# Fast three-dimensional generalized rectangular wide-angle beam propagation method using complex Jacobi iteration 

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#### Abstract

A fast and efficient three-dimensional generalized rectangular wide-angle beam propagation method (GR-WABPM) based on a recently proposed modified Padé $(1,1)$ approximant is presented. In our method, at each propagation step, the beam propagation equation is recast in terms of a Helmholtz equation with a source term, which is solved quickly and accurately by a recently introduced complex Jacobi iterative (CJI) method. The efficiency of the GR-WA-BPM for the analysis of tilted optical waveguides is demonstrated in comparison with the standard wide-angle beam propagation method based on Hadley's scheme. In addition, since the utility of the CJI method depends mostly on its execution speed in comparison with the traditional direct matrix inversion, several performance comparisons are also presented. © 2009 Optical Society of America

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## 1. INTRODUCTION

The wide-angle beam propagation method (WA-BPM) has become one of the most widely used techniques for the analysis of optical waveguide (WG) devices [1]. Different treatments of WA-BPM have been developed. There exist rational approximants of the square root operator [2], the exponential of the square root operator [3], the rational Hadley approximant operators [4], and the complex Padé approximant operators [5] for rectangular coordinates as well as an oblique coordinate system [6]. The Hadley-approximant-based WA-BPM, hereafter referred to as the standard wide-angle beam propagation method (S-WABPM), is one of the most commonly used techniques for modeling optical WG structures.

However, the efficiency and the accuracy of this method are limited by several factors resulting from either the approximation of partial derivatives with finite differences or the staircase approximation of structures calculated. In many cases the staircase approximation can be eliminated by using coordinate systems, which accurately describe the geometry of the studied devices. In particular, the nonorthogonal coordinate systems were employed for this purpose with a particular success [7,8]. Nevertheless, they still suffer from the staircase approximation problem when applying the finite difference beam propagation method (BPM) for the analysis of beam propagation in high-index-contrast structures. Recently, a solution for this problem was suggested in [9]. The proposed algorithm results in the so-called slanted-wall beam propagation, which is well suited for studying wide-angle (WA) propagation through a general class of optical WG structures defined by dielectric interfaces that may be slanted with respect to the propagation direction. When used with an appropriated grid-generation algorithm, the method allows the modeling of an extremely wide variety of high-
index-contrast structures with good phase accuracy and energy conservation. However, this method is limited for the two-dimensional (2D) beam propagation analysis of the transverse electric modes.

In addition, it was shown that the oblique coordinate system not only reduces the staircasing problem but also allows for arbitrary selection of the proper direction of propagation [10]. This results in relaxation of computational efforts in comparison with the standard Hadley-approximant-based WA-BPM in the rectangular coordinate. However, the oblique coordinate system is not orthogonal. Consequently, the power conservation cannot be general guaranteed.

Recently, by introducing a generalized envelope function, it was shown that these problems can be overcome [11]. It results in the so-called generalized rectangular WA-BPM, hereafter referred to as the GR-WA-BPM. The proposed algorithm keeps all the advantages of the S-WABPM in the rectangular coordinate system while adding flexibility in the selection of the preferred propagation direction. Since the propagation matrix can be described in a tridiagonal matrix form, it is usually solved by the wellknown direct matrix inversion (DMI). However, this method is too slow to deal with three-dimensional (3D) problems.
Here, we propose to use the recently introduced complex Jacobi iterative (CJI) method to solve the propagation equation. At each propagation step, the propagation equation is recast in terms of the Helmholtz equation with a source term, which is solved quickly and accurately by the CJI method. Via a performance comparison of the CJI and DMI methods for both 2D and 3D generalized rectangular beam propagations, it is convincingly demonstrated that the CJI method is very competitive for demanding problems.

## 2. FORMULATION

## A. GR-WA-BPM Based on Modified Padé Approximants

The 3D scalar Helmholtz equation is given by [1]

$$
\begin{equation*}
\frac{\partial^{2} \Psi}{\partial x^{2}}+\frac{\partial^{2} \Psi}{\partial y^{2}}+\frac{\partial^{2} \Psi}{\partial z^{2}}+k_{0}^{2} n^{2}(x, y, z) \Psi=0, \tag{1}
\end{equation*}
$$

where $n$ is the refractive index profile and $k_{0}$ is the vacuum wave vector. By introducing a generalized envelope function [11]

$$
\begin{equation*}
\Psi(x, y, z)=\Phi(x, y, z) \exp [i k \cos (\theta) z+i k \sin (\theta) x] \tag{2}
\end{equation*}
$$

where $k=k_{0} n_{\text {ref }}$ and $n_{\text {ref }}$ is the reference refractive index and inserting it into Eq. (1), we obtain

$$
\begin{equation*}
\frac{\partial^{2} \Phi}{\partial z^{2}}+2 j k \cos \theta \frac{\partial \Phi}{\partial z}+P \Phi=0 \tag{3}
\end{equation*}
$$

where the operator $P$ is given by

$$
\begin{equation*}
P=\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial x^{2}}+2 j k \sin \theta \frac{\partial}{\partial x}+k_{0}^{2}\left(n^{2}-n_{\mathrm{ref}}^{2}\right) . \tag{4}
\end{equation*}
$$

The generalized envelope function introduces two parameters, namely, $k$ and $\theta$. These parameters can be freely chosen to best match the requirements of the problem studied. It is known that the standard envelope function used in BPMs so far has only one adjustable parameter, which is typically referred to as the reference refractive index. This parameter has a major impact on the accuracy of the calculations and should be carefully selected. By adding another parameter to the envelope function, an additional degree of freedom is gained that allows for decoupling the preferred direction of propagation of BPMs from the coordinate system used.

Equation (3) can be rearranged as follows:

$$
\begin{equation*}
\frac{\partial \Phi}{\partial z}-\frac{j}{2 k \cos \theta} \frac{\partial^{2} \Phi}{\partial z^{2}}=\frac{j P}{2 k \cos \theta} \Phi \tag{5}
\end{equation*}
$$

which can be formally written as

$$
\begin{equation*}
\frac{\partial \Phi}{\partial z}=\frac{\frac{i P}{2 k \cos \theta}}{1-\frac{i}{2 k \cos \theta} \frac{\partial}{\partial z}} \Phi \tag{6}
\end{equation*}
$$

Equation (6) suggests the recurrence relation

$$
\begin{equation*}
\left.\frac{\partial}{\partial z}\right|_{n+1}=\left.\frac{\frac{i P}{2 k \cos \theta}}{1-\frac{i}{2 k \cos \theta} \frac{\partial}{\partial z}}\right|_{n} \Phi \tag{7}
\end{equation*}
$$

By using the initial value of $\partial /\left.\partial z\right|_{0}=0$, this gives us the well-known Padé ( $m, n$ ) approximant-based WA beam propagation formula as follows:

$$
\begin{equation*}
\frac{\partial \Phi}{\partial z} \approx i k \cos (\theta) \frac{N(m)}{D(n)} \Phi \tag{8}
\end{equation*}
$$

where $N(m)$ and $D(n)$ are polynomials in $X=P / k^{2} \cos ^{2}(\theta)$. However, as addressed in our earlier effort [5], Padé ( $m, n$ ) approximants incorrectly propagate evanescent modes. To overcome this problem we reported the modified Padé ( $m, n$ ) approximant. It not only allows more accurate approximations to the true Helmholtz equation but also gives the evanescent modes the desired damping. It is obtained by using the same recurrence formulation of Padé ( $m, n$ ) approximants but with a different initial value. Here, by following the same steps as in case of the S-WA-BPM based on modified Padé ( $m, n$ ) approximants, we found that the initial value for the recurrence relation (7) in the GR-WA-BPM based on modified Padé $(m, n)$ approximants is $\partial /\left.\partial z\right|_{0}=-k \cos (\theta) \beta$, where $\beta$ is a damping parameter, which can be chosen as well.

## B. Numerical Implementation of GR-WA-BPM

One of the most commonly used techniques to numerically deal with Eq. (8) is the finite difference method [4]. Finite difference equations may be derived from Eq. (8) by clearing the denominator and centering with respect to $z$ in the usual way,

$$
\begin{equation*}
D\left(\Phi^{n+1}-\Phi^{n}\right)=\frac{i k \cos (\theta) \Delta z}{2} N\left(\Phi^{n+1}+\Phi^{n}\right) . \tag{9}
\end{equation*}
$$

Equation (9) can be solved effectively by the multistep method whereby each component step is treated by the traditional DMI for 2D problems [12]. However, for large 3D problems requiring the frequently matrix inversion during a propagation direction, it is a numerically intensive task. Recently, we reported the approach solving these problems effectively and accurately by using the new CJI method [13]. The utility of the CJI technique depends mostly upon its execution speed dominated by the amount of effective absorption (or medium loss). If the medium loss is high, the convergence rate is fast. Here, for GR-WA-BPMs based on the modified Pade $(1,1)$ approximant, the propagation equation is given by [13]

$$
\begin{equation*}
(1+\xi P) \Phi^{n+1}=\left(1+\xi^{*} P\right) \Phi^{n} \tag{10}
\end{equation*}
$$

where $\quad \xi=1 /\left[4 k^{2} \cos ^{2}(\theta)(1+i \beta / 2)\right]-i \Delta z / 4 k \cos (\theta), \quad \xi^{*}$ $=1 /\left[4 k^{2} \cos ^{2}(\theta)(1+i \beta / 2)\right]+i \Delta z / 4 k \cos (\theta)$, and $\Delta z$ is the propagation step size, and is solved by the CJI method as follows. By dividing both sides of Eq. (10) by $\xi$, it may be rewritten as an inhomogeneous Helmholtz equation

$$
\begin{align*}
& {\left[\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial x^{2}}+2 j k \sin \theta \frac{\partial}{\partial x}+k_{0}^{2}\left(n^{2}-n_{\mathrm{ref}}^{2}\right)+\frac{1}{\xi}\right] \Phi^{n+1}} \\
& \quad=\left(\frac{\xi^{*}}{\xi} P+\frac{1}{\xi}\right) \Phi^{n} \tag{11}
\end{align*}
$$

or

$$
\begin{align*}
& {\left[\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial x^{2}}+2 j k \sin \theta \frac{\partial}{\partial x}+k_{0}^{2}\left(n^{2}-n_{\mathrm{ref}}^{2}\right)+\frac{1}{\xi}\right] \Phi^{n+1}} \\
& \quad=\text { source term. } \tag{12}
\end{align*}
$$

It is obvious that at each propagation step the 3D beam propagation equation is recast as a 2 D Helmholtz equation with a source term. Therefore, it can be solved effectively by the CJI.

## 3. BENCHMARK RESULTS AND DISCUSSIONS

The efficiency and the accuracy of the GR-WA-BPM in comparison with the S-WA-BPM were already shown in [11]. There, however, 3D methods were not practical in view of the slowness of the DMI. To show the efficiency of the CJI in comparison with the DMI for 3D GR-WA-BPM in terms of an execution speed, we perform several benchmark tests on both 2D and 3D optical WGs. All simulations were run on a notebook PC using Matlab.

For the 2D case, we consider a $5^{\circ}$ tilted WG. In the tilted WG the fundamental mode for the slab of width $w$ $=1 \mu \mathrm{~m}$ and with a cladding index of 3.17 is propagated through $10 \mu \mathrm{~m}$ at a wavelength of $\lambda=1.55 \mu \mathrm{~m}$ in a medium of refractive index $n=3.4$ and with the propagation step size of $\Delta z=0.05 \mu \mathrm{~m}$. With a very strict propagation error tolerance of $10^{-9}$, the CJI method only took 10.9 s , whereas the DMI method took 35.3 s . The resulting intensity profile for the S-WA-BPM is shown in Fig. 1(a). The intensity peaks of a beam propagating along a tilted WG calculated by the S-WA-BPM and the GR-WA-BPM are show in Fig. 2. As shown in the figures, the sudden changes in dielectric constant resulting from the stair-


Fig. 1. (Color online) Intensity profiles along a tilted WG for (a) the standard and (b) the generalized rectangular wide-angle propagations.


Fig. 2. Intensity peaks along a tilted WG for the standard (dotted curve) and the generalized rectangular (solid curve) wideangle propagations.


Fig. 3. (Color online) Magnitude of 3D Gaussian beam after propagating $1 \mu \mathrm{~m}$ calculated by the generalized rectangular WABPM based on (a) DMI and (b) CJI.

Table 1. Quantitative Comparison of Runtimes (in seconds) of the DMI and CJI methods for GR-WA Beam Propagation in WG Structures

|  | Structure |  |
| :--- | :---: | :---: |
|  | 2D | 3D |
|  | Tilted WG | Gaussian Beam Propagating in Free Space |
| Method | (s) | (s) |
| DMI | 35.3 | 323.6 |
| CJI | 10.9 | 36.7 |

stepping procedure have generated nonphysical ripples in the waveform and have led to a spurious radiation loss. This effect is sensitive to index contrast. Low-indexcontrast problems have been successfully addressed in the past using this standard method. However, high-index-contrast problems can often generate sufficient scattering so as to render the method completely useless. The corresponding intensity profile for the GR-WA-BPM is depicted in Fig. 1(b). In contrast to the previous case, all profiles are relatively uniform and smoother than those based on the S-WA-BPM as clearly seen in Fig. 2. It is worth confirming with the results addressed in previous work [11] that the GR-WA-BPM could be performed with a low loss of accuracy in terms of energy conservation.

For the 3D case, we consider a Gaussian beam with a waist radius of $w_{0}=1 \mu \mathrm{~m}$ propagating in free space (unity refractive index) with a $10^{\circ}$ tilt at a wavelength of $\lambda$ $=1.55 \mu \mathrm{~m}$. Due to the large memory required for the DMI, the small computational window of $3 \times 3 \mu \mathrm{~m}$ is discretized with a grid size of $\Delta x=\Delta y=0.1 \mu \mathrm{~m}$, and the short path length of $1 \mu \mathrm{~m}$ is discretized with a propagation step size of $\Delta z=0.05 \mu \mathrm{~m}$. The output beam calculated by the GR-WA-BPM using the CJI and the DMI is presented in Figs. 3(a) and 3(b), respectively. Definitely, the calculated results are the same since we are dealing with the same propagation equation. Due to the high effective loss in the propagation medium, the complex Jacobi method performed the propagation in only 36.7 s while the DMI required 323.6 s .

Table 1 shows the performance of the two methods for optical structures chosen here. It is clearly seen that the runtimes of the iterative method is substantially lower than that of the DMI method. For large problems requiring very large storage space and also for structures with a long path length with small propagation step size that require frequent matrix inversions, the DMI technique is numerically very intensive. In contrast, the CJI technique can offer rapid convergence and shorter runtimes.

## 4. CONCLUSIONS

In this paper, the modified Padé approximants for GR-WA-BPMs have been derived. Furthermore, by using the recently introduced complex Jacobi interative (CJI) method, a fast solution for the 3D GR-WA-BPM is obtained. Through a quantitative comparison of runtimes between the traditional DMI and the new CJI methods, it is convincingly demonstrated that the CJI method is very competitive for demanding problems.

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