

Three Dimensional Iterative Beam Propagation Method for Optical Waveguide Devices

Changbao Ma, Edward Van Keuren*

Department of Physics
Georgetown University
Washington, DC 20057

ABSTRACT

The finite difference beam propagation method (FD-BPM) is an effective model for simulating a wide range of optical waveguide structures. The classical FD-BPMs are based on the Crank-Nicholson scheme, and in tridiagonal form can be solved using the Thomas method. We present a different type of algorithm for 3-D structures. In this algorithm, the wave equation is formulated into a large sparse matrix equation which can be solved using iterative methods. The simulation window shifting scheme and threshold technique introduced in our earlier work are utilized to overcome the convergence problem of iterative methods for large sparse matrix equation and wide-angle simulations. This method enables us to develop higher-order 3-D wide-angle (WA-) BPMs based on Padé approximant operators and the multistep method, which are commonly used in WA-BPMs for 2-D structures. Simulations using the new methods will be compared to the analytical results to assure its effectiveness and applicability.

Keywords: 3-D BPM, iterative method, simulation.

1. INTRODUCTION

The finite difference beam propagation method (FD-BPM) is a widely used numerical method technique for simulating the propagation of optical fields.¹⁻⁵ In essence, the FD-BPM technique calculates how an input optical field distribution is changed by traveling through sections along the propagation direction, using the finite difference method to solve Helmholtz wave equation. The classical FD-BPMs¹⁻⁵ are based on the Crank-Nicholson scheme⁶ and solved in the tridiagonal form using the Thomas method.⁶ In 3-D FD-BPMs, the Fresnel wave equation can be split into two steps of 2-D equation using the alternating direction implicit (ADI) method.⁶ However, errors may be introduced when these methods are applied to wide-angle beam propagation. Efforts have been taken to develop wide-angle algorithms to resolve this problem.⁷⁻¹⁶ Of the several WA-BPMs that have been developed, the ones developed by Hadley based on Padé approximant operators¹³ and the multistep method¹⁴ are commonly employed to improve the accuracy for wide-angle simulations, especially for 2-D structures. Recently, some 3-D algorithms and techniques have also been developed to improve the accuracy for 3-D wide-angle simulations.^{17,18} In this work, we demonstrate a new type of BPM, in which the Fresnel wave equation is formulated into a large sparse matrix equation without splitting the wave equation, which will enable us to develop 3-D WA-BPMs based on Padé approximant operators¹³ and the multistep method.¹⁴

2. FORMULATION

2.1 Fresnel iterative BPM

The 3-D scalar Helmholtz equation is given by

$$\frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + \frac{\partial^2 E}{\partial z^2} + k_0^2 n^2(x, y, z)E = 0 \quad (1)$$

where k_0 denotes the free-space wavenumber, $E(x, y, z)\exp(i\omega t)$ is the electric field component with angular frequency ω , and $n(x, y, z)$ is the refractive index profile. If we assume the slowly varying envelope approximation (SEVA), then $E(x, y, z)$ can be separated into two parts: the complex field amplitude $\psi(x, y, z)$ (the axially slowly

* vankeu@physics.georgetown.edu; phone +1-202-687-5982

varying envelope term) and a propagation factor $\exp(-ik_0 n_0 z)$ (the rapidly varying phase term). The field is then expressed as

$$E(x, y, z) = \psi(x, y, z) \exp(-ik_0 n_0 z) \quad (2)$$

where n_0 is the refractive index in the cladding. Substituting Eq. (2) into Eq. (1) yields

$$ia \frac{\partial \psi}{\partial z} - \frac{\partial^2 \psi}{\partial z^2} = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + b \psi \quad (3)$$

with $a = 2k_0 n_0$ and $b = k_0^2 (n^2 - n_0^2)$. Neglecting the second-order derivative $|\partial^2 \psi / \partial z^2|$ in Eq. (3), by assuming the paraxial approximation $|ia \partial \psi / \partial z| \gg |\partial^2 \psi / \partial z^2|$, yields

$$ia \frac{\partial \psi}{\partial z} = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + b \psi \quad (4)$$

Assuming the electric field at the grid point of $x = m\Delta x$, $y = j\Delta y$ and $z = l\Delta z$ is expressed as $\psi(m\Delta x, j\Delta y, l\Delta z) = \psi_{m,j}^l$, eq.(4) can be discretized in z direction as

$$ia \frac{\psi_{m,j}^{l+1} - \psi_{m,j}^l}{\Delta z} = \frac{\partial^2}{\partial x^2} \left(\frac{\psi_{m,j}^{l+1} + \psi_{m,j}^l}{2} \right) + \frac{\partial^2}{\partial y^2} \left(\frac{\psi_{m,j}^{l+1} + \psi_{m,j}^l}{2} \right) + \frac{(b\psi)_{m,j}^{l+1} + (b\psi)_{m,j}^l}{2} \quad (5)$$

Instead of splitting eq. (5) into two equations using the ADI method as in the classical BPM,¹⁻⁵ we rearrange eq. (5) into the following

$$-\frac{1}{2} \frac{\partial^2 \psi_{m,j}^{l+1}}{\partial x^2} - \frac{1}{2} \frac{\partial^2 \psi_{m,j}^{l+1}}{\partial y^2} + \frac{ia}{\Delta z} \psi_{m,j}^{l+1} - \frac{1}{2} (b\psi)_{m,j}^{l+1} = \frac{1}{2} \frac{\partial^2 \psi_{m,j}^l}{\partial x^2} + \frac{1}{2} \frac{\partial^2 \psi_{m,j}^l}{\partial y^2} + \frac{ia}{\Delta z} \psi_{m,j}^l + \frac{1}{2} (b\psi)_{m,j}^l \quad (6)$$

Eq. (6) can be further discretized in transverse directions into

$$-\frac{\delta_x^2 \psi_{m,j}^{l+1}}{2\Delta x^2} - \frac{\delta_y^2 \psi_{m,j}^{l+1}}{2\Delta y^2} + \frac{ia}{\Delta z} \psi_{m,j}^{l+1} - \frac{1}{2} (b\psi)_{m,j}^{l+1} = \frac{\delta_x^2 \psi_{m,j}^l}{2\Delta x^2} + \frac{\delta_y^2 \psi_{m,j}^l}{2\Delta y^2} + \frac{ia}{\Delta z} \psi_{m,j}^l + \frac{1}{2} (b\psi)_{m,j}^l \quad (7)$$

with $\delta_x^2 = \psi_{m-1} - 2\psi_m + \psi_{m+1}$ and $\delta_y^2 = \psi_{j-1} - 2\psi_j + \psi_{j+1}$

After some rearrangements for eq. (7), we have

$$\begin{aligned} & A \psi_{m-1,j}^{l+1} + B \psi_{m,j-1}^{l+1} + C \psi_{m,j}^{l+1} + D \psi_{m,j+1}^{l+1} + E \psi_{m+1,j}^{l+1} \\ & = R \psi_{m-1,j}^l + S \psi_{m,j-1}^l + T \psi_{m,j}^l + U \psi_{m,j+1}^l + V \psi_{m+1,j}^l = P_{m,j}^l \end{aligned} \quad (8)$$

where

$$\begin{cases} A = E = -\frac{1}{\Delta x^2} \\ B = D = -\frac{1}{\Delta y^2} \\ C = 2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) + \frac{2ia}{\Delta z} - b_{m,j}^{l+1} \\ R = V = \frac{1}{\Delta x^2} \\ S = U = \frac{1}{\Delta y^2} \\ T = -2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) + \frac{2ia}{\Delta z} + b_{m,j}^l \end{cases} \quad (9)$$

Clearly, the numerical algebraic equation (8) is not tridiagonal and cannot be solved using the Thomas method as in classical BPMs.¹⁻⁵ The second-order truncation error of the algorithm is maintained as in the tridiagonal BPMs. The matrix equation of a 3 by 3 mesh grid, for example, is shown as

$$\begin{pmatrix} C'_{11} & D_{12} & 0 & E_{21} & 0 & 0 & 0 & 0 & 0 \\ B_{11} & C'_{12} & D_{13} & 0 & E_{22} & 0 & 0 & 0 & 0 \\ 0 & B_{12} & C'_{13} & 0 & 0 & E_{23} & 0 & 0 & 0 \\ A_{11} & 0 & 0 & C'_{21} & D_{22} & 0 & E_{31} & 0 & 0 \\ 0 & A_{12} & 0 & B_{21} & C_{22} & D_{23} & 0 & E_{32} & 0 \\ 0 & 0 & A_{13} & 0 & B_{22} & C'_{23} & 0 & 0 & E_{33} \\ 0 & 0 & 0 & A_{21} & 0 & 0 & C'_{31} & D_{32} & 0 \\ 0 & 0 & 0 & 0 & A_{22} & 0 & B_{31} & C'_{32} & D_{33} \\ 0 & 0 & 0 & 0 & 0 & A_{23} & 0 & B_{32} & C'_{33} \end{pmatrix} \begin{pmatrix} \psi^{l+1}_{11} \\ \psi^{l+1}_{12} \\ \psi^{l+1}_{13} \\ \psi^{l+1}_{21} \\ \psi^{l+1}_{22} \\ \psi^{l+1}_{23} \\ \psi^{l+1}_{31} \\ \psi^{l+1}_{32} \\ \psi^{l+1}_{33} \end{pmatrix} = \begin{pmatrix} P_{1,1}^l \\ P_{1,2}^l \\ P_{1,3}^l \\ P_{2,1}^l \\ P_{2,2}^l \\ P_{2,3}^l \\ P_{3,1}^l \\ P_{3,2}^l \\ P_{3,3}^l \end{pmatrix} \quad (10)$$

The coefficients with a prime sign in eq. (10) need to be calculated using the transparent boundary conditions (TBCs).¹⁹ As shown by Eq. (10) (a 9 by 9 matrix equation for a 3 by 3 mesh grid), an M by M mesh grid will generally need an M^2 by M^2 matrix equation, which requires a considerable amount of computer resources. However, since each row of the coefficient matrix of eq. (10) has no more than five non-zero values, the equation can be efficiently solved using iterative methods for sparse matrices, such as the Biconjugate Gradients Method (BICG).⁶

2.2 Wide-angle iterative BPM

In the following part, we demonstrate the derivation of a wide-angle iterative BPM based on Hoekstra's scheme and similar formulation as above. Rather than dropping this second order derivative, we can discretize the Helmholtz wave equation (3) in the z direction into the following

$$ia \frac{\psi^{l+1} - \psi^l}{\Delta z} - \frac{1}{\Delta z} \left[\left(\frac{\partial \psi}{\partial z} \right)^{l+1} - \left(\frac{\partial \psi}{\partial z} \right)^l \right] = \frac{\partial^2}{\partial x^2} \left(\frac{\psi^{l+1} + \psi^l}{2} \right) + \frac{\partial^2}{\partial y^2} \left(\frac{\psi^{l+1} + \psi^l}{2} \right) + \frac{(b\psi)^{l+1} + (b\psi)^l}{2} \quad (11)$$

and use Eq. (4) at the different z positions l and $l+1$ to find expressions for the first derivative with respect to z

$$\left(\frac{\partial \psi}{\partial z} \right)^l = \frac{1}{ia} \left[\frac{\partial^2 \psi^l}{\partial x^2} + \frac{\partial^2 \psi^l}{\partial y^2} + (b\psi)^l \right] \quad (12a)$$

$$\left(\frac{\partial \psi}{\partial z} \right)^{l+1} = \frac{1}{ia} \left[\frac{\partial^2 \psi^{l+1}}{\partial x^2} + \frac{\partial^2 \psi^{l+1}}{\partial y^2} + (b\psi)^{l+1} \right] \quad (12b)$$

Substituting eq. (12a) and (12b) into eq. (11), we find

$$\begin{aligned} ia \frac{\psi^{l+1} - \psi^l}{\Delta z} - \frac{1}{ia\Delta z} \left\{ \left[\frac{\partial^2 \psi^{l+1}}{\partial x^2} + \frac{\partial^2 \psi^{l+1}}{\partial y^2} + (b\psi)^{l+1} \right] - \left[\frac{\partial^2 \psi^l}{\partial x^2} + \frac{\partial^2 \psi^l}{\partial y^2} + (b\psi)^l \right] \right\} \\ = \frac{\partial^2}{\partial x^2} \left(\frac{\psi^{l+1} + \psi^l}{2} \right) + \frac{\partial^2}{\partial y^2} \left(\frac{\psi^{l+1} + \psi^l}{2} \right) + \frac{(b\psi)^{l+1} + (b\psi)^l}{2} \end{aligned} \quad (13)$$

Discretizing eq. (13) in the transverse directions x and y yields

$$\begin{aligned} ia \frac{\psi_{m,j}^{l+1} - \psi_{m,j}^l}{\Delta z} - \frac{1}{ia\Delta z} \left\{ \left[\frac{\delta_x^2 \psi_j^{l+1}}{\Delta x^2} + \frac{\delta_y^2 \psi_m^{l+1}}{\Delta y^2} + (b\psi)_{m,j}^{l+1} \right] - \left[\frac{\delta_x^2 \psi_j^l}{\Delta x^2} + \frac{\delta_y^2 \psi_m^l}{\Delta y^2} + (b\psi)_{m,j}^l \right] \right\} \\ = \frac{\delta_x^2 \psi_j^{l+1} + \delta_x^2 \psi_j^l}{2\Delta x^2} + \frac{\delta_y^2 \psi_m^{l+1} + \delta_y^2 \psi_m^l}{2\Delta y^2} + \frac{(b\psi)_{m,j}^{l+1} + (b\psi)_{m,j}^l}{2} \end{aligned} \quad (14)$$

After some rearrangements of eq. (14), we obtain a numerical equation in the same form as eq. (8) but with different coefficients from eq. (9)

$$\begin{cases} A = E = -\frac{1}{\Delta x^2} \left(1 - \frac{2i}{a\Delta z} \right) \\ B = D = -\frac{1}{\Delta y^2} \left(1 - \frac{2i}{a\Delta z} \right) \\ C = 2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \left(1 - \frac{2i}{a\Delta z} \right) + \frac{2ia}{\Delta z} - \left(1 - \frac{2i}{a\Delta z} \right) b_{m,j}^{l+1} \\ R = V = \frac{1}{\Delta x^2} \left(1 + \frac{2i}{a\Delta z} \right) \\ S = U = \frac{1}{\Delta y^2} \left(1 + \frac{2i}{a\Delta z} \right) \\ T = -2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \left(1 + \frac{2i}{a\Delta z} \right) + \frac{2ia}{\Delta z} + \left(1 + \frac{2i}{a\Delta z} \right) b_{m,j}^l \end{cases} \quad (15)$$

2.3 3-D Gaussian beam initialization

In order to show their applicability, accuracy and effectiveness, the algorithms derived above need to be applied to not only Gaussian beam propagation in homogeneous media and modal beam propagation in straight waveguide, but also to wide-angle beam propagation such as tilted Gaussian beam propagation and tilted waveguide beam propagation. In this part, we derive the electric field initialization expressions for tilted Gaussian beam and tilted waveguide.

The fundamental mode of the electric field complex amplitude of a 3-D Gaussian beam, propagating along the z axis of the coordinate system, measured a distance r from its centre, and a distance z from its waist, is given by

$$E(r, z) = E_0 \frac{W_0}{W(z)} \exp \left[-\frac{r^2}{W^2(z)} \right] \exp \left[-jkz - jk \frac{r^2}{2R(z)} + jG(z) \right] \quad (16)$$

with

$$r^2 = x^2 + y^2, \quad W(z) = W_0 \sqrt{1 + (z/z_0)^2}, \quad R(z) = z \left[1 + (z_0/z)^2 \right], \quad G(z) = \tan^{-1}(z/z_0), \quad W_0 = \sqrt{(\lambda_0 z_0)/(n\pi)}$$

where E_0 is a constant, λ_0 is the wavelength in vacuum and n is the refractive index of the media, k is wavevector and $W(z)$ is the beam radius at which the field amplitude drops to $1/e$. This parameter is called the beam radius or spot size of the beam. W_0 is the minimum value of $W(z)$, which is at $z=0$ and called waist radius. The beam radius increases gradually with $|z|$, reaching $\sqrt{2}W_0$ at $z=z_0$, which is known as Rayleigh range. $G(z)$ is referred to as Guoy phase.

If the beam is propagating along a vector with θ -degree tilted with respect to z axis, a coordinate system transform is needed to get the initialization in the input plane. The transform matrix for a clockwise rotation by an angle θ around a unit vector $\hat{v} = (x, y, z)$ is

$$M(v, \theta) = \begin{bmatrix} \cos\theta + (1-\cos\theta)x^2 & (1-\cos\theta)xy - z\sin\theta & (1-\cos\theta)xz + y\sin\theta \\ (1-\cos\theta)xy + z\sin\theta & \cos\theta + (1-\cos\theta)y^2 & (1-\cos\theta)zy - x\sin\theta \\ (1-\cos\theta)xz - y\sin\theta & (1-\cos\theta)zy + x\sin\theta & \cos\theta + (1-\cos\theta)z^2 \end{bmatrix} \quad (17)$$

As is shown in Figure 1, the z axis rotates θ degrees around the vector $\hat{v} = (\sin\phi, -\cos\phi, 0)$, then the coordinate system becomes $(\hat{x}_1, \hat{y}_1, \hat{z}_1)$ from $(\hat{x}, \hat{y}, \hat{z})$. The transform matrix for this rotation is

$$M(\phi, \theta) = \begin{bmatrix} \cos\theta + (1-\cos\theta)\sin^2\phi & (\cos\theta-1)\sin\phi\cos\phi & -\sin\theta\cos\phi \\ (\cos\theta-1)\sin\phi\cos\phi & \cos\theta + (1-\cos\theta)\cos^2\phi & -\sin\theta\sin\phi \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix} \quad (18)$$

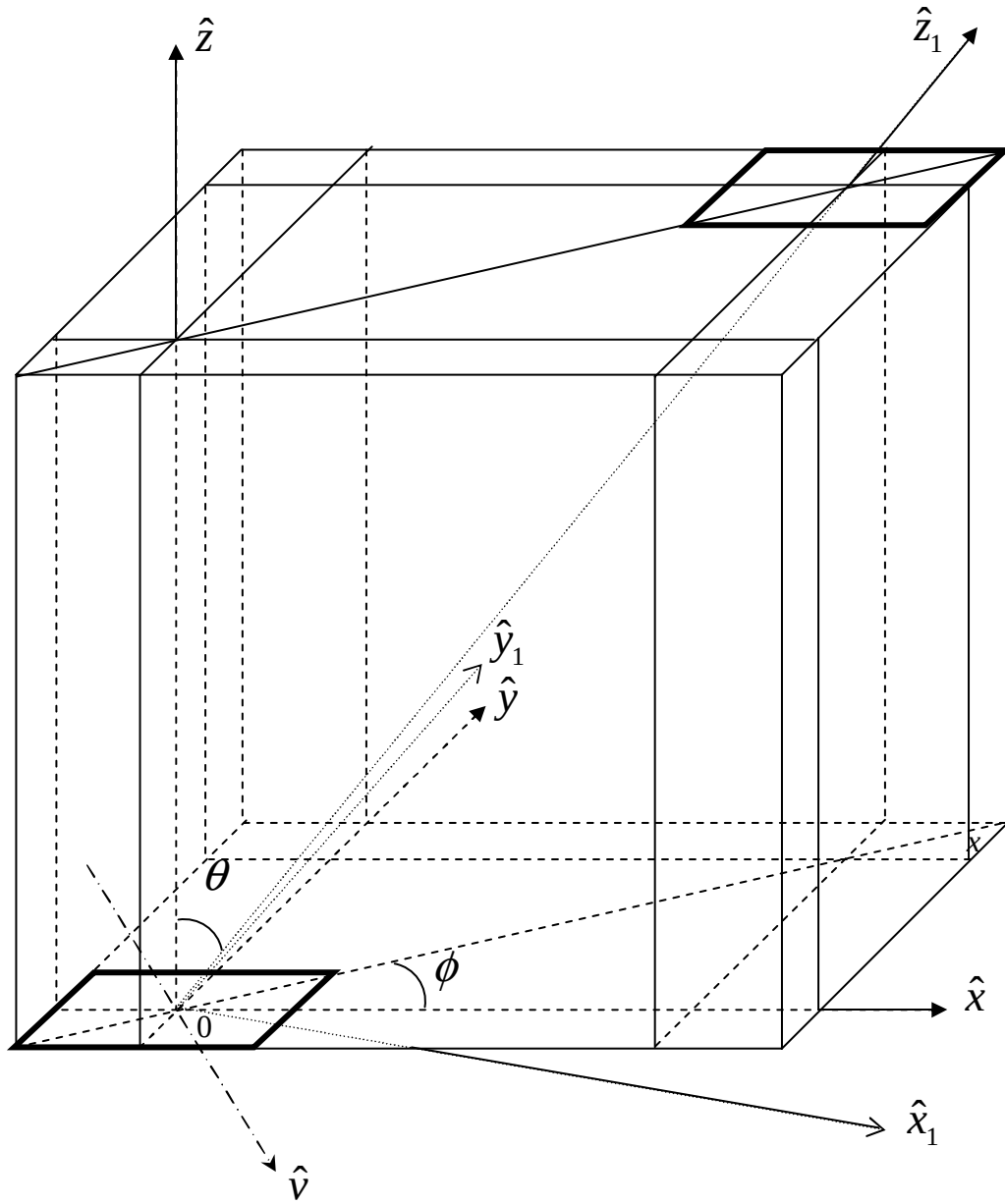


Figure 1 Schematic diagram of tilted beam and its coordinate systems

Therefore the transform equation is

$$(\hat{x}_1 \ \hat{y}_1 \ \hat{z}_1)' = M(\phi, \theta)(\hat{x} \ \hat{y} \ \hat{z})' \quad (19)$$

Here the prime in eq. (19) refers to as matrix transposition. Now we suppose the 3-D Gaussian beam is propagating along axis $\hat{z}_1$, then the Gaussian beam has the same form in the coordinate system $(\hat{x}_1, \hat{y}_1, \hat{z}_1)$ as in $(\hat{x}, \hat{y}, \hat{z})$, i.e.

$$E(r_1, z_1) = E_0 \frac{W_0}{W(z_1)} \exp\left[-\frac{r_1^2}{W^2(z_1)}\right] \exp\left[-jkz_1 - jk \frac{r_1^2}{2R(z_1)} + jG(z_1)\right] \quad (20)$$

Using the transform equation (19), the Gaussian beam (20) can be expressed in the coordinate system $(\hat{x}, \hat{y}, \hat{z})$. The question now is what the field distribution at $z=0$ is, because the numerical discretization is in the coordinate system $(\hat{x}, \hat{y}, \hat{z})$. This field distribution at $z=0$ is the initialization for the tilted waveguide, i.e.

$$\begin{cases} x_1 = x[\cos\theta + (1 - \cos\theta)\sin^2\phi] + y[(\cos\theta - 1)\sin\phi\cos\phi] \\ y_1 = x[(\cos\theta - 1)\sin\phi\cos\phi] + y[\cos\theta + (1 - \cos\theta)\cos^2\phi] \\ z_1 = x\sin\theta\cos\phi + y\sin\theta\sin\phi \end{cases} \quad (21)$$

2.4 3-D channel waveguide initialization

The electric field of the E_{pq}^x (also referred to as EH_{pq}) mode is assumed to be polarized in the x direction, i.e. $E_x \neq 0, E_y = 0$.²⁰ Here the Marcattili's method²¹ is used to analyze the modal distribution of 3-D optical waveguides. Figure 2 shows a cross section of a 3-D channel waveguide.

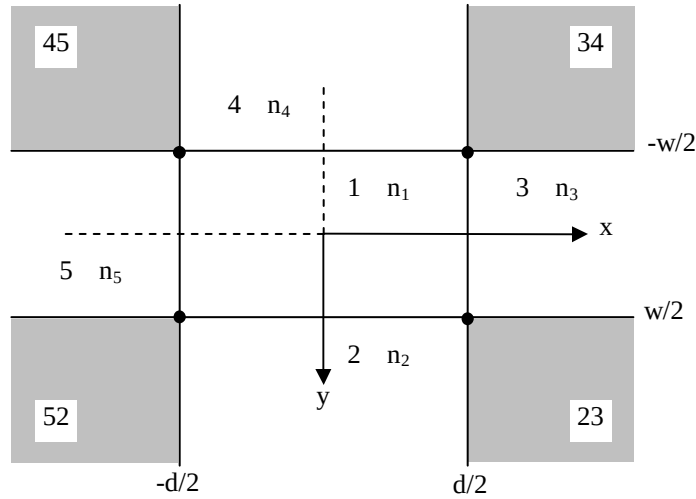


Figure 2 Cross section of a 3-D channel waveguide.

Assuming $\partial/\partial z = -ik_z$. The principal field component E_x of E_{pq}^x satisfies the wave equation

$$\frac{\partial^2 E_x}{\partial x^2} + \frac{\partial^2 E_x}{\partial y^2} + (\omega^2 \mu \epsilon - k_z^2) E_x = 0 \quad (22)$$

where ω is the circular frequency of the wave, μ is the permeability and ϵ is the permittivity of the materials. Note that the permeability of non-magnetic materials is one, i.e. $\mu = 1$. In Marcattili's method, the magnetic field and electric field are assumed to be confined to the core, region 1, and region 2 to 5, and do not exist in the four shadow regions. As a result, the continuity conditions of the fields are only applied to the boundaries between regions 1 and 2, 1 and 3, 1 and 4, and 1 and 5. The solution of the principal field component E_x takes the following forms in region 1 to 5²⁰

$$E_x = \exp(-ik_z z) \begin{cases} C_1 \cos(k_x x + \phi_x) \cos(k_y y + \phi_y) & (\text{in region 1}) \\ C_2 \cos(k_x x + \phi_x) \exp[-\alpha_2(y - w/2)] & (\text{in region 2}) \\ C_3 \exp[-\alpha_3(x - d/2)] \cos(k_y y + \phi_y) & (\text{in region 3}) \\ C_4 \cos(k_x x + \phi_x) \exp[\alpha_4(y + w/2)] & (\text{in region 4}) \\ C_5 \exp[\alpha_5(x + d/2)] \cos(k_y y + \phi_y) & (\text{in region 5}) \end{cases} \quad (23)$$

In order to include the field distribution in the four shadow regions, we extend E_x to region 23, 34, 45 and 52 in the following way

$$E_x = \exp(-ik_z z) \begin{cases} C_{23} \exp[-\alpha_2(y - w/2) - \alpha_3(x - d/2)] & (\text{in region 23}) \\ C_{34} \exp[-\alpha_3(x - d/2) + \alpha_4(y + w/2)] & (\text{in region 34}) \\ C_{45} \exp[\alpha_4(y + w/2) + \alpha_5(x + d/2)] & (\text{in region 45}) \\ C_{52} \exp[\alpha_5(x + d/2) - \alpha_2(y - w/2)] & (\text{in region 52}) \end{cases} \quad (24)$$

Where C 's are constants, α 's are attenuation coefficients and ϕ 's are phase shifts. C_i can be set to be any number, but usually one. C_{23} , C_{34} , C_{45} and C_{52} are field values at the corresponding corners. Using the boundary conditions at $y = \pm w/2$ and $x = \pm d/2$, we obtain two transcendental equations for k_x and k_d :

$$k_y w = \tan^{-1} \left(\frac{\sqrt{(n_1^2 - n_2^2)k_0^2 w^2 - (k_y w)^2}}{k_y w} \right) + \tan^{-1} \left(\frac{\sqrt{(n_1^2 - n_4^2)k_0^2 w^2 - (k_y w)^2}}{k_y w} \right) + q\pi \quad q = 0, 1, 2, \dots \quad (25)$$

$$k_x d = \tan^{-1} \left(\frac{k_0^2 n_1^2 - k_y^2}{k_0^2 n_3^2 - k_y^2} \cdot \frac{\sqrt{(n_1^2 - n_3^2)k_0^2 d^2 - (k_x d)^2}}{k_x d} \right) + \tan^{-1} \left(\frac{k_0^2 n_1^2 - k_y^2}{k_0^2 n_5^2 - k_y^2} \cdot \frac{\sqrt{(n_1^2 - n_5^2)k_0^2 d^2 - (k_x d)^2}}{k_x d} \right) + p\pi \quad p = 0, 1, 2, \dots \quad (26)$$

k_x and k_d can be obtained solving eqs. (25) and (26), then all the other coefficients can be calculated using some relations obtained during the derivation of eqs. (25) and (26).

If the waveguide is tilted as is shown in figure 1, its modal field expressions in coordinate system $(\hat{x}_1, \hat{y}_1, \hat{z}_1)$ have the same form as eqs. (23) and (24) but all independent variables having a subscript of 1. As a result, the initialization at $z=0$ can be obtained using eq. (21).

Note that the term $\exp(-ik_z z)$ for both cases is considered to be the fast changing phase term and removed during the derivation of the algorithms if the simulation and its numerical discretization are in the coordinate system $(\hat{x}, \hat{y}, \hat{z})$. As a result, this term also needs to be removed when calculating the field profile at z to compare with the simulation results.

3. SIMULATIONS AND DISCUSSIONS

We first apply these two algorithms to the simulations of 3-D Gaussian beam propagation in free space for 60 μm in the z direction, which is same for all simulations. The Gaussian beam profile has a waist radius $w_0 = 3.0 \mu\text{m}$ at the wavelength of 0.85 μm , which is used for all simulations. For the second example, we simulate fundamental mode propagation in a straight 4 μm by 4 μm channel waveguide with values of the refractive index of the core and the cladding being 1.55 and 1.532, respectively. The step sizes used for the two cases are $\Delta x = \Delta y = 0.15 \mu\text{m}$ and $\Delta z = 0.2 \mu\text{m}$. The results of both algorithms for both cases have good matches with the analytical solutions. The relative L^2 norm error with respect to the analytical solution of output field profile for the waveguide beam propagation is $\sim 10^{-4}$, which is 2 orders of magnitude higher than the same type of errors for the Gaussian beam propagation.

In order to check the effectiveness of the wide-angle scheme, in the following we apply the two algorithms to wide-angle beam propagation. However, a large simulation window is needed for wide-angle simulations, which is time-consuming and even inexecutable. As a result, we use the simulation window shifting technique introduced in our earlier work¹⁸ to ease the computational time required. In this shifting technique, we shift the window of simulation toward the transverse propagation direction every few steps. This keeps window centered on the main part of the pulse and avoids computations involving large numbers of edge cells. This is performed by removing cells at the two edges closer to the transverse origin and generating the same number of data at the two opposite edges using linear extrapolation. At the same time, the convergence problem accompanying the iterative methods is eased using the threshold technique introduced in our former work,¹⁸ in which those elements of the field vector below some small threshold are setting to zero to reduce the volatility of the field profile.

We apply the two algorithms to two examples: a tilted Gaussian beam propagation and mode propagation in a tilted channel waveguide. Both beams with the same parameters as the two above examples propagate along an angle of 30-degrees with respect to the z axis and along a direction mid way between the x and y axes. The step sizes used for the two wide-angle cases are $\Delta x = \Delta y = 0.1 \mu\text{m}$, $\Delta z = 0.2 \mu\text{m}$. As shown in figure 3, the results of the wide-angle scheme (middle pulse) have better matches with respect to the analytical solutions (pulse on the right side) than the results of the paraxial scheme (on the left side). Note that the output obtained using the wide-angle scheme is so close to the analytical solution that it is hard to distinguish in figure 3(a). Table 1 shows the relative L^2 norm errors the relative shift

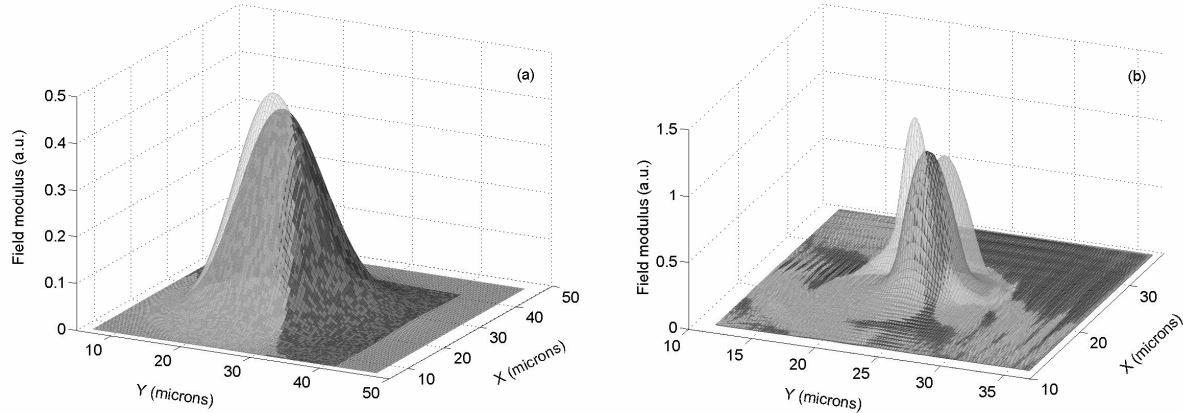


Figure 3 The output profiles obtained using the Fresnel scheme (on the left side), the wide-angle scheme (in the middle) and the analytical solution (on the right side), for (a) tilted Gaussian beam propagation, and (b) mode propagation in tilted channel waveguide.

errors with respect to the analytical solution of output field profiles for the tilted Gaussian beam propagation and the mode propagation in tilted waveguide. It is clearly seen that the wide-angle scheme is more accurate than the Fresnel scheme for both examples.

	Gaussian beam		Channel waveguide	
Scheme	L^2 norm	Shift	L^2 norm	Shift
Paraxial	7.67%	14.70%	14.32%	6.53%
Wide-angle	0.80%	3.27%	2.03%	4.08%

Table 1 The relative L^2 norm errors and the relative shift errors with respect to the analytical solution of output field profiles for the tilted Gaussian beam propagation and the mode propagation in tilted waveguide.

4. CONCLUSION

We have demonstrated the derivation of two iterative BPMs: one is the Fresnel scheme and the other one is a wide-angle scheme. Their applicability and effectiveness are shown by applying these two schemes to straight and tilted Gaussian beam propagation and mode propagation in straight and tilted channel waveguide. The simulations results show that the iterative BPMs are applicable, with the wide-angle scheme being more accurate than the Fresnel scheme. However, the applicability of the iterative BPMs is limited because large matrices have to be used and iterative methods can only be used to solve square matrix equations, despite the convergence problem being eased by using the threshold technique and the required computational resources lowered by reducing the dimension of the matrix using the simulation window shifting technique. These types of schemes can be combined with semivectorial formulations to improve the errors introduced by refractive index discontinuities between the core and cladding of waveguides. They also enable us to develop higher-order 3-D wide-angle BPMs using Padé approximant operators and multistep method.

5. ACKNOWLEDGEMENT

This material is based upon work supported by the National Science Foundation under Grant No. 0348955.

6. REFERENCES

1. M. D. Feit and J. A. Fleck, Jr., "Light propagation in graded-index optical fibers", *Appl. Opt.* **17**, p.3990-3998, 1978.
2. D. Yevick, "A guide to electric field propagation techniques for guided-wave optics", *Opt. Quantum Electron.* **26**, p.S185-S197, 1994.
3. R. Scarmozzino, A. Gopinath, R. Pregla, and S. Helfert, "Numerical techniques for modeling guided-wave photonic devices", *IEEE J. Selected Topics in Quantum Electron.*, **6**, p.150-161, 2000.
4. J. Van Roey, J. van der Donk, and P.E. Lagasse, "Beam-propagation method: analysis and assessment", *J. Opt. Soc. Am.*, **71**, p.803-810, 1981.
5. Y. Chung and N. Dagli, "Assessment of finite difference beam propagation," *IEEE J. Quantum Electron.*, **26**, p.1335-1339, 1990.
6. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical recipes: The art of scientific computing*, Cambridge University Press, New York, 1986.
7. J. Gerdes and R. Pregla, "Beam-propagation algorithm based on the method of lines", *J. Opt. Soc. Amer. A*, **8**, p.389-394, 1991.
8. R. P. Ratowsky and J. A. Fleck, Jr., "Accurate numerical solution of the Helmholtz equation by iterative Lanczos reduction", *Opt. Lett.*, **16**, p.787-789, 1991.
9. P. -C. Lee, D. Schulz, and E. Voges, "Three-dimensional finite difference beam propagation algorithms for photonic devices", *J. Lightwave Technol.*, **10**, p.1832-1838, 1992.
10. P. -C. Lee and E. Voges, "Three-dimensional semi-vectorial wave-angle beam propagation method", *J. Lightwave Technol.*, **12**, p.215-225, 1994.
11. A. Sharma and A. Agrawal, "New method for nonparaxial beam propagation", *J. Opt. Soc. Am. A*, **21**, p.1082-1087, 2004.
12. S. L. Chui and Y. Y. Lu, "Wide-angle full-vector beam propagation method based on an alternating direction implicit preconditioner", *J. Opt. Soc. Am. A*, **21**, p.420-425, 2004.
13. G. R. Hadley, "Wide-angle beam propagation using Padé approximant operators", *Opt. Lett.*, **17**, p.1426-1428, 1992.
14. G. R. Hadley, "Multistep method for wide-angle beam propagation", *Opt. Lett.*, **17**, p.1743-1745, 1992.
15. H. J. W. M. Hoekstra, G. J. M. Krijnen and P. V. Lambeck, "On the accuracy of the finite difference method for applications in beam propagating techniques", *Opt. Commun.*, **94**, p.506-508, 1992.
16. Z. Ju, J. Fu and E. Feng, "A simple wide-angle beam-propagation method for integrated optics", *Microwave Opt. Technol. Lett.*, **14**, p.345-347, 1997.
17. C. Ma and E. V. Keuren, "A simple three dimensional wide-angle beam propagation method", *Optics Express*, **14**, p.4668-4674, 2006.
18. C. Ma and E. V. Keuren, "A three dimensional iterative wide-angle beam propagation method", *Optics Express*, (submitted on June 15, 2006).
19. G. R. Hadley, "Transparent boundary condition for beam propagation", *Opt. Lett.*, **16**, p.624-626, 1991.
20. K. Kawano and T. Kitoh, *Introduction to optical waveguide analysis: solving Maxwell's equations and the Schrödinger equation*, John Wiley & Sons, INC., New York, 2001.
21. E. A. J. Marcatili, "Dielectric rectangular waveguide and directional coupler for integrated optics", *Bell Syst. Tech. J.*, **48**, p.2071-2102, 1969.