

# A Novel WA-BPM Based on the Generalized Multistep Scheme in the Propagation Direction in the Waveguide

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**Abstract.** A highly accurate wide-angle scheme, based on the generalized multistep scheme in the propagation direction, is developed for the finite difference beam propagation method (FD-BPM). Comparing with the previously presented method, the simulation shows that our method results in a more accurate solution, and the step size can be much larger

## 1. Introduction

The beam propagation method (BPM) has been one of the most popular techniques for modeling and simulation of optical guided-wave device. The original BPMs are derived from paraxial approximation of the scalar wave equation and hence can only perform the simulation of scalar wave propagation along waveguide axis in weakly guiding structures. To get rid of the paraxial restriction, several wide-angle (WA) BPMs have been developed in recent years. The original wide-angle algorithm was based on padé approximants given by Hadley[1,2]. The resulting formulas were derived by using the padé recurrence scheme to be approximated to the square root of the characteristic matrix. This formulation is, however, based on the Crank-Nicholson(CN) scheme with a truncation error of  $O(\Delta x^2)$  in the transverse direction. Yamauchi *et al.* [3,4] proposed an improved wide-angle BPM based on a generalized Douglas(GD) scheme for variable coefficients. In their algorithm, the second derivative of function E with respect to x was improved by replacing the Crank-Nicholson (CN) scheme with the Douglas scheme. The truncation error of their algorithm was deduced to  $O(\Delta x^4)$  in the transverse direction. Yevick *et al.*[5] introduced a wide-angle scheme using complex padé approximants. They rotated the branch-cut of standard padé expansion from the negative real axis into the lower half-plane. So the conventional real padé approximant is replaced by the modified padé approximant form with complex constants to evaluate the square-root operator in the exponential of the propagation operator. However, all of the above efforts were directed to the improvements in the transverse direction, i.e, x axis, while in the propagation direction, i.e, z axis, the operator was still approximated by the conventional CN scheme. This approximant have severely restricted the accuracy of the BPMs. To overcome this limitation, Chiou and Chang[6] proposed an improved WA-BPM in which they performed the padé approximants in the longitudinal directions as well as in the transverse direction. Although their method gives a more accurate result, it has to factor a polynomial of nth order in both the numerator and the denominator in the propagation equation in each step. So the efficiency is limited.

In this letter we propose a novel wide-angle beam propagation method based on the generalized multistep scheme in the propagation direction. The exponential of the square root operator is approximated by a continued-multiplication algorithm which is generalizable to arbitrarily high order in the longitudinal direction. Combining with the previously presented algorithm, the simulation results show that the accuracy of our method is much higher and the longitudinal step size can be much larger.

## 2. Formulation

We consider a slowly varying waveguiding structure characterized by the refractive index  $n(x, y, z)$ , where  $x$  and  $y$  are the transverse direction and  $z$  is the propagation direction. By using the slowly



varying envelope approximation formalism, the harmonic Maxwell equations can be reduced to the governing equation in

$$\frac{\partial^2 \phi}{\partial z^2} - 2jk_0 n_0 \frac{\partial \phi}{\partial z} + k_0^2 n_0^2 P \phi = 0 \quad (1)$$

in which  $\psi$  is a column vector of the transverse components of the electromagnetic field,  $k_0$  is the wave number in free space,  $n_0$  is the reference refractive index to be appropriately chosen, and  $P$  is the differential operator [5]. Hadley had solve Eq. (1) using the recurrence formula of the continued fraction expansion[2]. Here we solve Eq. (1) as a quadratic equation with respect to  $\partial \phi / \partial z$  and obtain the solution of one-way propagation scheme:

$$\frac{\partial \phi}{\partial z} = -jk_0 n_0 (\sqrt{P+1} - 1) \phi \quad (2)$$

Eq. (2) is often discretized directly with the standard Crank-Nicolson scheme, resulting in the midpoint scheme:

$$\frac{\phi^{l+1} - \phi^l}{\Delta z} = -jk_0 n_0 (\sqrt{P+1} - 1) \frac{\phi^{l+1} + \phi^l}{2} \quad (3)$$

This treatment will lead to the conventional CN scheme. Considering Eq. (2) as a first-order differential equation, the more accurate solution can be given as exponential form:

$$\phi^{l+1} = \exp \left[ -jk_0 n_0 (\sqrt{P+1} - 1) \Delta z \right] \phi^l \quad (4)$$

where  $\Delta z$  is the step size between the preceding field and the current field, and the superscript  $l$  indicates the position along the  $z$  axis. By using the standard padé approximate [7] to the square root of the transverse operator in Eq. (4), it becomes

$$\phi^{l+1} = \exp \left( -jk_0 n_0 \Delta z \sum_{k=1}^m \frac{a_{k,m} P}{1 + b_{k,m} P} \right) \phi^l \quad (5)$$

or denoted as

$$\phi^{l+1} = \prod_{k=1}^m \exp \left( -jk_0 n_0 \Delta z \frac{a_{k,m} P}{1 + b_{k,m} P} \right) \phi^l \quad (6)$$

Where

$$a_{k,m} = \frac{\sin^2(k\theta)}{m+0.5}, \quad b_{k,m} = \cos^2(k\theta)$$

for  $\theta = \pi / (2m+1)$ . By introducing the parameter  $\alpha$ , we rewritten the exponential of the square root operator as the following form:

$$\exp \left( \frac{-jk_0 n_0 \Delta z a_{k,m} P}{1 + b_{k,m} P} \right) = \frac{\exp \left[ (1-\alpha) \frac{-jk_0 n_0 \Delta z a_{k,m} P}{1 + b_{k,m} P} \right]}{\exp \left( -\alpha \frac{-jk_0 n_0 \Delta z a_{k,m} P}{1 + b_{k,m} P} \right)} \quad (7)$$

Here the original definition for the Euler's Number  $e$  is considered:

$$\lim_{x \rightarrow \infty} \left( 1 + \frac{1}{x} \right)^x = e \quad (8)$$

Substituting Eq. (8) into the numerator of Eq. (7), the numerator can be expressed as

$$\exp\left[(1-\alpha)\frac{-jk_0n_0\Delta za_{k,m}P}{1+b_{k,m}P}\right] = \left(\lim_{x \rightarrow \infty} \left(1 + \frac{1}{x}\right)^x\right)^{\left[\frac{(\alpha-1)jk_0n_0\Delta za_{k,m}P}{1+b_{k,m}P}\right]} \quad (9)$$

Now we introduce a positive integer  $r$  ( $r=1,2,3\cdots$ ) and a function  $f_r = r(1+b_{k,m}P)/[(\alpha-1)jk_0n_0\Delta za_{k,m}P]$ . Note that, when  $r$  approaches  $\infty$ ,  $f_r$  approaches  $\infty$  too. So we can replace the  $x$  in Eq.(9) with  $f_r$ , and rewrite Eq. (9) as follows:

$$\begin{aligned} & \exp\left[(1-\alpha)\frac{-jk_0n_0\Delta za_{k,m}P}{1+b_{k,m}P}\right] \\ &= \left(\lim_{r \rightarrow \infty} \left(1 + \frac{1}{\frac{r(1+b_{k,m}P)}{(\alpha-1)jk_0n_0\Delta za_{k,m}P}}\right)^{\frac{r(1+b_{k,m}P)}{(\alpha-1)jk_0n_0\Delta za_{k,m}P}}\right)^{\frac{(\alpha-1)jk_0n_0\Delta za_{k,m}P}{1+b_{k,m}P}} \\ &= \lim_{r \rightarrow \infty} \left(1 + \frac{(\alpha-1)jk_0n_0\Delta za_{k,m}P}{r(1+b_{k,m}P)}\right)^r \end{aligned} \quad (10)$$

Similarly the denominator in Eq. (7) can be rewritten as

$$\exp\left[-\alpha\frac{-jk_0n_0\Delta za_{k,m}P}{1+b_{k,m}P}\right] = \lim_{r \rightarrow \infty} \left(1 + \frac{\alpha jk_0n_0\Delta za_{k,m}P}{r(1+b_{k,m}P)}\right)^r \quad (11)$$

Then substituting Eq. (10) and Eq. (11) into Eq. (7), and using the basic limit theorem that is, the quotient of limits is a limit of the quotient, we obtain

$$\psi(z + \Delta z) \approx \prod_{k=1}^m \lim_{r \rightarrow \infty} \left( \frac{1 + \frac{1-\alpha}{r}(-jk_0n_0\Delta z)\frac{a_{k,m}P}{1+b_{k,m}P}}{1 + \frac{-\alpha}{r}(-jk_0n_0\Delta z)\frac{a_{k,m}P}{1+b_{k,m}P}} \right)^r \psi(z) \quad (12)$$

This is the exact solution for Eq.(6). It can be seen that when  $r$  is large enough, the formalism can be generalizable to arbitrarily high order, but it will lead a concomitant increase in numerical complexity. In actual simulation, we can choose a proper value for  $r$ , considering the calculation efficiency. Finally, assuming  $r = R$  and  $m = M$ , we obtain the following generalized multi-step algorithm as

$$\psi(z + \Delta z) \approx \prod_{k=1}^M \left( \frac{1 + \frac{1-\alpha}{R}(-jk_0n_0\Delta z)\frac{a_{k,M}P}{1+b_{k,M}P}}{1 + \frac{-\alpha}{R}(-jk_0n_0\Delta z)\frac{a_{k,M}P}{1+b_{k,M}P}} \right)^R \psi(z) \quad (13)$$

and reduced to

$$\psi(z + \Delta z) = \prod_{k=1}^{MR} \frac{1 + \left( b_{k,M} - \frac{1-\alpha}{R} a_{k,M} jk_0 n_0 \Delta z \right) P}{1 + \left( b_{k,M} + \frac{\alpha}{R} a_{k,M} jk_0 n_0 \Delta z \right) P} \psi(z) \quad (14)$$

where  $R$  is a positive integer which is the order of the continued-multiplication approximant of the exponential function in the propagation direction,  $M$  is the order of the padé approximant of the square root in the transverse direction, and  $\alpha$  ( $1/2 \leq \alpha \leq 1$ ) is a weighted factor employed to ensure the convergence.

The case with  $\alpha = 1/2$  corresponds to the Crank-Nicholson scheme and the case with  $\alpha = 1$  corresponds to the backward Euler method. Note that when  $R=1$  and  $\alpha = 1/2$ , Eq. (14) is deduced to the frequently used Hadley's wide-angle BPM with the CN implicit scheme:

$$\psi(z + \Delta z) = \prod_{k=1}^M \frac{1 + \left( b_{k,M} - \frac{1}{2} a_{k,M} jk_0 n_0 \Delta z \right) P}{1 + \left( b_{k,M} + \frac{1}{2} a_{k,M} jk_0 n_0 \Delta z \right) P} \psi(z) \quad (15)$$

The conventional Hadley's algorithm is the simplest case of our derived algorithm. From the derivation above, it can be proved that the higher the value of  $R$  is, the more approximate to the exact one the simulation result becomes. A higher value of  $R$  not only leads to a more accurate result but also means that the longitudinal step  $\Delta z$  can be much larger.

In the analysis of a wide-angle waveguide structure by the semi-vector or full-vector BPM, the  $z$ -varying structure is discretized by piecewise  $z$ -invariant segments. The discontinuousness of the refract index at the longitudinal interface will excite the evanescent modes which respond to the negative eigenvalues of the operator  $P+1$  of the eigenmode equation. Assuming that  $p$  is one of the eigenvalues of  $P$ , we have  $\left| \exp \left[ -jk_0 n_0 \left( \sqrt{p+1} - 1 \right) \Delta z \right] \right| < 1$ , for  $p < -1$ . This means that for the exact one-way beam propagation, the evanescent mode are always damped. But the conventional Hadley's scheme with CN scheme can not suppress the evanescent modes. It can be shown that the advancing  $\psi$  in spatial domain by one longitudinal step corresponds to the amplification factor  $g_z$  given by

$$g_z = \left[ 1 + \left( b_{k,M} - \frac{1-\alpha}{R} a_{k,M} jk_0 n_0 \Delta z \right) P \right] / \left[ 1 + \left( b_{k,M} + \frac{1-\alpha}{R} a_{k,M} jk_0 n_0 \Delta z \right) P \right] \quad (16)$$

It can be proved that the finite-difference propagation scheme are stable if  $|g_z| \leq 1$ . For the case of  $\alpha = 1/2$ , the formula is unconditionally stable and is ideally power conserving, since  $|g_z| = 1$ . Although the Crank-Nicholson method corresponding to  $\alpha = 1/2$  has the desirable power-conserving property for propagating modes in a straight waveguide, it incorrectly treats the evanescent modes as propagating modes. The evanescent modes are often excited in the analysis of semi-vector or full-vector BPM for three-dimension structures. If they are not suppressed efficiently, they will accumulate and give rise to a large error in the final solution. Our wide-angle method of Eq. (14) provide the desired damping for the evanescent modes, since  $|g_z| < 1$  for  $1/2 < \alpha < 1$ .

### 3. Simulation and discussions

We demonstrate the accuracy and usefulness of our method in a tilted slab waveguide shown in Fig.1. The refractive indices of core and cladding are  $n_1 = 1.469$  and  $n_2 = 1.460$ , respectively. The core width

is  $w=3 \mu\text{m}$ . The transverse sampling width is  $\Delta x=0.1 \mu\text{m}$ , and the tilt angle is  $\theta=30^\circ$ . The wavelength is  $\lambda=1.55 \mu\text{m}$ . The reference refractive index is  $n_0=(n_1+n_2)/2$ .

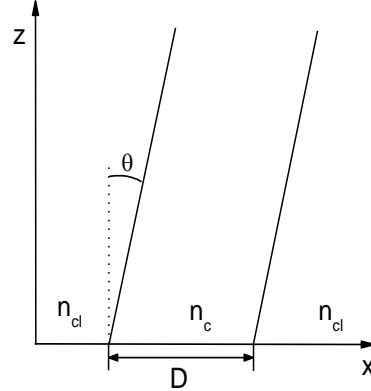


Fig.1. Geometry of a tilted step-index slab waveguide

For boundaries of numerical window, the transparent boundary condition (TBC) is used to suppress the reflections at the edges of the finite computational window. The (3,3) padé approximant operator is employed to the square root of the transverse operator. The second derivative in transverse direction is evaluated by the generalized Douglas(GD) scheme[3]. To validate the accuracy of the present method, we calculate the mode-mismatch loss  $\eta$ , which take into account the dissipation of the initial power as well as the deformation of the propagation field. In a two-dimensional waveguide,  $\eta$  is defined as

$$\eta = -10 \log \left[ \frac{\left| \int E_0 E^* \right|^2}{\left( \int |E_0|^2 dx \right)^2} \right] [dB] \quad (17)$$

where  $E$  is the propagating field and  $E_0$  is the incident field of the fundamental mode.

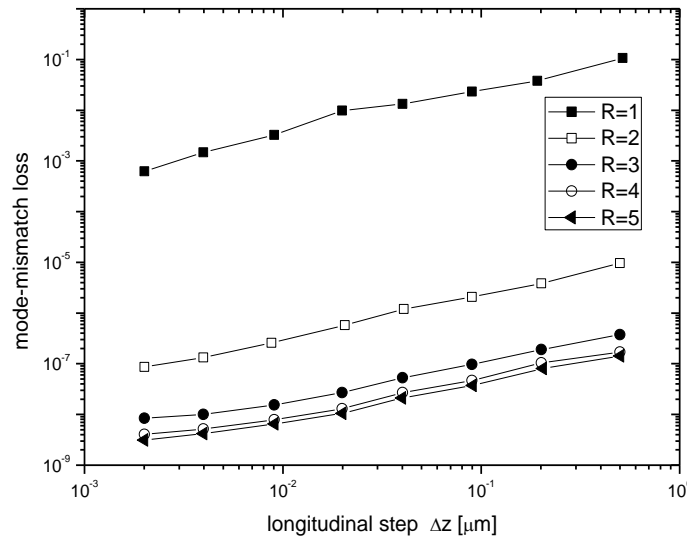


Fig.2. Mode-mismatch loss as a function of step size  $\Delta z$  in the longitudinal direction using the same weighted factor  $\alpha=1/2$ . The tilt angle is set at  $\theta=30^\circ$  and the order of padé is  $M=3$ .

Fig.2 shows the mode-mismatch loss  $\eta$  evaluated at a propagation distance of  $20 \mu\text{m}$  as a function of the step size in propagation direction. The curve denoted as  $R=1$  corresponds to the conventional Hadley's method. It can be seen that comparing with the conventional method, the accuracy of our method is greatly enhanced when the higher-order value of  $R$  is adopted. The presented formulation is generalizable to arbitrarily high order, with a concomitant increase in numerical complexity. Not that,

although the simulation results in a more accurate solution when a higher value  $R$  is used, the reduction of  $\eta$  descends progressively with the growth of  $R$ . In our simulation, the order of the generalized multistep scheme is set to be 4. It is also shown in Fig.2 that, for a fixed  $\eta$ , the step size of our methods can be much larger than that of the conventional method. This means that we could apply it to simulate the large-size photonic integrated devices.

### Conclusion

In conclusion, we have proposed an efficient and accurate wide-angle beam propagation method based on the generalized multi-step scheme in the propagation direction. Both two-dimension and three-dimension cases were demonstrated. Compared with the conventional method, our method show higher accuracy and the step size can be much larger.

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