An Efficient Method for Estimating the Electromagnetic Wave Propagation in Three Dimensional Optical Waveguide Structures

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Received 2 April 2018; Accepted (in revised version) 16 November 2018

Abstract. In this work, the full vectorial beam propagation methods (BPMs) are adopted for the calculations of the electromagnetic wave propagation from the two dimensional and three dimensional optical waveguide structures. First, the full vectorial BPM for the three dimensional optical waveguide structures is introduced. Next, in the transverse directions of the considered waveguide structures, we adopt the second order finite difference method to discretize the electromagnetic components. Then, the Lanczos/Arnoldi fast solvers are adopted to find the leading eigenvalues and eigenvectors of the square root operator in the BPM process of the optical waveguide structures. Furthermore, we propose the rational \([\frac{p-1}{p}]\) Padé approximation to approximate the exponential operator in the BPM process. To demonstrate the efficiency of the numerical solvers, the two dimensional symmetric and unsymmetric problems are considered, and good convergence results are obtained. Furthermore, the resulting full-vectorial BPM is adopted to simulate the wave propagation among the three dimensional rib and taper waveguide structures. Numerical results demonstrate the efficiency of the proposed method with respect to both the accuracies and convergence results.

AMS subject classifications: 78M25, 78M16, 78A45

Key words: Wave propagation, fast solver, Lanczos method, perfectly matched layer.

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1 Introduction

The beam propagation method (BPM) [1–6] is widely used in the numerical simulation of the wave propagation among the optical waveguides and optical fiber waveguide structures [7–10]. The simplest BPM is derived from the slowly varying envelope approximation [11], and more advanced variants are based on rational approximants of the square root operators [3] or the exponential of the square root operators [12, 13]. The limitation of the slowly varying envelope approximation is that it is only accurate for wave fields propagating in a small angle around the waveguide axis. For the planar waveguide structures, it is widely accepted that the scalar wide-angle BPM [3] is more accurate than the slowly varying envelope approximation BPM. Importantly, BPM is an efficient method for modeling wave propagation in slowly varying waveguides, including waveguide bends, branches, tapers, etc.

For two dimensional waveguide structures with the TE or TM polarized waves, the governing equation for the electromagnetic wave propagation is a scalar Helmholtz equation [14]. For the three dimensional guided-wave structures, the scalar and semi-vectorial formulations of the BPM are often not sufficient. A full vectorial formulation [15] is necessary for polarization-dependent optical waveguide structures. Most full vectorial BMPS [15–17, 19, 20, 34] could use the slowly varying envelope approximation. A wide-angle full vectorial BPM has already been formulated [12]. Recently, the full vectorical BMPS have been widely studied by the researchers from engineers, physicists and mathematicians. For instance, in [15], the simulations of three dimensional optical waveguides were described. The polarizations dependence and their coupling for the vectorial electromagnetic fields in nature were formulated in detail. The guided modes from the rib optical waveguide were investigated [18]. Specifically, the comparisons results of the simulation results via the scalar, semi-vectorial and full vectorial from the rib optical waveguide were made in detail. In [20], a novel full-vectorial beam-propagation method based on the McKee–Mitchell scheme was proposed. Compared to the Peaceman–Rachford scheme, the proposed McKee–Mitchell scheme demonstrates its better accuracy while maintaining the high computational accuracy. Moreover, the finite difference formulas with the consideration of the discontinuities of refractive index was developed. The three dimensional rib optical waveguide was considered with the eigenmode analysis with the aid of the proposed method in [20]. In [21], a numerical analysis of wave propagation through optical rib waveguide using Lanczos versions of the Fresnel, wide-angle, and Helmholtz propagation processes. Furthermore, the Lanczos algorithms combined with the finite-difference as opposed to the fast Fourier transform formulations of the transverse derivative operators from the Helmholtz propagation process were adopted. In [23], the typical beam propagation methods for the approximations to the one-way Helmholtz equation were considered first. Then, the efficient implementation of the beam propagation method based on the rational approximations of the propagator was developed successfully. Numerical results on the mode distribution from the taper optical waveguide were demonstrated.
For the simulation of the wave propagation along the optical waveguide structures, the Helmholtz equation converges very slowly. In this situation, as was given in [27], the full vectorial BPMs for three dimensional optical waveguides could be formulated with the rational approximants of a square root operator or the one-way propagator involved. Compared with the BPM from the slowly varying envelope approximation, the full vectorial BPM could gain high accuracies. In [27], the wide-angle full vectorial BPM was used to simulate the propagation of wave fields. In this work, the full vectorial electromagnetic wave propagation problem based on the BPM and the Lanczos/Arnoldi fast solvers is considered. The one-way Helmholtz equation to approximate the Maxwell’s equations is adopted. The \( \left( \frac{p-1}{p} \right) \) Padé approximation [23] for the square root propagator and the Lanczos/Arnoldi method are adopted in the process of BPM. The numerical results for two dimensional symmetric and unsymmetric waveguides are conducted, and then obtain the convergence results of the Lanczos/Arnoldi method. As the numerical examples of three dimensional waveguide, the waveguide structures with \( z \) as the propagation direction [5, 25] are analyzed. The subsequent full-vectorial BPM is used to simulate the propagation of the wave fields in the three dimensional rib and taper waveguide structures.

In this work, the reason why we adopt the full-vectorial wide angle BPM is that the waveguides have high index contrast, in this situation, the scalar BPM and the full-vectorial paraxial BPM are no longer accurate. Meanwhile, the reason why we use the Lanczos method is that the Lanczos method allows one to implement the full-vectorial wide-angle BPM efficiently, with the aid of the \( \left( \frac{p-1}{p} \right) \) Padé approximation for the square root propagator. The manuscript is organized as follows: Section 2 introduces the establishment of the mathematical formulations for the full vectorial BPM. The governing equations for the transverse electric field are described. In order to approximate the governing Helmholtz equation, the one-way Helmholtz equations are introduced. Then, a second order finite-difference scheme is adopted to solve the governing Helmholtz equation, and the implementation of the numerical dispersion for the propagation operator is discussed. In Section 3, we propose a new Lanczos/Arnoldi method to approximate the square root operator in one-way Helmholtz equation. To increase the convergence rate and accuracy of the solution, a \( \left( \frac{p-1}{p} \right) \) Padé approximation is introduced in Section 4. The application of the method to typical optical guided-wave structures is presented in Section 5, including both the two dimensional symmetric and unsymmetric waveguide structures, and three dimensional rib and taper waveguide structures. Finally, the conclusion is given in Section 6.

2 The full vectorial beam propagation method

In the frequency domain, the propagation of electromagnetic wave fields through an inhomogeneous medium is governed by the Maxwell’s equations:
\[ \nabla \times \mathbf{E} = i \omega \mu_0 \mathbf{H}, \quad (2.1) \]
\[ \nabla \times \mathbf{H} = -i \omega \varepsilon_0 \varepsilon(r) \mathbf{E}, \quad (2.2) \]
\[ \nabla \cdot (\varepsilon(r) \mathbf{E}) = 0, \quad (2.3) \]
\[ \nabla \cdot \mathbf{H} = 0, \quad (2.4) \]

where \( \varepsilon(r) = \varepsilon(x,y,z) \) is the permeability of the medium which is assumed to be isotropic. A time dependence of \( e^{-i \omega t} \) is assumed throughout this paper. In order to model and simulate the electromagnetic wave propagation in a medium characterized by \( \varepsilon(r) \), one could solve the two curl equations (2.1) and (2.2), simultaneously. As an efficient numerical methods, we could approximate the Helmholtz equations by one-way Helmholtz equation as follows.

In a \( z \)-invariant waveguide with \( \varepsilon = \varepsilon(x,y) \), the frequency domain Maxwell’s equations for the transverse magnetic components could be reduced as
\[ \partial_z^2 \mathbf{u} + A \mathbf{u} = 0, \quad (2.5) \]

where \( \mathbf{u} = [H_x, H_y]^T \).

The BPM is useful for the slowly varying waveguide where \( \varepsilon = \varepsilon(x,y,z) \) varies with \( z \) slowly. In this situation, Eq. (2.5) is an approximation of the Maxwell’s equations when \( n \) varies with \( z \) slowly. On invoking (2.5) in the BPM process, we could obtain
\[ \partial_z \mathbf{u} \approx i \sqrt{A} \mathbf{u}. \quad (2.6) \]

Here, the operation matrix is defined as follows:
\[
A = \begin{bmatrix}
\frac{\partial^2}{\partial x^2} + \varepsilon \frac{\partial}{\partial y} \left( \frac{1}{\varepsilon} \frac{\partial}{\partial y} \right) + k_0^2 \varepsilon & \frac{\partial^2}{\partial y \partial x} - \frac{\varepsilon}{\partial y} \left( \frac{1}{\varepsilon} \frac{\partial}{\partial x} \right) \\
\frac{\partial^2}{\partial x \partial y} - \frac{\varepsilon}{\partial x} \left( \frac{1}{\varepsilon} \frac{\partial}{\partial y} \right) & \frac{\partial^2}{\partial x^2} \left( \frac{1}{\varepsilon} \frac{\partial}{\partial x} \right) + \frac{\partial^2}{\partial y^2} + k_0^2 \varepsilon
\end{bmatrix},
\]

\( I \) is the \( 2 \times 2 \) identity matrix, \( n_* \) is the reference refractive index. And a \( 2 \times 2 \) operator matrix \( X \) is defined by
\[ A = k_0^2 n_*^2 (I + X), \quad (2.7) \]
and its entries are
\[
X_{11} = \frac{1}{k_0^2 n_*^2} \left[ n^2 \frac{\partial}{\partial x} \left( \frac{1}{n^2} \frac{\partial}{\partial x} \right) + \frac{\partial^2}{\partial y^2} + k_0^2 n^2 - k_0^2 n_*^2 \right],
\]
\[
X_{12} = \frac{1}{k_0^2 n_*^2} \left[ n^2 \frac{\partial}{\partial x} \left( \frac{1}{n^2} \frac{\partial}{\partial y} \right) - \frac{\partial^2}{\partial x \partial y} \right],
\]
\[
X_{21} = \frac{1}{k_0^2 n_*^2} \left[ n^2 \frac{\partial}{\partial y} \left( \frac{1}{n^2} \frac{\partial}{\partial x} \right) - \frac{\partial^2}{\partial y \partial x} \right],
\]
\[
X_{22} = \frac{1}{k_0^2 n_*^2} \left[ n^2 \frac{\partial}{\partial y} \left( \frac{1}{n^2} \frac{\partial}{\partial y} \right) + \frac{\partial^2}{\partial x^2} + k_0^2 n^2 - k_0^2 n_*^2 \right].
\]
Next, the propagation is discretized in \( z \) direction, for a discretized step from 
\( z_j \) to 
\( z_{j+1} = z_j + \Delta z \), subject to the starting field 
\( u = u_0 \) at 
\( z = z_0 \), we could get the numerical solution of (2.6) as follows

\[
    u_j = P(X)u_{j-1}, \quad j = 1, 2, 3, \ldots
\]

where

\[
    P(X) = e^{i\Delta z \sqrt{A}}.
\]

\[
    u_j(x, y, z) = u(x, y, z_0 + j\Delta z).
\]

In (2.8), \( u_j \) is an approximation of \( u \) at \( z_j \), and \( X \) is evaluated at 
\( z_{j+\frac{1}{2}} = z_j + \frac{\Delta z}{2} \). In order to find the approximate values of the propagation factor 
\( P(X) \), we could use the Lanczos/Arnoldi method to approximate the square of the operator matrix \( A \), and use the Padé approximation to approximate the value of the exponential function by a rational function, which are comprehensively given as follows.

Eq. (2.6) could be further formulated as

\[
    -\frac{\partial^2 H_x}{\partial z^2} = A_{xx} H_x + A_{xy} H_y, \quad \text{(2.9)}
\]

\[
    -\frac{\partial^2 H_y}{\partial z^2} = A_{yx} H_x + A_{yy} H_y, \quad \text{(2.10)}
\]

where the operators in (2.9) and (2.10) are defined as:

\[
    A_{xx} H_x = \frac{\partial^2 H_x}{\partial x^2} + \epsilon \frac{\partial}{\partial y} \left( \frac{1}{\epsilon} \frac{\partial H_x}{\partial y} \right) + k_0^2 \epsilon H_x, \quad \text{(2.11)}
\]

\[
    A_{xy} H_y = \frac{\partial^2 H_y}{\partial y \partial x} - \epsilon \frac{\partial}{\partial y} \left( \frac{1}{\epsilon} \frac{\partial H_x}{\partial x} \right), \quad \text{(2.12)}
\]

\[
    A_{yx} H_x = \frac{\partial^2 H_x}{\partial x \partial y} - \epsilon \frac{\partial}{\partial x} \left( \frac{1}{\epsilon} \frac{\partial H_y}{\partial y} \right), \quad \text{(2.13)}
\]

\[
    A_{yy} H_x = \frac{\partial^2 H_y}{\partial y^2} + \epsilon \frac{\partial}{\partial x} \left( \frac{1}{\epsilon} \frac{\partial H_y}{\partial x} \right) + k_0^2 \epsilon H_y. \quad \text{(2.14)}
\]

Eqs. (2.11)-(2.14) could be numerically solved by using a finite-difference method. In the finite-difference method, the continuous space is replaced by a discrete lattice structure defined in the computational region. The fields at the lattice point of \( x = m\Delta x, \ y = n\Delta y, \) and 
\( z = l\Delta z \) are represented by their discretized versions. Importantly, the operator components of \( A \) in (2.9) and (2.10) are approximated by a second order finite difference scheme. To decrease the error of the finite-difference approximation, we adopt the central finite-difference approximation scheme. In detail, the second order finite difference
formulations for the operator $A$ are given in the following.

$$A_{xx}H_x = \frac{H_x(m+1,n) - 2H_x(m,n) + H_x(m-1,n)}{(\Delta x)^2}$$

$$+ \frac{T^H_{m,n}H_x(m,n) + T^H_{m,n-1}H_x(m,n-1)}{(\Delta y)^2}$$

$$+ \frac{T^H_{m,n+1}H_x(m,n+1)}{(\Delta y)^2} - k_0^2 n^2 (m,n,l) H_x(m,n),$$  \hspace{1cm} (2.15)

$$A_{xy}H_y = \frac{1}{4\Delta x \Delta y} \left[ \left( 1 - \frac{n^2(m,n,l)}{n^2(m,n+1,l)} \right) H_y(m+1,n+1) \right.$$}

$$- \left( 1 - \frac{n^2(m,n,l)}{n^2(m,n-1,l)} \right) H_y(m+1,n-1) \right.$$}

$$- \left( 1 - \frac{n^2(m,n,l)}{n^2(m,n+1,l)} \right) H_y(m-1,n+1) \right.$$}

$$+ \left( 1 - \frac{n^2(m,n,l)}{n^2(m,n-1,l)} \right) H_y(m-1,n-1) \right],$$  \hspace{1cm} (2.16)

$$A_{yx}H_x = \frac{1}{4\Delta x \Delta y} \left[ \left( 1 - \frac{n^2(m,n,l)}{n^2(m,n+1,l)} \right) H_x(m+1,n+1) \right.$$}

$$- \left( 1 - \frac{n^2(m,n,l)}{n^2(m-1,n,l)} \right) H_x(m-1,n+1) \right.$$}

$$- \left( 1 - \frac{n^2(m,n,l)}{n^2(m+1,n,l)} \right) H_x(m-1,n-1) \right.$$}

$$+ \left( 1 - \frac{n^2(m,n,l)}{n^2(m-1,n,l)} \right) H_x(m-1,n-1) \right],$$  \hspace{1cm} (2.17)

$$A_{yy}H_y = \frac{H_y(m,n+1) - 2H_y(m,n) + H_y(m,n-1)}{(\Delta y)^2}$$

$$- \frac{T^H_{m+1,n}H_y(m,n) + T^H_{m-1,n}H_y(m-1,n)}{(\Delta x)^2}$$

$$+ \frac{T^H_{m+1,n}H_y(m+1,n)}{(\Delta x)^2} - n^2(m,n,l)k_0^2 H_y(m,n),$$  \hspace{1cm} (2.18)

where

$$T^H_{m\pm 1,n} = \frac{2\epsilon(m,n,l)}{\epsilon(m\pm 1,n,l) + \epsilon(m,n,l)},$$

$$T^H_{m,n\pm 1} = \frac{2\epsilon(m,n,l)}{\epsilon(m,n\pm 1,l) + \epsilon(m,n,l)}.$$

The numerical error for the finite difference method is $O((\Delta x)^2 + (\Delta y)^2)$ [30].
3 Implementation of Lanczos/Arnoldi method and the Padé approximation method

According to the Lanczos/Arnoldi method, for a given real symmetric matrix (or a general matrix) $X$ and a given unit vector $q_1$, the Lanczos/Arnoldi method will generate an orthogonal matrix $Q$ and a symmetric tridiagonal matrix (or an upper Hessenberg matrix) $T$, such that

$$XQ = QT,$$

(3.1)

where the first column of $Q$ is $q_1$. The Lanczos/Arnoldi method is useful for large sparse matrix $X$. In this case, for $m$ much smaller than the size of the matrix $n$, one could use the first $m$ columns of $Q$ and the leading $m \times m$ block of $T$ to get two applications. One is to approximate the eigenvalues of $X$. Another is to approximate $f(X)q_1$.

When one apply the Lanczos/Arnoldi method to calculate the eigenvalues and eigenvectors of a large real symmetric matrix $X$ (of size $m \times m$, $m$ is very large), one can use the Lanczos/Arnoldi method to find a few largest and smallest eigenvalues and eigenvectors of matrix $X$. One could start with an initial vector $b$, and let $q_1 = \frac{b}{\|b\|_2}$. Then, we calculate the coefficients of tri-diagonal matrix $T$. One may terminate at some steps $n$ and calculate the eigenvalues of $T_n$. Then, the extreme eigenvalues of $T_n$ are the approximation eigenvalues of the original matrix $X$.

After the eigenvalues $T_n$ is obtained, we can further approximate $f(X)b$. This process starts with implementing the Lanczos/Arnoldi method with $q_1 = \frac{b}{\|b\|_2}$. Then, we truncate at some $n$ steps. From the approximation relationship $XQ_n \approx Q_n T_n$, one has $f(X)Q_n \approx Q_n f(T_n)$. As a result, we have $f(X)q_1 \approx Q_n f(T_n)e_1$. The final expression is given as follows

$$f(X)b \approx \|b\|_2 Q_n f(T_n)e_1,$$

(3.2)

where $e_1 = [1,0,\cdots,0]^T$ is the first column of the $n \times n$ identity matrix.

In this work, in order to approximate the square-root operator $\sqrt{A}$, we could adopt the Lanczos/Arnoldi method to get the approximate eigenvalues and eigenvectors of the propagation matrix $A$ based on a starting vector $u_0$. Here, $u_0$ denotes the starting field $u$ at $z = z_0$ discretized along the transverse direction. Then, according to the aforementioned second application of the Lanczos/Arnoldi method, we could get the result $f(A)u_0 \approx \|u_0\|_2 Q_n f(T_n)e_1$. After this process, we could obtain the solutions of the square-root operator $\sqrt{A}$.

The algorithm could be outlined as follows. First, we get the approximation of the operator $\sqrt{A}$ by the Lanczos/Arnoldi method in Section 3. Next, the exponential of the square-root operator $P(X) = e^{i\Delta z \sqrt{A}}$ could be further approximated by its Padé rational approximation. In this work, we propose the $[(p-1)/p]$ Padé approximation of $P(X)$ [21].
In this work, we propose a \( \left( \frac{p-1}{p} \right) \) Padé approximation of \( P(x) \) to speed up the convergence, that is

\[
R(X) = \sum_{i=1}^{p} \frac{a_i}{1 + b_i X} \approx P(X), \quad (3.3)
\]

where \( a_i \) and \( b_i \) are new coefficients that depend on \( k_0 n, \Delta z \) and \( p \), and are related to (2.8). Then, we have

\[
v_j = P(X)v_{j-1} \approx \sum_{i=1}^{p} \frac{a_i}{1 + b_i X} v_{j-1}, \quad j = 1, 2, 3, \ldots. \quad (3.4)
\]

In Fig. 1, we obtain the comparisons of \(|P(x)|\) with \(|R(x)|\) for \( s = 5 \). We could see that \( R(x) \) approaches to 0 as \( x \to -\infty \), which ensures that the evanescent modes which are highly oscillatory in the transverse variable \( x \), are efficiently damped [23]. The error for the \( \left( \frac{p-1}{p} \right) \) Padé approximation can be expressed as

\[
\frac{|R(X) - P(X)|}{|P(X)|} = \left| \sum_{i=1}^{p} \frac{a_i}{1 + b_i X} - e^{i\Delta z \sqrt{1 + x}} \right| / \left| e^{i\Delta z \sqrt{1 + x}} \right|.
\]

In this work, \( u_1^{(m)} \) is used to denote the \( m \)-th Lanczos/Arnoldi iteration solution for (2.8), and \( v_1^{(m)} \) is used to denote the \( m \)-th iteration step Lanczos/Arnoldi solution for (3.4). The error from the Lanczos/Arnoldi method is [24]

\[
Er(m) = h_{m+1,m} \left| e_m^T \phi_2(H_m) \beta e_1 \right| \| H_m \|_F. \quad (3.5)
\]
Here, $h_{m+1,m}$ is the coefficients of the $m \times m$ upper Hessenberg matrix, $H_m$ represents the projection of the linear transformation, $\beta$ is a coefficient as $\beta = \|v\|_2$ and $\phi_2(H_m)$ is a function, all of which are defined and described in detail in [24], $\|H_m\|_F$ represents the scaled Frobenius norm.

To denote the relative errors, we use

$$ E_m(u_1) = \frac{\|u_1^{(m)} - u_1\|}{\|u_1\|}, \quad E_m(v_1) = \frac{\|v_1^{(m)} - v_1\|}{\|v_1\|}. \tag{3.6} $$

Here, $u_1$ and $v_1$ correspond to the values after one iteration with an initial value $u_0$, respectively.

## 4 Numerical examples

### 4.1 Two dimensional symmetric and unsymmetric waveguides

For the two dimensional (2-D) numerical example, we consider the general symmetric and unsymmetric optical waveguide structures. The considered structures of waveguide are shown in Fig. 2. We adopt a gaussian beam $u_0(x) = u(x,z_0) = e^{-x^2/2}$ as the wave impinging into the optical waveguide.

For the unsymmetric and symmetric waveguide structures as shown in Fig. 2, we get the relative errors after one iteration with the variation of the discretization step $\Delta x$ along the $x$-direction, respectively. From Figs. 3-4 we could see that for a fixed $\Delta z$ and $\Delta x$, the decay rate of $E_m(v_1)$ is much faster than that of $E_m(u_1)$ as the iteration step $m$ going large. Therefore, it is efficient to use $R(x)$ in the Lanczos/Arnoldi method. Moreover, from the

![Figure 2: For the unsymmetric waveguide structure, the permeability parameters of the optical waveguide structure are $\varepsilon_1 = 1.0$, $\varepsilon_2 = 3.34$, $\varepsilon_3 = 3.44$. The widths of the waveguide structure are $h_1 = 3\mu m$, $h_2 = 1\mu m$, $h_3 = 5\mu m$. For the symmetric waveguide, the permeability parameters of the optical waveguide structure are $\varepsilon_1 = \varepsilon_3 = 3.17$, $\varepsilon_2 = 3.24$. The widths of the waveguide structure are $h_2 = 1\mu m$, $h_1 = h_3 = 4\mu m.
Figure 3: For the unsymmetric waveguide, the relative errors $E_m(u_1)$ ("blue □") and $E_m(v_1)$ ("red .") as the Arnoldi iteration step $m$ increases from 1 to 20, with $\Delta x = 0.1$ and 0.05 for the left and right sub-figures, respectively.

Figure 4: For the unsymmetric waveguide, the corresponding relative errors $E_m(u_1)$ ("blue □") and $E_m(v_1)$ ("red .") as the Arnoldi iteration steps $m$ increasing from 1 to 150. The finite difference discretization step is $\Delta x = 0.0125$.

right subfigures of Figs. 3-4, as $\Delta x$ decreases, more Arnoldi iteration steps (i.e. larger $m$) are needed to reach a desired accuracy for both $u_1$ and $v_1$.

To demonstrate the efficiency of the convergence rate and the relative error, we compare the results between (2.8) that uses the typical Lanczos/Arnoldi method and (3.4) that uses the Lanczos/Arnoldi method with the $[1/2]$ Padé rational approximation. We consider the unsymmetric waveguide. In order to let $E_m(v_1)$ achieve the accuracy of $10^{-5}$, the corresponding iteration number of the Arnoldi steps $m$ with the variations of the discretization step in the finite difference method is shown in Table 1. Here, the $[1/2]$ Padé approximation is adopted with $\Delta z = 0.25$, $\lambda = 1.55$, and $\epsilon_s = 3.3885$. Similarly, for the symmetric waveguide, the required relative error of $E_m(v_1)$ and the corresponding iteration number of Arnoldi steps are given in Table 2. In order to let $E_m(v_1)$ achieve
Table 1: For the unsymmetric waveguide, in order to make $E_m(v_1)$ achieve $10^{-5}$ error accuracy, the corresponding iteration number of Arnoldi steps $m$ is required. Here, the parameter $\Delta x$ corresponds to the finite difference discretization step.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$m$</th>
<th>$E_m(v_1)$</th>
<th>$E_m(u_1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>16</td>
<td>9.2875e-005</td>
<td>0.0690</td>
</tr>
<tr>
<td>0.075</td>
<td>21</td>
<td>9.0622e-005</td>
<td>0.0916</td>
</tr>
<tr>
<td>0.05</td>
<td>31</td>
<td>8.4067e-005</td>
<td>0.0822</td>
</tr>
<tr>
<td>0.03</td>
<td>51</td>
<td>8.6606e-005</td>
<td>0.0758</td>
</tr>
<tr>
<td>0.025</td>
<td>60</td>
<td>9.4542e-005</td>
<td>0.0811</td>
</tr>
<tr>
<td>0.0125</td>
<td>119</td>
<td>9.4103e-005</td>
<td>0.0790</td>
</tr>
</tbody>
</table>

Table 2: For symmetric waveguide, in order to make $E_m(v_1)$ achieve $10^{-5}$ error accuracy, the corresponding iteration number of Arnoldi steps $m$ is required. Here, the parameter $\Delta x$ corresponds to the finite difference discretization step.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$m$</th>
<th>$E_m(v_1)$</th>
<th>$E_m(u_1)$</th>
</tr>
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<td>6.8928e-005</td>
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<td>74</td>
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$10^{-5}$ accuracy, we show the corresponding iteration number of Arnoldi steps $m$ in Table 2, where $\Delta z = 0.25$, $\lambda = 1.55\mu m = 3.3885$, with a $[1/2]$ Padé approximation.

From Figs. 3-6 and Tables 1-2, we conclude that $E_m(v_1)$ converges much faster than $E_m(u_1)$. Furthermore, $E_m(v_1)$ has a higher accuracy than $E_m(u_1)$ when the iteration number of Arnoldi steps remains as the same. Hence, the $[1/2]$ Padé approximation of the exponential function in (2.8) could increase both the convergence rate and computational accuracy of the wave propagation along the optical waveguides.

### 4.2 The three dimensional optical waveguide structures

The efficient simulations of the wave propagation along three dimensional optical waveguides are important. To demonstrate the efficiency of the proposed method, we consider the wave propagation of the wave fields in the rib and taper waveguide structures. The computational domain of the rib waveguide is given by $|x| < 4 \mu m$ and $|y| < 4 \mu m$ in Fig. 7. Our calculations are carried out in the free space with the wavelength $\lambda = 1.55 \mu m$. At $z = 0$, we use the gaussian beam $u_0(x,y) = u(x,y,0) = e^{-\frac{x^2+y^2}{2\lambda^2}}$ (for $z \leq 0$) as the incident electromagnetic wave field, which is discrete with the grid sizes $\Delta x = \Delta y = 0.05 \mu m$. A second order finite difference scheme is adopted to approximate the operator $A$ in (2.6). To
Figure 5: For the symmetric waveguide, the relative errors $E_m(u_1)$ ("blue □") and $E_m(v_1)$ ("red .") to the Arnoldi iteration step $m$ increasing from 1 to 20, with the finite difference discretization step $\Delta x = 0.1$.

Figure 6: For the symmetric waveguide, the corresponding relative errors $E_m(u_1)$ ("blue □") and $E_m(v_1)$ ("red .") to the Arnoldi iteration steps $m$ increasing from 1 to 150, with the finite difference discretization step $\Delta x = 0.0125$.

Figure 7: The three dimensional rib waveguide, $h_1 = h_2 = 1.1 \mu m$, for the second example with the linear taper waveguide, $h_1 = 1.1 \mu m$, $h_2 = 0.5 \mu m$. 
suppress the reflections from the edges of the computational domain, a perfectly matched layer (PML) [26, 28] is adopted, with the thickness of the PML as 0.25 \( \mu m \).

In the BPM process, the structure is discretized along z-direction with \( \Delta z = 0.1 \mu m \). Hence, a total of 400 steps are required to propagate along z-direction from \( z = 0 \) to \( z = L \). We calculate the electromagnetic wave field at \( z = 40 \mu m \) based on (3.4) by using the Padé [1/2] approximation and the Arnoldi iteration method. Here, the Arnoldi steps \( m = 30 \) are adopted.

Next, we consider the three dimensional linear taper optical waveguide structures [27], which is shown in Fig. 7. For \( z < 0 \), the structure is a straight rib waveguide. From \( z = 0 \) to \( z = 40 \mu m \), the height of the rib linearly decreases from 1.1 \( \mu m \) to 0.5 \( \mu m \). For \( z \geq 40 \mu m \), the structure is a straight rib waveguide with the constant height of 0.5 \( \mu m \). At \( z = 0 \), we use the fundamental mode of the straight waveguide (for \( z \leq 0 \)) as the starting field. The x-y plane is discretized with the grid sizes \( \Delta x = \Delta y = 0.05 \mu m \), and the propagate direction of \( z \) is discretized with \( \Delta z = 0.1 \mu m \). The mode is scaled such that the maximum of \( H_y \) is 1 by using the same Arnoldi iteration steps \( m = 30 \).

In Figs. 8-9, the calculated results of the first rib waveguide excited by a gaussian beam are demonstrated. Figs. 11-12 are the calculation results of the three dimensional
Figure 10: The magnitude of $H_y$ from the three dimensional linear taper structure in [27] at $z = L$ (Padé $[3/4]$ approximation).

Figure 11: The magnitude of $H_y$ from the three dimensional linear taper structure using (3.6) at $z = L$ (Padé $[1/2]$ approximation). The Arnoldi iteration steps are $m = 30$.

liner taper structures excited by its fundamental mode of the optical waveguide which has been analyzed in [27], Fig. 11 is the magnitude of $H_y$ at $z = L$ for the taper based on the BPM method with the fast solver proposed in this work, and the generated results agree well with the results in [27], which is shown in Fig. 10. Figs. 14-15 are the calculated results for the third rib waveguide excited by its fundamental mode of the optical waveguide, which has been analyzed in [28]. Fig. 14 depicts the transverse magnetic field component $H_x$ of the fundamental mode of the rib waveguide structure. Fig. 15 is the transverse magnetic field component $H_y$ of the fundamental mode of the rib waveguide. Again, the simulation results of the two components of transverse field agree well with the results in [28]. On invoking the full vectorial beam propagation method, these results imply that the proposed Lanczos/Arnoldi method with the Padé $[1/2]$ approximation is efficient in the simulation of the three-dimensional optical waveguides.

The third example is a rib waveguide that was studied in [28, 29, 31, 32]. We consider the rib waveguide structure [28]. The sketch with its refractive-index distribution of this
Figure 12: The magnitude of $H_x$ from the three dimensional linear taper structure using (3.6) at $z = L$ (Padé $[1/2]$ approximation). The Arnoldi iteration steps are $m = 30$.

Figure 13: A rib waveguide structure.

rib waveguide is shown in Fig. 13. Our calculations are carried out for the free-space wavelength $\lambda = 1.55 \mu m$. At $z = 0$, we use the fundamental mode of the straight waveguide as the starting incident field. The computational domain is given by $|x| < 2 \mu m$ and $-1 \mu m < y < 2 \mu m$. The transverse structure of the rib waveguide is discretized with the grid sizes $\Delta x = \Delta y = 0.013 \mu m$ along the $x$- and $y$-directions, respectively. A second-order finite-difference scheme is used to approximate the operator $A$. To suppress the reflections from the edges of the computational domain, a perfectly matched layer is adopted in [26, 33], with the thickness of the perfectly matched layer as 0.25 $\mu m$. On the basis of the reference refractive index $\varepsilon_s = 3.388687$, we first use the Lanczos/Arnoldi method to get the approximate solution of the square-root operator $\sqrt{A}$. As is shown in Figs. 14-15, the transverse magnetic field components are efficiently calculated among this rib waveguide. Moreover, the generated results agree well with those in [28].
5 Conclusions

In this work, we propose the full vectorial BPMs for analyzing the electromagnetic wave propagation from the two and three dimensional optical waveguide structures. The rational Padé approximation (a \([(p-1)/p]\) approximation) is adopted to approximate the exponential operator in the BPM process. In the transverse directions of the optical waveguide structures, the second order finite difference method is adopted. Then, the Lanczos/Arnoldi method is used to speed up the BPM process. Numerical results demonstrate the mode distributions from the two dimensional symmetrical and unsymmetrical optical waveguides. Furthermore, we consider the wave propagation among the three di-
mensional rib and taper waveguides, and a rib waveguide structure with large refractive index step. The efficiencies of the proposed method with respect to both wave propagation accuracy and convergence results are demonstrated for both two dimensional and three dimensional optical waveguide structures.

Acknowledgments

This work was supported in part by National Key R&D Program of China under Grant No. 2017YFB0502703, in part by the Science Challenge Program under Grant No. JCKY2016212A502, in part by National Natural Science Foundation of China under Grant No. 11571196, No. 11671099 and No. 61971144, in part by the Foundation of Science and Technology on Electromagnetic Scattering Laboratory under Grant No. 621802Y010101, in part by Open Research Fund of State Key Laboratory of Pulsed Power Laser Technology under Grant SKL2018KF08.

References