n \neq n(z)$, an operator ∇ is replaced as $\nabla = \nabla_t + \nabla_z$; the similar equation states for the transverse magnetic field \mathbf{H}_t . The BPM methods are developed under the paraxial approximation of (1), [3-5],

$$j2kn_0\frac{\partial \mathbf{E}_t}{\partial z} = \nabla_t \left[\frac{1}{n^2}\nabla_t (n^2 \mathbf{E}_t)\right] + k^2(n^2 - n_0^2)\mathbf{E}_t, \quad (2)$$

where $j = \sqrt{-1}$, $\mathbf{E}_t = E_t e^{-j k n_0 z}$ and n_0 denotes a reference refractive (modal) index. Equation (2) is known as the one-way paraxial wave equation, or Fresnel's equation. Note that in TEM case (1) simplifies to

$$\nabla_t \left[\frac{1}{n^2} \nabla_t (n^2 \mathbf{E}_t) \right] + k^2 n^2 \, \mathbf{E}_t = 0, \tag{3}$$

and within the 2D static approximation $k \rightarrow 0$, so we have

$$\nabla_t \left[\frac{1}{n^2} \nabla_t (n^2 \mathbf{E}_t) \right] \tag{4}$$

The conventional FDMs schemes are obtained by directly discretizing eqs. (1-4) and in the case of the transverse plane step-index devices they are generally arranged to avoid the discontinuity problem, for example by assuming the graded-index approximation. The improved FD formulas approaches take into account boundary conditions for the field and its derivatives near the dielectric interfaces.

2.1. Improved FDM formulas formulation

We will focus our attention on the rectangular FD meshes and improved full-vectorial FD formulation given in [12], where optical waveguides with step-index profiles have been treated for oblique even curved interfaces. Derivation procedure employs the Taylor series expansion and matching the interface conditions of the field components. The derivation methodology for the transverse electric field E_c , c = x or y, will be briefly presented here only.



Figure 1. Cross-section of a linear oblique interface discretized with a uniform grid in x and y directions.

In the case of the linear oblique interface between two dielectric regions, Fig. 1, a task is to derive the relationship between the fields in two neighbouring grid points $E_c|_{(i,j)}$ and $E_c|_{(i+1,j+1)}$ taking in the account all grid points around centered point (i, j). $E_c|_L$ and $E_c|_R$, Fig. 1, represent the fields at just to the left and right sides of the interface, respectively. Taylor series expansion for $E_c|_L$ in terms of $E_c|_{(i,j)}$ and its derivatives is

$$E_{c}\Big|_{L} = E_{c}\Big|_{(i,j)} + \Delta x_{L} \frac{\partial E_{c}}{\partial x}\Big|_{(i,j)} + \Delta y_{L} \frac{\partial E_{c}}{\partial y}\Big|_{(i,j)} + \frac{\Delta x_{L}^{2}}{2!} \frac{\partial^{2} E_{c}}{\partial x^{2}}\Big|_{(i,j)} + \frac{2\Delta x_{L} \Delta y_{L}}{2!} \frac{\partial^{2} E_{c}}{\partial x \partial y}\Big|_{(i,j)} + \frac{\Delta y_{L}^{2}}{2!} \frac{\partial^{2} E_{c}}{\partial y^{2}}\Big|_{(i,j)} + \cdots$$
(5)

By successively differentiating of (5) with respect to x or y, one could arrange a matrix equation

$$[E_L] = [[M_{L:(i,j)}]] \cdot [E_{(i,j)}] + H.O.T. , \qquad (6)$$

where $[E_L]$ is a vector assembled of E_{xL} , E_{yL} and their derivatives in respect to x and y, $[E_{(i,j)}]$ is a vector assembled of $E_{x_{(i,j)}}$, $E_{y_{(i,j)}}$ and their derivatives in respect to x and y, $[[M_{L:(i,j)}]]$ is a resulting square matrix in terms of Δx_L and Δy_L , and H.O.T. denotes "higher order terms". In a similar fashion, starting from Taylor series expansion for $E_c|_{R}$, we arrive to the next matrix equation

$$[E_{(i+1,j+1)}] = [[M_{(i+1,j+1):R}]] \cdot [E_R] + H.O.T.$$
(7)

By introducing local co-ordinate system (n, t), unit vectors (\hat{n}, \hat{t}) shown in Fig. 1, in a matrix form, then linking vectors $[E_L]$ and $[E_R]$ via the interface conditions, again in a matrix form, and combining these matrix equations we obtain

$$[E_{(i+1,j+1)}] = [[M_{(i+1,j+1):R}]] \cdot [[M]]_{RC} \cdot [[M]]_{RL} \cdot \\ \cdot [[M]]_{CL} \cdot [[M]]_{L:(i,j)} \cdot [E_{(i,j)}] + H.O.T. ,$$
(8)

where $[[M]]_{RC}$ and $[[M]]_{CL}$ are local co-ordinates transformation matrices and $[[M]]_{RL}$ is a matrix where boundary conditions are packed, all matrices being square. The crucial point in the improved FD formulas approaches is deriving and packing a matrix $[[M]]_{RL}$. In the case of the transverse electric field, in terms of normal E_n and tangential E_t field components, boundary conditions are

$$E_{n}\Big|_{R} = \frac{\varepsilon_{L}}{\varepsilon_{R}}E_{n}\Big|_{L}, \quad E_{t}\Big|_{R} = E_{t}\Big|_{L}, \quad \frac{\partial E_{n}}{\partial n}\Big|_{R} = \frac{\partial E_{n}}{\partial n}\Big|_{L},$$

$$\frac{\partial E_{n}}{\partial t}\Big|_{R} = \frac{\varepsilon_{L}}{\varepsilon_{R}}\frac{\partial E_{n}}{\partial t}\Big|_{L}, \quad \frac{\partial E_{t}}{\partial t}\Big|_{R} = \frac{\partial E_{t}}{\partial t}\Big|_{L},$$

$$\frac{\partial E_{t}}{\partial n}\Big|_{R} = \frac{\partial E_{t}}{\partial n}\Big|_{L} + \left(\frac{\varepsilon_{L}}{\varepsilon_{R}} - 1\right)\frac{\partial E_{n}}{\partial t}\Big|_{L},$$

$$\frac{\partial^{2} E_{n}}{\partial n^{2}}\Big|_{R} = \frac{\varepsilon_{L}}{\varepsilon_{R}}\frac{\partial^{2} E_{n}}{\partial n^{2}}\Big|_{L} + k^{2}\frac{\varepsilon_{L}}{\varepsilon_{R}}(\varepsilon_{L} - \varepsilon_{R})E_{n}\Big|_{L},$$

$$\frac{\partial^{2} E_{t}}{\partial n^{2}}\Big|_{R} = \frac{\partial^{2} E_{t}}{\partial n^{2}}\Big|_{L} + k^{2}(\varepsilon_{L} - \varepsilon_{R})E_{t}\Big|_{L}, \quad (9)$$

and so on, where ε_L and ε_R are the permittivities on the lefthand and right-hand sides of the interface, respectively. The same conditions (9) were acquired and used in multiple of papers in the derivation of improved FD formulas [7-15]. Note that (9) represent exact boundary conditions and can be used in the electrostatic case as well, with approximation $k \rightarrow 0$. Improved FD formula (8) is with $O(h^2)$ truncation error. Higher accuracy is difficult to obtain because of singular problems with matrix inversion in (8), [12]. In [11] the same approach was used with a generalized Douglas scheme to improve the accuracy to $O(h^3)$ for arbitrarily positioned interfaces and $O(h^4)$ where interfaces lie on nodes or are centered between them, however for structures with rectangular cross-sections and within the semi-vectorial formulation only.

2.2. Hadley's FDM formulation

In [14,15] Hadley utilized 2D solutions of the Helmholtz's equation in cylindrical co-ordinates. This approach resulted in the tremendous increase in accuracy, however with increase in algebraic and numerical efforts in formulas derivation and implementation. Three distinct cases of uniform regions, dielectric interfaces and dielectric corners are handled separately and these derivations are finally incorporated into a TE mode waveguide modeling tool.

Hadley started by assuming a uniform grid in both transverse directions, and from the TE eigenmode-solving form of (1) in polar co-ordinates (r, θ) , in terms of the transverse magnetic field $\mathbf{H}_t = \mathbf{H}_t(r, \theta)$,

$$\nabla_t \left[\frac{1}{n^2} \nabla_t (n^2 \mathbf{H}_t) \right] + k^2 (n^2 - n_0^2) \, \mathbf{H}_t = 0, \tag{10}$$

with the general series solution for $\mathbf{H}_t(r, \theta)$,

$$\mathbf{H}_t(r,\theta) = \sum_{n=0}^{\infty} J_n(\xi r)(c_n \cos n\theta + d_n \sin n\theta), \qquad (11)$$

where $J_n(\xi r)$ denotes the *n*th order Bessel function of the first kind and $\xi^2 = k^2(n^2 - n_0^2)$. FD formula is evaluated under (10) and (11) over nine-point stencil formed from the centered grid point and 8 neighbouring FD grid points, giving $O(h^6)$ order of the truncation error ($O(h^4)$ for non-uniform grid) in homogeneous regions. An intrinsic drawback of this approach is a need for additional computation of multitudes of Bessel functions in the final FD formula.

The derivation of similar FD formulas on a dielectric interface is even more demanding because of the discontinuities of higher field derivatives on the interface. Cumbersome formulas was derived in [14] giving $O(h^5)$ order of the truncation error for the uniform grid and points placed exactly at the dielectric interface, finally resulting in $O(h^6)$ -order accuracy for the modal index and $O(h^4)$ -order accuracy for the value of the small field component for problems containing no dielectric corners, and somewhat lower order of accuracy for realistic problems including corners (e.g. rib waveguides eigenmode analysis).

Although Hadley's FD formulas are rather tedious to derive and implement, they have been incorporated in the improved accuracy eigenmode solvers for benchmark purposes in some waveguide simulations (e.g. buried and rib waveguides with rectangular cross-sections).

2.3. Structure-related FDM formulation

Successful approach to eliminate non-physical scattering due to the staircasing effect in FD discretization of oblique dielectric interfaces in rectangular co-ordinate system is the use of the co-ordinate transformation methods, such as structure related (SR) FD-BPM, [8-10]. SR co-ordinate systems, such as tapered, oblique, bi-oblique co-ordinate systems, naturally follow the local geometry of the structure under analysis. Eqs. (1-4) can be rewritten in any orthogonal or non-orthogonal transverse co-ordinate system. The general theory of the SR non-orthogonal co-ordinate systems was given in [16]. As an example, in the case of a tapered coordinate system (t, v) in the transverse plane, in which $t = \tan \theta$, $x = t(y - y_0)$, v = y, where the origin of tapered co-ordinate system (x_0, y_0) is given as $v_0 = y_0 = x_0 \cot \theta$, the scalar paraxial wave equation, in the uniform regions and in terms of the electric field E_t , can be derived as

$$j2kn_0\frac{\partial E_t}{\partial z} = \frac{\partial^2 E_t}{\partial v^2} - \frac{2t}{v - v_0}\frac{\partial^2 E_t}{\partial v\partial t} + \frac{1}{(v - v_0)^2}\frac{\partial}{\partial t}\left[(1 + t^2)\frac{\partial E_t}{\partial t}\right] + k(n^2 - n_0^2)E_t.$$
 (12)

In (12) a slowly-varying scalar envelope approximation of the electric field $E_t = E_t(t, v, z)$ and the refractive index n = n(t, v) are functions of a tapered co-ordinates t and v. Derivation details of (12) can be found in [16,17].

In spite being scalar, the resulting SR FD-BPM algorithm allows simulations with noticeably reduced numerical noise and shortened simulation time. The non-orthogonal coordinate FD-BPM has been applied to the analysis of structures with oblique, bi-oblique, tapered, and taperedoblique cross-sections in the transverse plane.



Figure 2. Discretization of the rib waveguide with sloped walls in the transverse plane, by using "ROTOR" – rectangular-oblique-tapered-oblique-rectangular - FD mesh, [17,18].

In the "ROTOR" scheme, Fig. 2, rectangular, oblique and tapered co-ordinate systems are utilized together. This scheme shows that rectangular can be combined with other non-orthogonal co-ordinate systems. In general, SR FD-BPM algorithms allow considerable relaxing of the mesh size, offering savings in both computational time and memory.

2.4. Two-dimensional full-vectorial FDM formulation

FD formulas proposed in [19] have been derived under the power series expansion of the electric field components in respect to co-ordinates x and y. The 2D static field (e.g. electrostatics), TEM field (e.g. transmission line field, $\mathbf{E}_z = 0$, $\mathbf{H}_z = 0$) and TM mode field ($\mathbf{H}_z = 0$) have been considered. In linear and isotropic source-free media, by using Maxwell's equations scalar forms,

$$\frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} = 0, \qquad \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} = 0, \qquad (13)$$

the transverse electric field components can be expressed as

$$\mathbf{E}_x(x,y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 x y - a_3 y^2 + \cdots, \quad (14)$$

$$\mathbf{E}_{y}(x,y) = b_{0} + a_{2}x - a_{1}y + \frac{a_{4}}{2}x^{2} - 2a_{3}xy - \frac{a_{4}}{2}y^{2} + \cdots$$
(15)

Assuming that the dielectric interface has no charge, we can apply the integral form of the Maxwell's eqs.,

$$\oint_{S} \mathbf{D} \cdot d\mathbf{s} = 0, \qquad \oint_{C} \mathbf{E} \cdot d\mathbf{l} = 0, \tag{16}$$

on the Gaussian surface S and contour C enclosing two subsequent FD grid points placed close to the interface. If the x and y component of the field are expanded in (14) and (15) up to the 5th order, FD-formulas for E_{x_0} , E_{y_0} and their first, second... derivatives with $O(h^5)$ accuracy can be derived, see [19] for details. Performed test-computations in simple electrostatic and full-vectorial FD-BPM field and eigenmode test-simulations have demonstrated accuracy and stability of derived FD formulas. These results have been expected, as a consequence of the true two-dimensional FD approach. Results obtained in simple TM mode field FD-BPM testsimulations of buried dielectric waveguides are shown in Fig. 3. It can be seen that approach proposed in [19] exhibits a superior behavior in comparison to other improved FD formulas approaches.



Figure 3. Modal index versus mesh size for buried waveguide, [19], cross-section and simulation parameters given in insets of figure, calculated by using different FDM approaches.

FDM Scheme	Formulation	Accuracy	Advantages	Deficiencies
Improved – Yamauchi et al. [8,9]	Semi-vectorial	$O(h^2) - O(h^4)$		Require special positions of the interface and FD grid
Improved – Yamauchi et al. [10]	Full-vectorial	$O(h^2)$		Included the graded-index approximation
Improved – Chiou et al. [11]	Semi-vectorial	$O(h^3) - O(h^4)$	Accurate	Only for rectangular cross- sections
Improved – Chiang et al. [12]	Full-vectorial	$O(h^2)$	Applicable to oblique and curved interfaces	Difficult to improve the accuracy
Benchmark improved – Hadley [14,15]	Full-vectorial	$O(h^4) - O(h^6)$	Very accurate for mode solvers, can be used in benchmark code simulations	Rather tedious FD formulas; a need to calculate Bessel functions; only for TE case and rectangular cross-sections
Structure-related – Djurdjevic et al.[17,18]	Scalar, Semi- vectorial	$O(h^2)$	Enable accurate simulations with reduced computer time	Analytically complex, full-vec- torial formulation does not exist
Improved – Djurdjevic [19]	Full-vectorial	${\cal O}(h^4)$ and higher	Very accurate; true 2D; easy to incorporate in a code	Still under research

Table 1. Summary and comparison of discussed improved FD schemes.

3. CONCLUSION

A few attractive numerical concepts that allow accurate FD treatment of dielectric interfaces are reviewed and compared. So-called improved FD formulas approach has become a standard in CAD simulations in optoelectronics and photonics, although some other approaches are available as well. The comparison of discussed methods is given in Table 1, emphasizing their intrinsic advantages and deficiencies.

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