New Finite-Difference Formulas for Dielectric Interfaces

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Abstract: The finite difference method is often-used numerical simulation method in electromagnetics. In this paper a new methodology is presented that allows the derivation of finite difference formulas near dielectric interfaces with high accuracy. Derived finite difference formulas have been used in the electric field computations in electrostatics (the two-dimensional Laplace’s equation is employed) and in full-vectorial waveguide simulations in photonics (the three-dimensional Helmholtz’s equation and the beam propagation simulation technique in frequency domain are employed). The finite difference formulas derivation is made under a power series expansion of the transverse field components in the case for uniform rectangular discretization mesh. The resulting finite difference formulas provide highly accurate solutions, both for electrostatic and waveguide propagation problems even on coarse grids and thus enable a very cost-effective and rapid numerical field simulations. Reported methodology and derived formulas have not been used in finite difference method formulations in literature. Some results for the electric field computation and dielectric waveguide eigenmode and propagation analysis are presented.

Keywords: Finite difference method, finite difference formulas, finite difference beam propagation method, structure related beam propagation method, staircasing effect, electric field computation, Laplace’s Equation, Helmholtz’s Equation.

1 Introduction

Electromagnetic phenomena are well-presented and described by partial differential equations (PDE).

Except for few elementary and geometrically well-defined cases, closed form analytical solutions are not available for solving PDE, representing electromagnetic boundary value problems. Numerical methods offer a remedy, providing often the only-one and usually the best and the most economical solution.

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Finite difference method (FDM) is perhaps one of the oldest numerical technique for solving PDE. FDM is conceptually simple, straightforward and flexible. Although numerous numerical techniques have been developed and successfully applied for solving PDE in recent decades, FDM remains the most often-used numerical and simulation tool in a broad range of static, steady-state and dynamic electromagnetic problems and applications, covering both frequency and time domain formulations, 2D and 3D cases. FDM is ideally suited and often a favorite approach for CAD simulation software in microwaves, optoelectronics and photonics.

FDM technique has two conceptually different approaches in electromagnetics. If the space dependent partial derivatives in PDE are replaced by approximative difference equations, the standard FDM, or FDM in frequency domain (FDM-FD) is employed. Contrary, if both space and time discretization is present in difference equations, the time domain FDM is implemented. Usually, space and time discretization are performed directly on Maxwell’s equations, so we arrive to the finite difference method in time domain (FD-TD). The latest became increasingly popular in electromagnetic community in recent decade, allowing both simple and accurate time and space electromagnetic field simulations of a wide variety of structures. Unfortunately, tiny time steps in FD-TD simulations require more powerful computers and FD-TD field calculation can be very often time consuming. These are the reasons why FDM-FD still stands as a very attractive concept enabling electromagnetic field simulations at reduced time and computer costs. In this paper the standard FDM and FDM-FD are discussed only.

In this work a new formulation for FD discretization is proposed. The approach is based on a power series expansion of the transverse field components of the electromagnetic field. This approach allows the derivation of novel high accurate FD formulas. Derived FD formulas enable accurate treatment of dielectric interfaces and they have been used in the electric field computations in electrostatics and in full-vectorial waveguide field propagation simulations and eigenmode analysis, based on the frequency domain beam propagation algorithm, in photonics. The FD formulas derivations are given in Section 2, followed by a description of numerical implementation in Section 3. It has been shown that the use of derived FD formulas provide highly accurate solutions and therefore they are ideally suited for implementations in CAD simulation software. The conclusion is drawn in Section 4.
2 Outline of the method

2.1 Basic theoretical concept

In this subsection the basic equations and ideas involved in the standard FDM and FDM-FD approaches will be explained, while more extensive treatment and bibliography can be found for example in [1–3]. Standard FDM usually refers to time and frequency independent problems described by Laplace’s and Poisson’s equations, while FDM-FD is more sophisticated approach. In a waveguide analysis it is the best known and used as the finite difference beam propagation method (FD-BPM). Generally, the FD-BPM is a particular FDM-FD technique for the numerical finite difference solution of an exact vector Helmholtz’s wave equation, [1, 3].

In linear and isotropic media, under the assumption that propagation is in perfectly insulating and \( z \)-invariant dielectric media of refractive index \( n \), in terms of transverse electric field \( \mathbf{E}_t \), Helmholtz’s equation has a well-known form [1],

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

where \( k = \omega \sqrt{\varepsilon_0 \mu_0}, \ n = \sqrt{\varepsilon_r} \) and a differential operator \( \nabla \) is replaced as a sum of transverse and longitudinal part, \( \nabla = \nabla_t + \nabla_z \). The similar equation can be derived for the transverse magnetic field \( \mathbf{H}_t \). In homogeneous regions in the transverse plane, the right-hand side in (1) vanishes, thus (1) becomes

\[
\frac{\partial^2 \mathbf{E}_t}{\partial z^2} = - \left( \nabla_t^2 + k^2 n^2 \right) \mathbf{E}_t.
\]

One could recognize (2) as a near-to-exact starting point for deriving various simplified forms under certain further assumptions and approximations. The most general approximations are:

- **TEM propagation** (e.g. transmission line field, \( \mathbf{E}_z = 0, \mathbf{H}_z = 0 \)) and **TM mode propagation** (\( \mathbf{H}_z = 0 \)), \( \mathbf{E}_t \) is \( z \)-invariant, a second derivative on the left in (2) is zero, giving
  \[
  \left( \nabla_t^2 + k^2 n^2 \right) \mathbf{E}_t = 0.
  \]

- **2D** (\( z \)-invariant) static and quasistatic approximation, \( k \to 0 \), so we could rewrite (3) as
  \[
  \nabla_t^2 \mathbf{E}_t = 0.
  \]

- The most typical approximation of (2) in photonics (lightwave electromagnetics) is the paraxial (or parabolic, or Fresnel) approximation. Assuming

\[
(\nabla_t^2 + \nabla_z^2) \mathbf{E}_t + k^2 n^2 \mathbf{E}_t = \nabla_t \left[ \nabla_t \cdot \mathbf{E}_t - \frac{1}{n^2} \nabla_t (n^2 \mathbf{E}_t) \right],
\]
that the forward travelling wave of typical photonics waveguide-based structures has rapid phase variations and a slowly-varying envelope $E_t$ along the guiding axis $z$, we could rewrite (2) as, [1, 3],

$$\frac{\partial E_t}{\partial z} = \frac{1}{j2n_0k} \left[ \nabla_t^2 + k^2(n^2 - n_0^2) \right] E_t.$$  \hspace{1cm} (5)

In (5) $j = \sqrt{-1}$ and $E_t = E_te^{-j\beta z} = E_t e^{-j\beta n_0 z}$, where $\beta = kn_0$ is the propagation constant and $n_0$ denotes a reference (modal) index. The further assumption used in (5) is that the field envelope variation with $z$ is sufficiently small and the field propagation is dependent only on the first derivative of $z$. Equation (5) is known as the paraxial full-vectorial approximation of (2) and has initiated the development of the very efficient and well-established numerical simulation techniques in photonics and optoelectronics, recognized today as ”the beam propagation methods - (BPM)”, [3]. In the single most often-used BPM, by using finite difference discretization techniques, we arrive to FD-BPM, [1,3–8]. In FD-BPM the transverse (e.g. xy) field is propagated in certain subsequent $z > 0$ ”slices”. The transverse field in one $z$ plane is calculated from the discrete finite difference distribution in the preceding plane, so numerical propagation along the photonics structure is obtained. Note that (3) and (4) can be considered as the special cases or approximations of (5).

In the finite difference approaches of (4) (the standard FDM) and (3), (5) (frequency domain FD-BPM), the main research interests are: developing of so-called improved FD schemes with more accurate treatment of the dielectric interfaces, [9–12], and extending the range of FD-BPM applicability to the waveguide structures changing in the direction of propagation, [5,6,13,14].

FD treatment and discretization of structures with constant cross-section with the refractive transverse index step at the interface between two dielectric regions suffer from reduced accuracy due to the necessary staircase approximation employed by most algorithms, [1,4]. Improved FD-schemes, [8–12,15], enable better accuracy. However, the error introduced at a dielectric interface in all FD implementations is of the order $n - 1$, assuming the order of the uniform region discretization is given by $n$. Dielectric corner points truncate the overall accuracy to the order of $n - 2$, [16]. The use of higher order numerical FD schemes can slightly improve the overall accuracy, [10,15,16], however, staircasing effects at dielectric interfaces and corner points require considerably greater treatment effort.

In this paper a new, simple methodology for FD discretization is proposed. It can be applied in a uniform dielectric region, at a step-like dielectric interface of the arbitrary shape and near dielectric corner points. The details are explained briefly in the next subsection. Bearing in mind that the methodology is still under research,
some of very promising results obtained from the initial numerical experiments are presented.

2.2 Derivation of FD formulas

We begin with power series expansion of the electric field components as functions of two variables, e.g. Cartesian coordinates $x$ and $y$.

\[ E_x(x, y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 xy + a_5 y^2 + a_6 x^3 + a_7 x^2 y + a_8 xy^2 + a_9 y^3 + \cdots, \]  
\[ E_y(x, y) = b_0 + b_1 x + b_2 y + b_3 x^2 + b_4 xy + b_5 y^2 + b_6 x^3 + b_7 x^2 y + b_8 xy^2 + b_9 y^3 + \cdots. \]

We consider 2D $(xy)$ static field (e.g. electrostatics), or TEM field (e.g. transmission line field), when $E_z = 0$, $H_z = 0$ and $E_t = E_x \hat{x} + E_y \hat{y}$. In linear and isotropic source-free media, directly from Maxwell’s equations,

\[ \nabla \cdot E_t = 0, \quad \nabla \times E_t = 0, \]  
\[ \nabla \cdot E_t = 0, \quad \nabla \times E_t = 0, \]  
\[ \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} = 0, \quad \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} = 0. \]

Next, we evaluate power series expansion coefficients in (6) and (7), by using (9),

\[ E_x(x, y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 xy + a_5 y^2 + a_6 x^3 + a_7 x^2 y + a_8 xy^2 + a_9 y^3 + \cdots, \]  
\[ E_y(x, y) = b_0 + b_1 x + b_2 y + b_3 x^2 + b_4 xy + b_5 y^2 + b_6 x^3 + b_7 x^2 y + b_8 xy^2 + b_9 y^3 + \cdots. \]

Comparing two expansion sets, (6) and (7) with (10) and (11), (up to the third order), we can conclude that, actually, only 8 unknown coefficients are sufficient in power series expansions for transverse field components $E_x$ and $E_y$ of the third order, (10) and (11), instead of 20 unknowns, (6) and (7). In general, $n$th order expansions in (6) and (7) require $(n+1)(n+2)$ unknown coefficients $a_i$ and $b_i$, $i = 0, \cdots, n$, but only $2(n+1)$ unknowns in fact. As an example, 8th order power expansion can be completely represented by 18 unknown coefficients only, instead of 90!

The aforementioned expansions (10) and (11) lead us to the very accurate approximative FD-formulas for the field near the dielectric interface.

If we assume that the dielectric interface has no charge, we can apply the integral form of the Gauss’ law,

\[ \int_S \mathbf{D} \cdot \mathbf{ds} = 0, \]
on the Gaussian surface $S$ (a contour $S'$ in Fig. 1 is a cross-section of $S$ in the transverse plane). Recalling $D = \varepsilon E$, and by using expansions (10) and (11), we evaluate

$$\varepsilon_1 2h \left[ b_0 + \frac{a_4 h^2}{6} \right]_{M_1} = \varepsilon_2 2h \left[ b_0 + \frac{a_4 h^2}{6} \right]_{M_2},$$

(13)

and after rearranging (13) we get

$$\varepsilon_r \varepsilon_1 \left[ b_0 + \frac{a_4 h^2}{6} \right]_{M_1} = \varepsilon_r \varepsilon_2 \left[ b_0 + \frac{a_4 h^2}{6} \right]_{M_2}.$$  

(14)

It is obvious, from (10) and (11), that $E_y \big|_{M_1} = b_0 \big|_{M_1}$, $E_y \big|_{M_2} = b_0 \big|_{M_2}$, with

$$a_{4M_1} = \left. \frac{\partial^2 E_y}{\partial x^2} \right|_{M_1} = -\left. \frac{\partial^2 E_y}{\partial y^2} \right|_{M_1} = \left. \frac{\partial^2 E_x}{\partial x \partial y} \right|_{M_1},$$

(15)

and

$$a_{4M_2} = \left. \frac{\partial^2 E_y}{\partial x^2} \right|_{M_2} = -\left. \frac{\partial^2 E_y}{\partial y^2} \right|_{M_2} = \left. \frac{\partial^2 E_x}{\partial x \partial y} \right|_{M_2}.$$  

(16)

Thus, equation (14) can be written in the following form,

$$\varepsilon_{r1} E_y \big|_{M_1} - \varepsilon_{r2} E_y \big|_{M_2} = \frac{h^2}{6} \left[ \varepsilon_{r2} \left. \frac{\partial^2 E_x}{\partial x \partial y} \right|_{M_2} - \varepsilon_{r1} \left. \frac{\partial^2 E_x}{\partial x \partial y} \right|_{M_1} \right] + O(h^2).$$

(17)
Applying the integral form of the second equation in (8),

$$\oint \mathbf{E} \cdot d\mathbf{l} = 0,$$

on contour $C$ in Fig. 1, by using expansions (10) and (11), we evaluate

$$2h \left[ a_0 + \frac{a_3}{3} h^2 \right]_{M_1} = 2h \left[ a_0 + \frac{a_3}{3} h^2 \right]_{M_2}. \quad (19)$$

From (10) and (11) it is obvious that

$$E_x \bigg|_{M_1} = a_0 \bigg|_{M_1}, \quad E_x \bigg|_{M_2} = a_0 \bigg|_{M_2},$$

with

$$a_3 \bigg|_{M_1} = -\frac{\partial^2 E_x}{\partial x^2} \bigg|_{M_1} = -\frac{1}{2} \frac{\partial^2 E_y}{\partial x \partial y} \bigg|_{M_1}, \quad (20)$$

and similarly for $a_3 \bigg|_{M_2}$, thus, (19) can be written in the following form,

$$E_x \bigg|_{M_1} - E_x \bigg|_{M_2} = \frac{h^2}{6} \left[ \frac{\partial^2 E_y}{\partial x \partial y} \bigg|_{M_1} - \frac{\partial^2 E_y}{\partial x \partial y} \bigg|_{M_2} \right] + O(h^2). \quad (21)$$

In a more realistic case when dielectric interface is arbitrarily placed between two subsequent grid lines, integrations in (12) and (18) over $S$ and $C$, Fig. 2, (a contour $S'$ in Fig. 2 is a cross-section of $S$ in the transverse plane), yield

$$\varepsilon_1 \left[ b_0 + \frac{a_4}{6} h^2 - a_1 h_1 - \frac{a_4}{2} h_1^2 \right]_{M_1} = \varepsilon_2 \left[ b_0 + \frac{a_4}{6} h^2 - a_1 h_2 - \frac{a_4}{2} h_2^2 \right]_{M_2}, \quad (22)$$

$$\left[ a_0 + \frac{a_3}{3} h^2 + a_2 h_1 - a_3 h_1^2 \right]_{M_1} = \left[ a_0 + \frac{a_3}{3} h^2 + a_2 h_2 - a_3 h_2^2 \right]_{M_2}, \quad (23)$$

where $h_1 + h_2 = h$, and $h = \Delta x = \Delta y = \Delta$ is a distance between two subsequent grid lines in the transverse rectangular FD-mesh adopted, uniformly spaced both in $x$ and $y$ directions, Fig. 2. We have considered only first 6 terms in (10) and (11) expansions (up to the second order). Choosing the derivation form of coefficients $a_i, i = 1, \cdots, 4$, $a_3$ and $a_4$ are defined in (15) and (20), $a_1$ and $a_2$ can be easily obtained from (10) and (11),

$$a_1 \bigg|_{M_1} = \frac{\partial E_x}{\partial x} \bigg|_{M_1} = -\frac{\partial E_y}{\partial y} \bigg|_{M_1}, \quad a_2 \bigg|_{M_1} = \frac{\partial E_x}{\partial y} \bigg|_{M_1} = \frac{\partial E_y}{\partial x} \bigg|_{M_1}. \quad (24)$$
Fig. 2. Non-square 2D rectangular cell arbitrarily placed at the interface of two dielectric media. Points $M_1$ and $M_2$ are placed at two subsequent grid lines.

and similarly for $a_1|_{M_2}$ and $a_2|_{M_2}$, equations (22) and (23) can be rewritten as

$$
\varepsilon_{r1}E_y|_{M_1} - \varepsilon_{r2}E_y|_{M_2} = \frac{h^2}{6} \left[ \left( p_2 \frac{\partial E_x}{\partial x} + q_2 \frac{\partial^2 E_x}{\partial x \partial y} \right)_{M_2} - \left( p_1 \frac{\partial E_x}{\partial x} + q_1 \frac{\partial^2 E_x}{\partial x \partial y} \right)_{M_1} \right] + O(h^2),
$$

(25)

$$
E_x|_{M_1} - E_x|_{M_2} = \frac{h^2}{6} \left[ \left( r_1 \frac{\partial E_y}{\partial x} + s_1 \frac{\partial^2 E_y}{\partial x \partial y} \right)_{M_1} - \left( r_2 \frac{\partial E_y}{\partial x} + s_2 \frac{\partial^2 E_y}{\partial x \partial y} \right)_{M_2} \right] + O(h^2).
$$

(26)

In (25) and (26) new coefficients $p, q, r$ and $s$ are

$$
p_1 = -\varepsilon_{r1} \frac{6h_1}{h^2}, \quad q_1 = \varepsilon_{r1} \left( 1 - \frac{3h_1^2}{h^2} \right), \quad p_2 = -\varepsilon_{r2} \frac{6h_2}{h^2}, \quad q_2 = \varepsilon_{r2} \left( 1 - \frac{3h_2^2}{h^2} \right),
$$

(27)

$$
r_1 = -\frac{6h_1}{h^2}, \quad s_1 = \left( 1 - \frac{3h_1^2}{h^2} \right), \quad r_2 = -\frac{6h_2}{h^2}, \quad s_2 = \left( 1 - \frac{3h_2^2}{h^2} \right).
$$

(28)

Formulas (17), (21), (25) and (26) are second order accurate. Formulas with higher order of accuracy can be derived in the similar way, by extending the order of power series in (10) and (11) expansions. Those formulas give the relation between transverse field components $E_x$ and $E_y$ and their derivatives calculated at two adjacent points $M_1$ and $M_2$ near, but on the opposite sides of the dielectric interface. Earlier reported improved finite difference formulas, [9, 10, 12], have been constructed under the similar concept. However, improved formulas are derived under one-dimensional expansions with the accuracy limited to the 2nd order, $O(h^2)$, if a
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dielectric interface is placed symmetrically between two FD grid lines. Otherwise the accuracy decreases to the 1st order. Much more accurate improved formulas have been proposed by Hadley, [15, 16], yielding 5th order of accuracy, but only if a grid line coincides with an interface. Advantages of the methodology and FD formulas presented in this paper are: 1) they are derived under two-dimensional expansions; 2) the location of the interface and grid lines does not affect the accuracy; and 3) formulas with higher order of accuracy can be derived in the similar manner with the small amount of additional computational effort.

Fig. 3 shows the uniform rectangular grid scheme, in xy coordinate system, used in derivation of the finite difference formulas near a dielectric interface. Five adjacent points to the interface point \( M \) are used to obtain formulas with the 5th order of accuracy.

For the \( x \) component of the field we can evaluate (10) and (11) up to the 5th order of the power series expansion, over the stencil diagram in Fig. 3, in the following systematic way:

\[
(E_x)_{i,j} = E_x(0,0) = E_{x0} = a_0, \tag{29}
\]

\[
(E_x)_{i+1,j} = E_x(h,0) = E_{x2} = a_0 + a_1 h + a_3 h^2 + a_6 h^3 + a_{10} h^4 + a_{15} h^5 + \cdots, \tag{30}
\]

\[
(E_x)_{i,j+1} = E_x(0,h) = E_{x3} = a_0 + a_2 h - a_3 h^2 - \frac{1}{3} a_7 h^3 + a_{10} h^4 + \frac{1}{5} a_{16} h^5 + \cdots, \tag{31}
\]

and similarly for \((E_x)_{i-1,j} \), \((E_x)_{i+1,j+1} \) = \( E_{x5} \) and \((E_x)_{i-1,j+1} \) = \( E_{x4} \).

For the \( y \) component of the electric field,

\[
(E_y)_{i,j} = E_y(0,0) = E_{y0} = b_0, \tag{32}
\]

\[
(E_y)_{i+1,j} = E_y(h,0) = E_{y2} = b_0 + a_2 h + \frac{1}{2} a_4 h^2 + \frac{1}{3} a_7 h^3 + \frac{1}{4} a_{11} h^5 + \frac{1}{5} a_{16} h^5 + \cdots, \tag{33}
\]

\[
(E_y)_{i,j+1} = E_y(0,h) = E_{y3} = b_0 - a_1 h + \frac{1}{2} a_4 h^2 + a_6 h^3 + \frac{1}{4} a_{11} h^5 - a_{15} h^5 + \cdots, \tag{34}
\]

and similarly for \((E_y)_{i-1,j} \), \((E_y)_{i+1,j+1} \) = \( E_{y5} \) and \((E_y)_{i-1,j+1} \) = \( E_{y4} \).

Presented methodology provides us with 10 linear algebraic equations. Unknowns can be calculated, yielding FD-formulas for \( E_{x0}, E_{y0} \) and their derivatives with 5th order of accuracy. Calculations lead to the results for \( E_{x0} \) and \( E_{y0} \),

\[
E_{x0} = \frac{1}{10} \left[ 3E_{x1} - 3E_{x2} + 3E_{y3} - 3E_{y5} - \left( E_{x1} + E_{x2} - 10E_{x3} - E_{x4} - E_{x5} \right) \right] + O(h^5), \tag{35}
\]

\[
E_{y0} = -\frac{1}{10} \left[ 3E_{x1} - 3E_{x2} + 3E_{y4} - 3E_{y5} + \left( E_{y1} + E_{y2} - 10E_{y3} - E_{y4} - E_{y5} \right) \right] + O(h^5), \tag{36}
\]
and for derivatives, in terms of coefficients $a_i$,

$$a_1 = \frac{1}{10h} \left[ E_{x_4} - E_{x_2} + E_{x_4} - E_{x_5} + (20E_{y_0} - 3E_{y_1} - 3E_{y_2} - 10E_{y_3} - 2E_{y_4} - 2E_{y_5}) \right] + O(h^5),$$ (37)

$$a_2 = \frac{1}{10h} \left[ 20E_{x_0} - 3E_{x_1} - 3E_{x_2} - 10E_{x_3} - 2E_{x_4} - 2E_{x_5} - \left( E_{y_1} - E_{y_2} + E_{y_4} - E_{y_5} \right) \right] + O(h^5),$$ (38)

$$a_3 = \frac{1}{4h^2} \left[ -10E_{x_0} + 2E_{x_1} + 2E_{x_2} + 4E_{x_3} + E_{x_4} + E_{x_5} + \left( 2E_{y_1} - 2E_{y_2} + E_{y_4} - E_{y_5} \right) \right] + O(h^5),$$ (39)

$$a_4 = \frac{1}{2h^2} \left[ -2E_{x_1} + 2E_{x_2} - E_{x_4} + E_{x_5} - \left( 10E_{y_0} - 2E_{y_1} - 2E_{y_2} - 4E_{y_3} - E_{y_4} - E_{y_5} \right) \right] + O(h^5).$$ (40)

Expressions (37-40) give formulas for the first and the second derivatives in $x$ and $y$ only. Higher order derivatives can be computed by the similar procedure.

Similar FD-formulas can be derived for the stencils given in Fig. 4, Fig. 5 and Fig. 6. In convenience, only (35-36)-like formulas are presented here. For stencil depicted in Fig. 4, formulas for $E_{x_0}, E_{y_0}$ are:

$$E_{x_0} = -\frac{1}{10} \left[ 3E_{x_1} - 3E_{x_2} + 3E_{x_3} - 3E_{x_4} + \left( E_{x_1} + E_{x_2} - 10E_{x_3} - E_{x_4} - E_{x_5} \right) \right] + O(h^5),$$ (41)

$$E_{y_0} = +\frac{1}{10} \left[ 3E_{x_1} - 3E_{x_2} + 3E_{x_3} - 3E_{x_4} - \left( E_{x_1} + E_{x_2} - 10E_{x_3} - E_{x_4} - E_{x_5} \right) \right] + O(h^5).$$ (42)

For stencil depicted in Fig. 5, FD-formulas for $E_{x_0}, E_{y_0}$ are:

$$E_{x_0} = \frac{1}{10} \left[ 3E_{x_1} - 3E_{x_2} + 3E_{x_3} - 3E_{x_4} - \left( E_{x_1} + E_{x_2} - 10E_{x_3} - E_{x_4} - E_{x_5} \right) \right] + O(h^5),$$ (43)

$$E_{y_0} = -\frac{1}{10} \left[ 3E_{x_1} - 3E_{x_2} + 3E_{x_3} - 3E_{x_4} + \left( E_{x_1} + E_{x_2} - 10E_{x_3} - E_{x_4} - E_{x_5} \right) \right] + O(h^5).$$ (44)
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3 Numerical results

To illustrate the effectiveness of the new FD formulas we will consider a simple electrostatic test problem and a FD-BPM simulation example. In both examples the iterative FD solution of the transverse electric field components $E_x$ and $E_y$ is calculated and presented in terms of computational error.

3.1 Electrostatic test example

The efficiency and accuracy of resulting finite difference formulas have been tested using a simple electrostatic problem with known analytical solution and with Dirichlet’s boundary conditions. The cross-section of an isolated line charge of
uniform density $q'$ parallel to the dielectric interface separating whole space in two half-spaces with different permittivities $\varepsilon_1$ and $\varepsilon_2$ is shown in Fig. 7, assuming $|X_0, Y_0| > |L_w, L_{wd}, L_{wu}|$.

The electric field components $E_x$ and $E_y$ at the boundaries are computed analytically, but the field inside the square computational window ($L_{wd} + L_{wu} = 2L_w$) is computed numerically.

Although a problem is simple, the goal has been to measure accuracy and stability of derived FD formulas.

![Fig. 7. Coordinate system and geometry for the test problem. FD grid lines are uniformly spaced in the $x$ and $y$ directions and arbitrarily placed in respect to the dielectric interface.](image)

For the adopted geometry, $Y_0 > 0$, the electric field components at any $(x_i, y_j)$ point inside the computational window or at the window boundaries, normalized by the factor $\frac{2\pi}{q'}$, are well-known to be,

$$E_{x_{ij}} = \frac{x_i - X_0}{R^2} + \alpha \frac{x_i - X_0}{R'^2}, \quad E_{y_{ij}} = \frac{y_j - Y_0}{R^2} + \alpha \frac{y_j + Y_0}{R'^2},$$

(47)

for $y \geq 0$, and

$$E_{x_{ij}} = \beta \frac{x_i - X_0}{R'^2}, \quad E_{y_{ij}} = \beta \frac{y_j - Y_0}{R'^2},$$

(48)

for $y \leq 0$. In (47) and (48) $R$ and $R'$ are

$$R^2 = (x_i - X_0)^2 + (y_j - Y_0)^2, \quad R'^2 = (x_i - X_0)^2 + (y_j + Y_0)^2,$$

(49)

while coefficients $\alpha$ and $\beta$ are defined as

$$\alpha = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}, \quad \beta = \frac{2\varepsilon_1}{\varepsilon_1 + \varepsilon_2}.$$

(50)
Formulas (47-50) are used to calculate the exact Dirichlet’s boundary conditions at the window edges, and later to obtain the exact values of the field for comparison with the numerical results.

Computations within this test problem have been performed on a variety of uniform grids in respect to grid density and placement, for $y = 0$ and for $x = 0$ dielectric interface, for different positions of the line charge $q'(X_0, Y_0)$ and for several values of permittivities $\varepsilon_1$ and $\varepsilon_2$, including the cases when one half-space permittivity tends to infinity imitating therefore the perfectly conducting medium. In uniform region the well-known five-point (2nd order of accuracy) and the nine-point (better than 6th order of accuracy) FD formulas have been incorporated in the algorithm.

Performed computations have confirmed that presently derived finite difference formulas have truncation error proportional to the grid size, with the expected 5th order of accuracy for the FD formulas (35-36) and (41-46) and the 2nd order of truncation order for formulas (25) and (26). Accuracy order of (25) and (26) can be easily improved by adding higher order derivatives in formulas.

Fig. 8 and Fig. 9 show the normalized surface error distribution in $E_x$ and $E_y$ computations inside the square computational window ($L_w = L_wd = L_wu = 1$). The $x$ axis coincides with the dielectric interface of two dielectric media ($\varepsilon_{r1} = 1$ and $\varepsilon_{r2} = 5$). In uniform regions the nine-point FD formula has been used (yielding in all test computations an apparent eight order truncation error for the uniform FD mesh). Figures show the surface error distribution evaluated for the $50 \times 50$ mesh with $\Delta_x = \Delta_y = h = \Delta = 0.04$.

For both field components $E_x$ and $E_y$, the normalized relative error is calculated as

$$\text{error}_{\text{norm}} = \frac{\text{error}_{\text{relative}}}{\Delta^5} = \frac{1}{\Delta^5} \frac{E_{\text{exact}} - E_{\text{calculated}}}{E_{\text{exact}}}.$$  (51)
From diagrams shown in Fig. 8 and Fig. 9 it can be seen that normalized error is less than 1, insuring $O(h^5) = O(\Delta^5)$ order of accuracy. Thus, the use of the standard five-point FD formula, $O(h^2)$, in the uniform region will give considerably higher magnitude of the error in comparison to the interface discretization, $O(h^5)$!

### 3.2 Photonics example

Unfortunately, the analytical solution for any of 3D optoelectronic waveguide structures with the rectangular cross-section is not known.

In keeping with the topic of this paper, a simple buried waveguide has been analyzed (Fig. 10) and the most realistic and practical case has been considered - the full-vectorial beam propagation and eigenmode computation. The full-vectorial FD-BPM is adopted because of the presence of both transverse field components. Although much simpler, the scalar and polarized numerical simulations could have not lead us to the appropriate conclusions. Only TM propagation has been treated in this paper, but the same methodology could be straightforwardly applied to TE cases, even possibly with the higher accuracy.

In TM case, using the FD-BPM numerical simulation technique, the transverse electric field $E_t$ of the waveguide structure is propagated, equation (5), numerically from one $z_i$ to subsequent $z_{i+1}$ "slice". If the structure cross-section is $z$-invariant, the paraxial steady-state field regime occurs after certain $z$ steps, under the conditions that the reference index is properly determined and the open waveguide boundaries are properly treated canceling the leakage of the energy out from the
computational window. The numerical simulation of the field propagation along the structure and the reference (modal) index evaluation are highly dependent on the electric field discretization accuracy in the transverse plane, especially near the step-index interfaces and dielectric corners. If the discretization accuracy is low, increasing the accuracy of the result requires a finer discretization grid and thus significant increase in numerical effort and computer simulation time.

Scalar equations (9) are valid for the static and TEM fields in the source-free region. However, having in mind that in TM propagation the $z$ component of the magnetic field is equal to zero, $H_z = 0$, (9) can be used in TM case as well, providing us with benefits of the methodology proposed in this paper.

It is well-known that certain components of the electric field exhibit singular behavior near a dielectric corner (see for example [16]). To avoid as much as possible the influence of corners on the overall result, discretization in the transverse plane, performed in this paper, has been done by placing interfaces at the middle between two grid lines, see Fig. 10, thus using formulas (25) and (26) everywhere near interfaces, except in corner neighbouring discretization points. Referring to the dielectric corner in Fig. 10, for the field in points A, B, C and D, the following formulas, with truncation error of the order 3, have been derived and used:

$$E_x|_c = E_{x,i,j} = E_{x,i+1,j+1} - E_{y,i+1,j} + E_{y,j+1} + O(h^3),$$  \hspace{1cm} (52)
\[
E_y|_c = E_{y,i} = E_{y,i+1,j+1} + E_{x,i+1,j} - E_{x,i,j+1} + O(h^3), \\
E_x|_d = E_{x,i} = E_{x,i-1,j+1} + E_{y,i-1,j} - E_{y,i,j+1} + O(h^3), \\
E_y|_d = E_{y,i} = E_{y,i-1,j+1} - E_{x,i-1,j} + E_{x,i,j+1} + O(h^3), \\
E_{x,a} = E_{x,i} = E_{x,i-1,j-1} - E_{y,i-1,j} + E_{y,i,j-1} + O(h^3), \\
E_{y,a} = E_{y,i} = E_{y,i-1,j-1} + E_{x,i-1,j} - E_{x,i,j-1} + O(h^3), \\
E_{x,b} = E_{x,i} = E_{x,i+1,j-1} + E_{y,i+1,j} - E_{y,i,j-1} + O(h^3), \\
E_{y,b} = E_{y,i} = E_{y,i+1,j-1} - E_{x,i+1,j} + E_{x,i,j-1} + O(h^3).
\]

Table 1. Reference (modal) index $n_{ref}$ of the buried waveguide, cross-section given in Fig. 10, low-index contrast case, for different mesh sizes. Table gives the uniform mesh step, $\Delta$, the relative computational error, and the used CPU run-time in the imaginary distance BPM simulations.

<table>
<thead>
<tr>
<th>mesh size</th>
<th>$\Delta$ [$\mu$m]</th>
<th>$n_{ref}$</th>
<th>error$_{relative}$</th>
<th>CPU time [min:s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>42 × 42</td>
<td>0.12500</td>
<td>1.2722253</td>
<td>0.000727</td>
<td>00:01</td>
</tr>
<tr>
<td>82 × 82</td>
<td>0.06250</td>
<td>1.2715934</td>
<td>0.000231</td>
<td>00:07</td>
</tr>
<tr>
<td>122 × 122</td>
<td>0.04166</td>
<td>1.2714600</td>
<td>0.000125</td>
<td>00:22</td>
</tr>
<tr>
<td>162 × 162</td>
<td>0.03125</td>
<td>1.2714077</td>
<td>0.000084</td>
<td>00:51</td>
</tr>
<tr>
<td>202 × 202</td>
<td>0.02500</td>
<td>1.2713807</td>
<td>0.000063</td>
<td>01:36</td>
</tr>
<tr>
<td>242 × 242</td>
<td>0.02083</td>
<td>1.2713645</td>
<td>0.000050</td>
<td>02:39</td>
</tr>
<tr>
<td>282 × 282</td>
<td>0.01785</td>
<td>1.2713538</td>
<td>0.000041</td>
<td>05:04</td>
</tr>
<tr>
<td>322 × 322</td>
<td>0.01562</td>
<td>1.2713462</td>
<td>0.000036</td>
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</tr>
<tr>
<td>362 × 362</td>
<td>0.01389</td>
<td>1.2713405</td>
<td>0.000031</td>
<td>09:50</td>
</tr>
<tr>
<td>402 × 402</td>
<td>0.01250</td>
<td>1.2713361</td>
<td>0.000028</td>
<td>11:00</td>
</tr>
</tbody>
</table>

In the uniform regions of the refractive index $n_0$ and $n$ the standard five-point FD formula has been used, so discretization of the whole computational domain has been utilized by using formulas with $O(h^2)$ and $O(h^3)$ order of accuracy. A standard Crank-Nicolson method has been used to simulate propagation in the $z$ direction, and due to the well confined waveguide field Hardley’s transparent boundary conditions (TBC), [17], have been introduced at the edges of the computational window. For eigenmode solving, the efficient imaginary distance beam propagation algorithm has been applied, [18].

Numerical simulations have been performed for two different buried waveguide structures: low-index contrast one, with $n = 1.5$ ($\varepsilon_r = n^2 = 2.25$), 2$d = 1 \mu$m, and the strong-index contrast waveguide, with $n = 3.4$ ($\varepsilon_r = 11.56$), 2$d = 0.5 \mu$m.

The wavelength has been kept at $\lambda = 1.5 \mu$m in both cases. BPM step used in imaginary distance and one-way propagation has been chosen to be $\Delta z =$
0.1 μm, dimensions of the square computational domain have been truncated at $L_{w} = 2.5 \mu m$ in low, and at $L_{w} = 1.25 \mu m$ in strong-index contrast simulations. The imaginary distance algorithm has been set to enable $10^{-7}$ order of accuracy (seven significant digits).

![Fig. 11. Calculated modal index versus mesh size for buried waveguide shown in Fig. 10, low-index contrast case.](image)

Results for $n_{ref}$ obtained in simulations in low-index contrast case are tabulated in Table 1, together with data showing the total CPU use during the C++ code execution on PC (32-bit OS, 2.0 GHz) and the relative error computed against the extrapolated value for $n_{ref}$ (the simple, but efficient, Aitken $\delta^2$ method has been used to yield $n_{ref, extr.} = 1.271301$, low-index contrast case, and $n_{ref, extr.} = 2.844921$, for strong-index contrast case). Values for CPU evaluation time represent the necessity to perform as more accurate FD discretization as possible, since the mesh refinement implies a drastic increase of computer run-time.

Fig. 11 and Fig. 12 show the computed TM modal index $n_{ref}$ versus number of grid lines in the $x$ ($N_x$), and the $y$ ($N_y$) directions. Also shown in figures Fig. 11 and Fig. 12 are comparisons with results obtained by using methods published in [9, 12]. Figures demonstrate the faster convergence of the present discretization model as the grid size is reduced, specially in the strong-index contrast case. Those results have been expected, as a consequence of the present approach where the true two-dimensional FD formulas for interfaces and corners have been employed. Note that proposed improved FD formulas in [9, 12] are, in fact, one-dimensional.
4 Conclusion

Novel FD formulas have been derived and successfully applied to the electric field analysis in electrostatics and optoelectronics. Numerical simulations, based on efficient algorithm built under proposed approach, have been carried out to solve eigenmodes and to study the beam-propagation in some simple waveguide structures with step-index sections. The propagation of the fundamental TM mode of the buried waveguide in the rectangular coordinate system is studied and results compared with those obtained from simulations based on previously reported improved finite difference mesh algorithms. The simulated results demonstrate the advantages and generality of the proposed approach and presently derived FD formulas over standard and improved formulas in rectangular coordinate system, namely the propagation error is reduced enabling very accurate analysis with coarser meshes, consequently offering significant computational resource savings. In addition, the flexibility of the approach can allow the comfortable analysis of TEM structures and TE and TM waveguide-based optoelectronic circuits, which are frequently used today in the photonics design.

References

New Finite-Difference Formulas for Dielectric Interfaces


