Ultra-Wide-Angle Beam Propagation Method Based on High-Order Finite-Difference

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Abstract - The true fourth-order finite-difference scheme is incorporated into an ultra wide-angle beam propagation method (BPM) based on Padé series expansion. A comprehensive study for the accuracy of various finite-difference (FD) formulas in literature for the wide-angle beam propagation method is presented. It is demonstrated that the new high-order FD wide-angle BPM is highly accurate for efficient simulation of wide-angle field propagation and is superior to the other FD schemes in the case of high index contrast and/or ultra wide-angle propagation.

Index Terms - Beam propagation method (BPM), discontinuities, finite difference methods, step-index optical waveguides.

I. INTRODUCTION

Beam propagation method (BPM) based on finite-difference (FD) schemes is one of the most popular numerical techniques for simulation of electromagnetic field propagation in optical waveguides and photonic integrated circuits. The wide-spread acceptance and application of the FD-based BPM are primarily due to its relative ease of mesh implementation in comparison with other methods such as the finite element methods (FEM) [1]. It is well-known that one of the main limiting factors for the accuracy of the FD-BPM arises from the finite difference schemes for the second-order derivatives in the transverse direction. The conventional central differencing [2] is of second-order in the transverse mesh discretization (i.e., Δx and Δy). Several improved formulations with lower truncation errors have been derived for the optical waveguide mode solvers [3]-[6]. Parallel development has also occurred to the beam propagation methods, where most of the applications of high-order FD formulas have been restricted to the paraxial approximations [7]-[9].

Yamauchi et al. first introduced the Douglas scheme to a wide-angle FD-BPM [10], [11] in which the truncation error is reduced to the fourth order for the case of graded-index waveguides. The discussion is limited to the TE polarization only. Vassallo formulated a wide-angle algorithm based on high-order formulas by using Taylor series expansions to approximate the exponential function of the square root operator [12], [13]. The treatment of discontinuities in the refractive index results in the second-order accurate FD formula even at the discontinuities as long as the index interfaces lie midway between the adjacent grid points. Hadley proposed a quasi-fourth-order scheme [14] for step-index waveguides in which the grid points coincide with the dielectric boundary, and applied this scheme for the wide-angle beam propagation using the Padé (1.1) approximation [15]. The higher-order field derivatives are evaluated through the Helmholtz propagation equation and complex averaging techniques. So far, no attempt has been made to generalize the wide-angle algorithm to the ultra wide-angle propagation schemes involving higher-order Padé approximation.

Chiou et al. derived a fourth-order accuracy FD formula by the Taylor series expansion and matching the interface conditions for a step-index profile regardless of the existence of the interface [16]. Different from the previous high-order finite differing schemes, the formulas developed in [16] maintains the fourth-order
truncation error even in the presence of index discontinuities. Because of its general and simple algebraic form, Chiou’s truly fourth-order scheme can be applied to both mode solvers and propagation analyses. In this work, by taking advantage of the Padé approximation to the square root operator [17], we have successfully incorporated the truly fourth-order formula into an ultra-wide-angle scheme based on Padé series expansion. In the case of 2D waveguide structures, the high-order FD discretization and the implementation of the PML numerical boundary conditions lead to a tridiagonal matrix and can be readily solved. Both TE and TM polarizations are considered for waveguide structures with high index contrast and/or ultra-wide angle propagation. For the sake of comparison, the conventional central-differencing scheme and several other high-order finite-difference formulas are also incorporated into the BPM and their scope of validity and degree of accuracy are accessed in a systematic fashion. Section II gives the procedure for the combination of high-order formulas with the ultra-wide-angle algorithm. Various formulas are assessed through numerical results in section III. Section IV summarizes the main conclusions.

II. FORMULATIONS

A. Governing Equation

For the sake of simplicity, we confine our discussions to two-dimensional structures throughout this paper. If the refractive index varies slowly along \( z \) (the propagation direction), the governing Helmholtz equation in terms of the transverse electric fields is given by [18]

\[
\left( \frac{\partial^2}{\partial z^2} + P \right) E = 0
\]  

(1)

where \( E \) represents \( E_y \) for TE polarization (\( y \) polarized transverse E field) or \( E_x \) for TM polarization (\( x \) polarized transverse E field), and the operator \( P \) is defined as

\[
P = \begin{cases} 
\frac{\partial^2}{\partial x^2} + k_0^2 n^2 & \text{TE polarization} \\
\frac{\partial}{\partial x} \left[ \frac{1}{n^2} \frac{\partial}{\partial x} \right] + k_0^2 n^2 & \text{TM polarization}
\end{cases}
\]

(2)

where \( k_0 \) is the vacuum wave vector and \( n = n(x, z) \) is the refractive index of the medium. The time dependence of the field is assumed to be \( e^{j\omega t} \). By assuming the wave propagates along \(+z\) direction, the field \( E(x, z) \) can be expressed as

\[
E(x, z) = \Psi(x, z) e^{-jk_0 n_0 z}
\]

(3)

where \( \Psi(x, z) \) represents the slow varying field and \( n_0 \) is the reference refractive index. Substituting (3) into (1), we obtain the Helmholtz equation written in terms of the slow varying field

\[
\frac{\partial^2 \Psi}{\partial z^2} - j2k_0 n_0 \frac{\partial \Psi}{\partial z} + k_0^2 n_0^2 \Psi = 0
\]

(4)

where the operator \( \overline{P} \) takes the form of

\[
\overline{P} = \begin{cases} 
\frac{1}{k_0^2 n_0^2} \left[ \frac{\partial^2}{\partial x^2} + k_0^2 \left(n^2 - n_0^2\right) \right] & \text{TE} \\
\frac{1}{k_0^2 n_0^2} \left[ \frac{\partial}{\partial x} \left( \frac{1}{n^2} \frac{\partial}{\partial x} \right) + k_0^2 \left(n^2 - n_0^2\right) \right] & \text{TM}
\end{cases}
\]

(5)

Ignoring the backward field yields the following one-way Helmholtz equation [15]

\[
\frac{\partial \Psi}{\partial z} = -jk_0 n_0 \left( \sqrt{1 + \overline{P}} - 1 \right) \Psi
\]

(6)

B. Ultra-Wide-Angle Scheme Based on Padé Series Approximations

Note that (6) contains the square root operator which is not amendable to direct numerical solution without rationalization. In this respect,
several approaches have been proposed to resolve this problem in both underwater acoustics [17], [19] and integrated optics [15], [20], [21]. Since the emphasis of this paper is the application of the high-order FD formulas to the ultra wide-angle scheme, we employ the efficient multi-step method based on the Padé series approximation [22].

Given the field at the propagation distance \( z \), the analytical solution of (6) at \( z + \Delta z \) is

\[
\Psi(z + \Delta z) = \exp \left[ -jk_0n_0\Delta z (\sqrt{1 + \frac{P}{\rho}} - 1) \right] \Psi(z). \tag{7}
\]

The square root operator on the right side of (7) is approximated by [22]

\[
\sqrt{1 + X} \approx 1 + \sum_{k=1}^{m} \frac{a_{k,m}X}{1 + b_{k,m}X}
\]

where

\[
a_{k,m} = \frac{2}{2m+1} \sin^2 \left( \frac{k\pi}{2m+1} \right)
\]

\[
b_{k,m} = \cos^2 \left( \frac{k\pi}{2m+1} \right). \tag{10}
\]

The multi-step scheme is achieved by rewriting (7) as

\[
\Psi(z + \Delta z) = \exp \left( -jk_0n_0\Delta z \sum_{k=1}^{m} \frac{a_{k,m}P}{1 + b_{k,m}P} \right) \Psi(z)
\]

\[
= \prod_{k=1}^{m} \exp \left( -jk_0n_0\Delta z \frac{a_{k,m}P}{1 + b_{k,m}P} \right) \Psi(z) \tag{11}
\]

from which the \( k \)th step takes the form

\[
\Psi \left[ z + k\Delta z / m \right] = \exp \left( -jk_0n_0\Delta z \frac{a_{k,m}P}{1 + b_{k,m}P} \right) \Psi \left[ z + (k-1)\Delta z / m \right]. \tag{12}
\]

With the Crank-Nicholson scheme [23] for the exponential function in (12), we obtain the following approximate equation in which only the transverse differential operator is retained

\[
\Psi \left[ z + k\Delta z / m \right] = \frac{1 + c_{k,m}P}{1 + c_{k,m}P} \Psi \left[ z + (k-1)\Delta z / m \right] \tag{13}
\]

where

\[
c_{k,m} = b_{k,m} - \frac{jk_0n_0\Delta z}{2} a_{k,m}. \tag{14}
\]

### C. High-Order FD Formulas

To obtain the numerical solution of (13), FD formulas are required to replace differential operators. Following the procedure proposed by Chiu et al. [16], we derive the E-field formulation as follows.

Consider the three consecutive points shown in Fig. 1, where refractive index discontinuities exist between sampling points.

Fig. 1. Schematics of grid points with discontinuities.

Using the Taylor series expansion within a uniform medium, \( \Psi_L \) is expanded in terms of \( \Psi_i \) as

\[
\Psi_L = \Psi_i + \frac{p}{1!} \frac{\partial \Psi_i}{\partial \chi} + \frac{p^2}{2!} \frac{\partial^2 \Psi_i}{\partial \chi^2} + \frac{p^3}{3!} \frac{\partial^3 \Psi_i}{\partial \chi^3} + \frac{p^4}{4!} \frac{\partial^4 \Psi_i}{\partial \chi^4} + \frac{p^5}{5!} \frac{\partial^5 \Psi_i}{\partial \chi^5} + O(h^6). \tag{15}
\]

Similarly, \( \Psi_{i+1} \) is expressed in terms of \( \Psi_R \) as
\[
\Psi_{i+1} = \Psi_R + \Psi_L + \frac{q}{2!} \frac{\partial^2 \Psi_R}{\partial x^2} + \frac{q^2}{3!} \frac{\partial^3 \Psi_R}{\partial x^3} + O(h^5) \\
+ \frac{q^3}{4!} \frac{\partial^4 \Psi_R}{\partial x^4} + \frac{q^4}{5!} \frac{\partial^5 \Psi_R}{\partial x^5} + O(h^6)
\]  
(16)

To guarantee the fourth-order accuracy, we let the refractive index discontinuity lie midway between sampling points, i.e., \( p = q = h/2 \). The boundary conditions require that

\[
\Psi_R = \theta \Psi_L 
\]  
(17)

\[
\Psi_R' = \Psi_L' 
\]  
(18)

where

\[
\theta = \begin{cases} 
1 & \text{TE polarization} \\
\frac{n_1^2}{n_2^2} & \text{TM polarization}
\end{cases}
\]  
(19)

The higher-order derivatives of \( \Psi_R \) and \( \Psi_L \) are connected by the one-dimensional Helmholtz equation

\[
\beta^2 \Psi = \left( \frac{\partial^2}{\partial x^2} + k_n^2 n_i^2 \right) \Psi.
\]  
(20)

From (17) and (20), we have

\[
\left( \frac{\partial^2}{\partial x^2} + k_n^2 n_{i+1}^2 \right) \Psi_R = \left( \frac{\partial^2}{\partial x^2} + k_n^2 n_i^2 \right) \theta \Psi_L
\]  
(21)

or

\[
\Psi_R'' = \theta \left( \Psi_L'' + \eta \Psi_L' \right).
\]  
(22)

Similarly, the higher-order derivatives of \( \Psi_R \) and \( \Psi_L \) are connected as

\[
\Psi_R^{(3)} = \Psi_L^{(3)} + \eta \Psi_L' \]  
(23)

\[
\Psi_R^{(4)} = \theta \left( \Psi_L^{(4)} + 2 \eta \Psi_L'' + \eta^2 \Psi_L' \right)
\]  
(24)

\[
\Psi_R^{(5)} = \Psi_L^{(5)} + 2 \eta \Psi_L^{(3)} + \eta^2 \Psi_L'
\]  
(25)

where \( \eta = k_0 \left( n_i^2 - n_{i+1}^2 \right) \). By substituting (17), (18), and (22)-(25) into (16) and appropriately differentiating (15), \( \Psi_{i+1} \) can be expressed in terms of \( \Psi_i \) as

\[
\Psi_{i+1} = f_0 \Psi_i + f_1 \Psi_i' + f_2 \Psi_i'' + f_3 \Psi_i^{(3)} + f_4 \Psi_i^{(4)} + f_5 \Psi_i^{(5)} + O(h^6)
\]  
(26)

The following expression can be similarly obtained:

\[
\Psi_{i+1} = e_0 \Psi_i + e_1 \Psi_i' + e_2 \Psi_i'' + e_3 \Psi_i^{(3)} + e_4 \Psi_i^{(4)} + e_5 \Psi_i^{(5)} + O(h^6)
\]  
(27)

where the coefficients are given in Appendix. The difference forms of \( \Psi_i' \) and \( \Psi_i'' \) are derived as follows by ignoring the higher-order terms containing \( \Psi_i^{(3)} \), \( \Psi_i^{(4)} \), and \( \Psi_i^{(5)} \) in (26) and (27)

\[
\Psi_i' = f_1 \Psi_i' + f_2 \Psi_i'' + f_3 \Psi_i^{(3)} + f_4 \Psi_i^{(4)} + f_5 \Psi_i^{(5)} + O(h^5)
\]  
(28)

\[
\Psi_i'' = g_1 \Psi_i'' + g_2 \Psi_i^{(3)} + g_3 \Psi_i^{(4)} + g_4 \Psi_i^{(5)} + O(h^5)
\]  
(29)

Eliminating \( \Psi_i' \) and \( \Psi_i^{(5)} \) simultaneously in (26) and (27), we obtain

\[
f_1 \Psi_{i+1} + \left( f_2 e_1 - e_2 f_1 \right) \Psi_i + \eta \Psi_i'' + \eta^2 \Psi_i' + O(h^5) = 0
\]  
(30)

where \( g_1 \) and \( g_2 \) are given in Appendix. Replacing the first and second differential operators in the brackets of (30) with (28) and (29), respectively, we finally obtain the fourth-

\[
\Psi_{i+1} = f_0 \Psi_i + f_1 \Psi_i' + f_2 \Psi_i'' + f_3 \Psi_i^{(3)} + f_4 \Psi_i^{(4)} + f_5 \Psi_i^{(5)} + O(h^6)
\]  
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\]  
(28)

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\[
f_1 \Psi_{i+1} + \left( f_2 e_1 - e_2 f_1 \right) \Psi_i + \eta \Psi_i'' + \eta^2 \Psi_i' + O(h^5) = 0
\]  
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\[
\Psi_{i+1} = f_0 \Psi_i + f_1 \Psi_i' + f_2 \Psi_i'' + f_3 \Psi_i^{(3)} + f_4 \Psi_i^{(4)} + f_5 \Psi_i^{(5)} + O(h^6)
\]  
(26)

The following expression can be similarly obtained:

\[
\Psi_{i+1} = e_0 \Psi_i + e_1 \Psi_i' + e_2 \Psi_i'' + e_3 \Psi_i^{(3)} + e_4 \Psi_i^{(4)} + e_5 \Psi_i^{(5)} + O(h^6)
\]  
(27)
order FD formula:

\[
\Psi_i^* = \frac{D^2 \Psi_i}{1 + g_1 D_x + g_2 D_x^2} + O(h^4)
\]

(31)

which is referred to as the true FD4 scheme in this paper. If we ignore the refractive index discontinuities, (31) is reduced to

\[
\Psi_i^* \approx \frac{\partial \Psi_i}{\Delta x^2(1 + \delta / 12)}
\]

(32)

where \( \partial \Psi_i = \Psi_{i+1} - 2\Psi_i + \Psi_{i-1} \). Equation (32) is of the 4th-order accuracy only for transverse waveguide structures with graded index profile and/or weak index difference and therefore referred to as the quasi-FD4. This FD formulas are employed in [10], [11], and [13].

The second-order FD formula (referred to as the FD2) can be obtained when the high-order terms up to third derivative are retained in the derivation. Doing so leads to the following expression:

\[
\Psi_i^* = \frac{b_1 \Psi_{i+1} + (b_2 a_i - a_i b_2) \Psi_j - a_i \Psi_{i+1}}{a_i b_1 - b_2 a_i} + O(h^2).
\]

(33)

The coefficients in (33) are summarized in Appendix. By neglecting the refractive index discontinuity in the coefficients of (33), the conventional central difference (CD) schemes [24] are obtained as:

\[
\Psi_i^* \approx \frac{\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}}{\Delta x^2}
\]

(34)

for TE polarization and

\[
\Psi_i^* \approx \frac{a_i \Psi_{i-1} - 2b_i \Psi_i + c_i \Psi_{i+1}}{\Delta x^2}
\]

(35)

for TM polarization, where

\[
a_i = \frac{2n_{i-1}^2}{n_{i-1}^2 + n_i^2}
\]

(36)

\[
b_i = n_i^2 \left( \frac{1}{n_{i-1}^2 + n_i^2} + \frac{1}{n_{i-1}^2 + n_{i+1}^2} \right)
\]

(37)

\[
c_i = \frac{2n_{i+1}^2}{n_{i+1}^2 + n_i^2}.
\]

(38)

All these FD formulas, i.e., the true FD4, the quasi-FD4, the FD2, as well as the conventional CD schemes, will be applied to the wide-angle beam propagation method and compared in terms of accuracy under different situations.

III. NUMERICAL RESULTS AND COMPARISONS

As the first example for comparison, we simulated the radiation from a line source in free space, which propagates in all directions evenly. As such, this example provides us with an excellent opportunity to check the accuracy of the different numerical solutions intuitively and precisely. The excitation is generated by the Hankel function [25]. Simulations are carried out based on the central differencing (CD) and the fourth-order differencing (FD4) by using the wide-angle BPMs with different Padé orders. Since the refractive index is uniform, there is no difference between the true and quasi FD4 and between the CD and the FD2 schemes, respectively. As the focus of this study is on performance of the FD-based wide-angle schemes, both coarse mesh and fine mesh are used for the sake of comparison. The computation window is chosen as 20 µm, in which a PML [26] of 5 µm is placed adjacent to the edge of the window. At the edge of the window, the conventional transparent boundary condition is employed. In the simulation, we propagate the field originated from the line source along +z direction for total of 10 µm with a longitudinal step size equal to Δz = 0.05 µm. The wavelength is \( \lambda = 1.55 \) µm.

Figures 2(a)-(d) show the field patterns simulated by the paraxial scheme in which the CD and the
FD4 are used with coarse ($\Delta x = 0.4 \, \mu m$) and fine ($\Delta x = 0.05 \, \mu m$) meshes, respectively. It is noted that the paraxial schemes do not reproduce the correct radiation patterns as expected. Further, we see that, while the fine mesh simulations of both FD schemes yield the same results, considerable difference is noted for the coarse mesh calculations. The errors inherent in the paraxial approximation are reduced successively by increasing the Padé order in the wide-angle scheme and the simulation results of Padé (11,11) for the CD and FD4 formulas are illustrated in Fig. 3(a)-(d) for the coarse and fine meshes, respectively. The wide-angle BPMs can produce the expected radiation patterns for the fine mesh case, whereas the FD4 is seen to be more accurate than the CD for the coarse mesh. In this sense, the high-order FD scheme does produce more accurate results than the conventional CD scheme for the ultra-wide angle BPMs.

Fig. 2. Field distributions of the radiation from a line source obtained by the paraxial BPM. (a) CD in coarse mesh; (b) FD4 in coarse mesh; (c) CD in fine mesh; (d) FD4 in fine mesh. Coarse mesh $\Delta x = 0.4 \, \mu m$, fine mesh: $\Delta x = 0.05 \, \mu m$, and longitudinal step-size: $\Delta z = 0.05 \, \mu m$. 
To gain some quantitative results for the comparison, we calculate the relative errors for the intensities and the phases of the radiation field as functions of Padé orders. The results obtained by the two differencing schemes are compared in Fig. 4. It is observed that the relative errors decrease rapidly as the Padé order increases and become stabilized at Padé (3,3). The conventional central differencing (CD) and the fourth-order differencing (FD4) produce similar results in the case of fine mesh ($\Delta x = 0.05 \mu m$). In contrast, the fourth-order difference scheme yields more accurate results than the central difference scheme when the relatively coarse mesh ($\Delta x = 0.4 \mu m$) is employed. This conclusion is consistent with the observation made for the field patterns in Fig. 2 and 3.

Fig. 3. Field distributions of line source obtained by Padé (11,11) wide-angle BPM. (a) CD in coarse mesh; (b) FD4 in coarse mesh; (c) CD in fine mesh; (d) FD4 in fine mesh. The other parameters are the same as in Fig. 2.

Fig. 4. The comparison of CD and FD4 for coarse and fine meshes, respectively. (a) The relative error for the intensity; (b) The relative error for the phase.
As the second example for the comparison, we consider a step-index slab waveguide. It is well known that the improper choice of reference refractive index causes severe errors in the paraxial beam propagation analysis, due to the fast phase variations in the complex field $\Psi(x,z)$. A wide-angle scheme based on Padé approximations can alleviate this problem to some degree since the second derivative of $\Psi(x,z)$ is included in the governing equation. To assess various FD formulas, we calculate the relative errors in the propagation constants due to the fast oscillation in $\Psi(x,z)$ along $z$ for both TE and TM polarizations by choosing $n_0$ to be different from the mode effective index. The relative error in the propagation constants is defined as

$$
\varepsilon = \left| \frac{\beta_{\text{calculated}} - \beta_{\text{exact}}}{\beta_{\text{exact}}} \right|
$$

where $\beta_{\text{exact}}$ and $\beta_{\text{calculated}}$ are the exact and the numerically calculated propagation constants, respectively. $\beta_{\text{calculated}}$ can be found as follows:

$$
\beta_{\text{calculated}} = k_0 n_0 + \frac{\Delta \phi}{\Delta L}
$$

where $\Delta \phi$ is the phase shift and $\Delta L$ is the propagation distance. The phase shift is extracted from the overlap integral between the input and the output fields expressed as

$$
\int \Psi_{\text{output}} \cdot \Psi_{\text{input}}^* \, dx.
$$

The refractive indices of the core and the cladding are $n_i = 1.5$ and $n_c = 1.0$, respectively. The wavelength is $\lambda = 1.0$ µm. The core width is chosen to be $D = 0.427$ µm so as to form a single-mode waveguide. The effective indices for TE and TM polarizations of this waveguide are $n_{\text{eff}} \approx 1.336$ and $n_{\text{eff}} \approx 1.2495$, respectively. The step sizes are chosen to be $\Delta x = 0.10675$ µm and $\Delta z = 0.1$ µm. The width of the computation window is $W = 5.978$ µm. The PML boundary condition [26] is employed at the edges of the computation window. The electric fields of the fundamental mode are launched as the incident fields. Fig. 5 shows the effects of the variation in the reference refractive index on the relative errors of the propagation constants for the paraxial and wide-angle schemes. The results obtained using the CD scheme, FD2, and FD4 are presented in the same figure for comparison. Fig. 5(a) and (b) are for the cases of TE and TM polarizations, respectively. For each polarization, it can be seen that the best results are obtained with the fourth-order FD formula for both paraxial and wide-angle schemes. As expected, the multi-step wide-angle scheme yields accurate results over a wider range of reference index values, compared to paraxial approximations. For each curve the best results are achieved when $n_0$ is chosen to be $n_{\text{eff}}$. 
Fig. 5. Effect of the variation in the reference index on the relative error of the propagation constant. (a) TE mode; (b) TM mode.

We now proceed to study the convergence of various FD formulas as a function of transverse step size $\Delta x$. The reference index is fixed at $n_0 = 1.8$ and other parameters are the same as in Fig. 5. The relative errors of the propagation constant for TE and TM modes versus $\Delta x$ are shown in Fig. 6(a) and (b). In general, the discretization errors increase with the increase of $\Delta x$ as illustrated in the curves corresponding to the wide-angle scheme based on CD and FD2. It should be noted that the wide-angle scheme based on FD4 maintains high accuracy even with very coarse grids. In paraxial cases, it is observed that the results obtained with various FD formulas are nearly superimposed. This indicates that the main source of error arises from the paraxial approximation.

Fig. 6. Relative error in the propagation constant as a function of the transverse step size (a) TE mode; (b) TM mode.

To emphasize the effectiveness of treatment of interface conditions, we compare the quasi-FD4 and the true FD4 schemes based on Padé (3,3) approximation as shown in Fig. 7 in a higher index contrast waveguide with a different core index $n_1 = 2.0$. The cladding index $n_2$ is fixed to be 1.0. We take $\lambda = 1.0$ $\mu$m and $D = 0.27566$ $\mu$m so that only the fundamental mode propagates. The longitudinal step size is $\Delta z = 0.1 \mu$m. The reference indices for TE and TM polarizations are chosen to be 1.9605 and 2.162, respectively, which are far different from their respective effective indices. For both TE and TM polarizations, the relative error of the propagation constants observed for FD4 is much smaller than that for quasi-FD4 when the coarse grids are employed. Since these two formulas are obtained from the same order Taylor series expansions, the improvement of FD4 in accuracy is contributed to the proper treatment of interface conditions.

Fig 7. Relative error in the propagation constant as a function of the transverse step size for quasi-FD4 and true FD4. (a) TE mode; (b) TM mode.
Finally, the comparison of quasi-FD4 and true FD4 scheme is conducted by calculating the mode-mismatch loss [8] as a function of the relative refractive index difference ($\Delta n/n_2$) between the core and cladding regions. The wavelength is $\lambda = 1.0 \, \mu m$, the cladding index $n_2$ is 1.0, and the relative refractive index difference is set successively at $\Delta n/n_2 = 0.002$, 0.01, 0.1, and 1.0. The single-mode condition is guaranteed by choosing the waveguide width to fix the normalized frequency around 1.5. The mode-mismatch loss obtained with paraxial BPM is plotted versus $\Delta n/n_2$ in Fig. 8 at the propagation distance of 100 $\mu m$ with $\Delta z = 0.1 \mu m$ for both coarse mesh ($\Delta x = 0.068915 \mu m$) and fine mesh ($\Delta x = 0.0068915 \mu m$). It is confirmed that the strongly guiding structures suffer larger mode-mismatch loss. In the case of fine mesh, the two FD schemes appear to converge as the guidance becomes weak. In the case of coarse mesh, big difference between the results obtained by the two schemes is observed from weak guidance to strong guidance, which indicates that the FD4 scheme is able to provide accurate results with high efficiency.

![Fig. 8. The mode-mismatch loss as a function of relative refractive index difference for quasi-FD4 and true FD4. (a) TE mode; (b) TM mode.](image)

**IV. CONCLUSION**

We have successfully applied the fourth-order finite-difference formula to an efficient ultra-wide-angle scheme based on Padé approximations, in which the Padé approximations can go to any higher order. For the 2D cases, the resulting FD equations are tridiagonal in the form of matrix and solvable by the standard solver such as Thomas algorithm. We have compared the accuracy of various FD formulas by simulating the propagation of a cylindrical wave in free space and a TE/TM mode in a step-index slab waveguide. It is demonstrated that the fourth-order formulation takes into account interface conditions and therefore offers highly accurate results, especially when simulating waveguide structures of high index contrast with relatively coarse grids.

**APPENDIX**

The coefficients used in (26) are as follows:

$$f_0 = \theta \left(1 + \frac{q^2 \eta}{2} + \frac{q^4 \eta^2}{24}\right) + O(h^6) \quad (A1)$$
\[ f_1 = \theta \left( p + \frac{pq^2 \eta}{2} + \frac{pq^4 \eta^2}{24} \right) + q + \frac{q^3 \eta}{6} + \frac{q^5 \eta^2}{120} + O(h^6) \quad (A2) \]

\[ f_2 = \theta \left( p + \frac{q^2}{2} + \frac{p^2 q^2 \eta}{4} + \frac{q^4 \eta}{12} \right) + pq + \frac{pq^3 \eta}{6} + O(h^6) \quad (A3) \]

\[ f_3 = \theta \left( p + \frac{pq^2}{2} - \frac{p^3 q^2 \eta}{12} + \frac{pq^4 \eta}{12} \right) + \frac{p^2 q}{2} + \frac{q^3 \eta}{6} + \frac{q^5 \eta^2}{60} + O(h^6) \quad (A4) \]

\[ f_4 = \theta \left( p + \frac{pq^2 q^2}{24} + \frac{q^4}{24} \right) + \frac{p^2 q}{6} + \frac{pq^3}{6} + O(h^6) \quad (A5) \]

\[ f_5 = \theta \left( p + \frac{p^2 q}{120} + \frac{pq^4}{24} + \frac{p^2 q}{24} \right) + \frac{p^3 q}{12} + \frac{q^5}{120} + O(h^6) \quad (A6) \]

The coefficients used in (27) can be obtained by replacing \( p \), \( q \) and \( n_{i+1} \) with \(-c\), \(-d\) and \( n_{i-1} \), respectively.

The coefficients used in (30) are expressed as

\[ g_1 = \frac{e_3 f_1 - f_2 e_1}{e_2 f_1 - f_2 e_1} \quad (A7) \]

\[ g_2 = \frac{e_4 f_1 - f_4 e_1}{e_2 f_1 - f_2 e_1} \quad (A8) \]

The coefficients \( b_j \)'s used in (33) are given by

\[ b_0 = \theta \left( 1 + \frac{q^2 \eta}{2} \right) + O(h^4) \quad (A9) \]

\[ b_1 = \theta \left( p + \frac{pq^2 \eta}{2} \right) + q + \frac{q^3 \eta}{6} + O(h^4) \quad (A10) \]

\[ b_2 = \theta \left( p^2 + \frac{q^2}{2} \right) + pq + O(h^4) \quad (A11) \]

\[ b_3 = \theta \left( \frac{p^3}{6} + \frac{pq^2}{2} \right) + \frac{p^2 q}{2} + \frac{q^3}{6} + O(h^4) \quad (A12) \]

The coefficients \( a_j \)'s used in (33) can be obtained by replacing \( p \), \( q \) and \( n_{i+1} \) with \(-c\), \(-d\) and \( n_{i-1} \), respectively.

REFERENCES


