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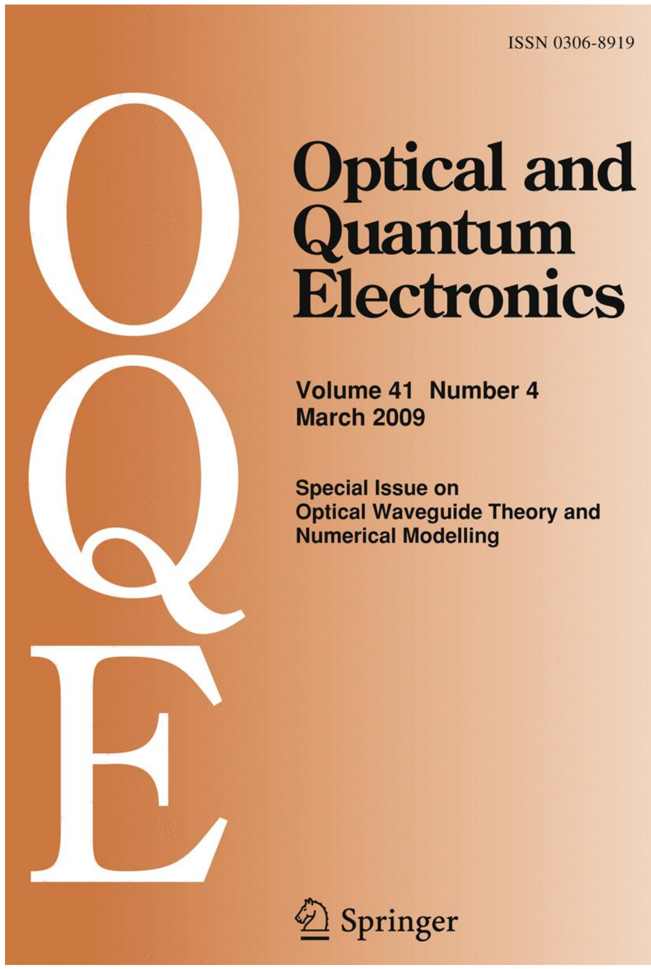

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# A stable complex Jacobi iterative solution of 3D semivectorial wide-angle beam propagation using the iterated Crank–Nicholson method

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**Abstract** An extension of the recently proposed three-dimensional (3D) wide-angle (WA) beam propagation method (BPM) using complex Jacobi iteration (CJI) taken into account polarization effects is presented. The resulting iterative BPM is faster than BPMs based on the traditional direct matrix inversion for waveguides with unchanging refractive index profiles during propagation direction. However, for varying refractive index waveguides the iterative method suffered from the fact that the iteration count between two successive cross-sections increases dramatically during the propagation direction. To overcome this problem, we propose the utility of the iterated Crank–Nicholson method. At each propagation step, the propagation equation is divided in multiple stages by the iterated Crank–Nicholson method and then each stage is recast in terms of a Helmholtz equation with source term, which is solved effectively by the complex Jacobi iterative method. The resulting approach is stable and well-suited for large structures with long propagation paths.

**Keywords** 3D semivectorial BPM · Complex Jacobi iteration · Iterated Crank–Nicholson

## 1 Introduction

Efforts to improve the limitations of the paraxial approximation in the beam propagation method have so far made use of wide-angle formulations. Different treatments of WA-BPM based on the slowly varying envelope approximation (SVEA) have been developed. In these approaches the field is assumed to be separated into two parts including the complex field amplitude and a propagation factor. There exist real Padé approximant operators (Hadley 1992) and complex Padé approximant operators (Le 2009). In addition, treatments of WA-BPM without having to make the SVEAs have also been reported, including the series expansion technique of the propagator (Lee and Voges 1994), the split-step of beam propaga-

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tion equation (Sharma and Agrawal 2004), and the recently proposed rational KP approximant operators (Le and Bienstman 2009).

The real Padé-approximant-based WA-BPMs have become one of the most commonly used techniques for modeling of optical waveguide structures. However, it was shown that the real Padé approximant propagators incorrectly propagate the evanescent modes. These modes can cause serious instability problems when implementing WA-BPMs based on real propagators. To circumvent this problem, we recently proposed modified Padé approximant operators, which give evanescent waves the desired damping and allow more accurate approximation to the Helmholtz equation than the conventional operators (Le 2009).

In those WA-BPMs, the beam propagation equation can be described in a tridiagonal matrix form, which is usually solved by the well-known direct matrix inversion (DMI). However, these equations need to be solved efficiently since numerous propagation steps are routinely required during the course of a problem solution. For this purpose the recently introduced complex Jacobi iterative (CJI) method (Hadley 2005) was proposed for the solution of WA beam propagation and shown to be highly efficient. At each propagation step, the beam propagation equation is recast in terms of Helmholtz equation with source term, which is solved quickly and accurately by the CJI method (Le et al. 2008).

However, this method is based on scalar propagation, in which the field and its spatial derivatives are assumed to be continuous across dielectric interfaces. This approximation does not hold for modeling optical propagation in waveguides on semiconductor substrates which frequently involve abrupt index changes. For these cases a full vectorial analysis is needed (Bhattacharya and Sharma 2009). Unfortunately, full vectorial schemes require large computational efforts. For most of optical devices where the polarization coupling is weak and may be neglected, the semivectorial BPM is very convenient for analyzing polarization effects (Mitomi and Kasaya 1998).

In this paper, an extension of our recently proposed WA-BPM using complex Jacobi iteration (Le et al. 2008) taken into account polarization effects is presented. Also, the investigation of the convergence rate of the CJI method and its execution speed in comparison with the DMI method is reported. The resulting semivectorial iterative approach still has fast convergence even though the effect of refractive index changes in the transverse direction of waveguides is included. The method is very competitive in comparison with the traditional DMI method.

However, for waveguides with refractive index profiles varying both in the transverse direction and along the propagation direction, the CJI method suffers from the fact that the iteration count between two successive cross-sections increases dramatically during the propagation direction. To circumvent this problem, we propose the utility of the iterated Crank–Nicholson (ICN) method (Teukolsky 2000; Leiler and Rezzolla 2006), in which at each propagation step, rather than solving the propagation equation directly, it is divided in multiple stages by the ICN method and then each stage is recast as an inhomogeneous Helmholtz equation and solved by the CJI method. The resulting approach is stable and well-suited for high-index-contrast waveguides with very long propagation paths.

## 2 Formulation

We begin by considering the semivectorial Helmholtz equation for the electric field component (Bhattacharya and Sharma 2009)

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial n^2}{\partial x}\Psi\right) + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + k_0^2 n^2(x, y, z)\Psi = 0 \tag{1}$$

where $n$ is the refractive index profile and $k_0$ is the vacuum wavevector. At any interface perpendicular to the $x$-direction, the refractive index and the electric field component is discontinuous; thus if the polarization is ignored in high-index-contrast waveguides (the second term in Eq. 1 is ignored), numerical evaluation of their derivatives would lead to large errors. However, it will be overcome if we investigate the first two terms in Eq. (1) together (Bhattacharya and Sharma 2009).

Using the SVEA, in which the wave function $\Psi(x, y, z)$ propagating in the $z$ direction can be separated into a slowly varying envelope function $\Phi(x, y, z)$ and a very fast oscillating phase term $\exp(-ikz)$, the Helmholtz equation is given by:

$$\frac{\partial \Phi}{\partial z} - \frac{i}{2k}\frac{\partial^2 \Phi}{\partial z^2} = \frac{iP}{2k}\Phi, \tag{2}$$

where $P = \nabla_\perp^2 + k_0^2(n^2 - n_{ref}^2) = \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial n^2}{\partial x}\right) + \frac{\partial^2}{\partial y^2} + k_0^2(n^2 - n_{ref}^2)$ with $k = k_0 n_{ref}$, $n_{ref}$ the reference refractive index. The finite difference discretization of the term $\frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial n^2}{\partial x}\Phi\right)$ is given as follows: (Kawano and Kitoh 2001)

$$\begin{aligned}\frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial n^2}{\partial x}\Phi\right) = \frac{1}{\Delta x^2}\Bigg[&\frac{n^2(i+1,j) - n^2(i,j)}{n^2(i+1,j) + n^2(i,j)}(\Phi_{i+1,j} + \Phi_{i,j}) \\ &- \frac{n^2(i,j) - n^2(i-1,j)}{n^2(i,j) + n^2(i-1,j)}(\Phi_{i,j} + \Phi_{i-1,j})\Bigg].\end{aligned} \tag{3}$$

From Eq. 2, different treatments of WA-BPM can be developed. In this work, the modified Padé(1,1) approximant operator for a wide-angle propagator is used and leads to the beam propagation equation as follows (Le et al. 2008):

$$(1 + \xi P)\Phi^{n+1} = (1 + \xi^* P)\Phi^n, \tag{4}$$

where $\xi = \frac{1}{4k^2(1+1i)} - \frac{i\Delta z}{4k}$, $\xi^* = \frac{1}{4k^2(1+1i)} + \frac{i\Delta z}{4k}$ and $\Delta z$ the propagation step size.

The adaptation of the CJI method for the solution of Eq. (4) is given as follows:

By dividing both sides of this equation by $\xi$, it may be written as an inhomogeneous Helmholtz equation

$$\left[\nabla_\perp^2 + k_0^2(n^2 - n_m^2) + \frac{1}{\xi}\right]\Phi^{n+1} = \left(\frac{\xi^*}{\xi}P + \frac{1}{\xi}\right)\Phi^n, \tag{5}$$

or

$$\left[\nabla_\perp^2 + k_0^2(n^2 - n_{ref}^2) + \frac{1}{\xi}\right]\Phi^{n+1} = source\ term, \tag{6}$$

It is clearly seen that the beam propagation equation is recast as a Helmholtz equation with source term in an effective medium with loss determined by the imaginary part of $\frac{1}{\xi}$. Thus, it is easy to solve this equation effectively by the CJI method. Its convergence rate is mostly dominated by the amount of effective absorption (or medium loss). If the loss is high, rapid convergence is obtained.

However, for waveguides with refractive index profiles varying through the propagation direction the iteration count between two successive cross-sections increases dramatically. This problem can be remedied, however, by considering multistage solving Eq. (4) by the iterated Crank–Nicholson method. In (Teukolsky 2000) the author proved that for dealing with the so-called advective equation when using the ICN method, one should use two stages. In this work, it is numerically shown in the next section that the complex Jacobi iterative solution of Eq. (4) using the ICN method is stable and results in significant advantages in view of an execution speed of the CJI method for semivectorial beam propagation of very long path length. The implementation of the ICN method is described as follows:

Rather than solving Eq. (4) directly by the CJI method, it is divided in multiple stages as follows:

First, we calculate the initial estimated field ${}^{(1)}\Phi^{n+1}$ at the next propagation cross-section $(n+1)$ using Eq. (4):

$$(1+\xi P)^{(1)}\Phi^{n+1} = (1+\xi^* P)\Phi^n. \tag{7}$$

Equation (7) is solved by the iterative procedure described above. Then the field at the mid-step cross-section $(n+1/2)$ is made by weighting equally the newly predicted solution ${}^{(1)}\Phi^{n+1}$ and the previous solution $\Phi^n$. This can be seen as the special case of a more generic averaging of the type

$${}^{(1)}\Phi^{n+\frac{1}{2}} = \theta^{(1)}\Phi^{n+1} + (1-\theta)\Phi^n, \tag{8}$$

where $\theta$ is the ICN weight coefficient, here set to 0.1.

Similarly, the final estimated field $\Phi^{n+1}$ at the next propagation cross-section $(n+1)$ is recalculated by

$$(1+\xi P)\Phi^{n+1} = (1+\xi^* P)^{(1)}\Phi^{n+\frac{1}{2}}. \tag{9}$$

This happens again in an iterative way.

## 3 Benchmark results

That polarization effects on high-index-contrast waveguides play an important role on an accuracy of BPM was already shown in (Bhattacharya and Sharma 2009). In this paper, we will investigate how polarization effects affect the convergence rate of the CJI method and its execution speed in comparison with the DMI method. We consider Gaussian beam propagation in the 3D rib waveguide (Lee and Voges 1994). The iteration count of the CJI method with respect to propagation steps through the propagation direction is shown in Fig. 1. From the figure, it is shown that due to polarization effects through discontinuous interfaces in the waveguide the CJI method requires larger iterations to perform propagation than the method where these effects are ignored. However, the CJI for the semivectorial BPM is still faster than the DMI method. With a relatively large propagation step size $\Delta z = 0.1\,\mu$m in a small $4\,\mu\text{m} \times 4\,\mu\text{m}$ computational window, the resulting runtime of CJI for WA-BPM is only 3.1 s whereas the DMI requires 61.4 s to perform propagation.

It is clearly seen that the runtime 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, for typical choices of $k\Delta z$ the CJI technique offers rapid convergence and shorter runtimes.

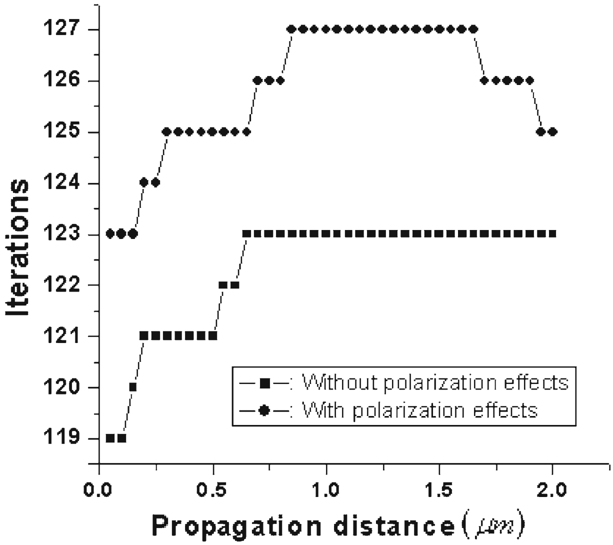


**Fig. 1** The iteration count per propagation step for a Gaussian beam propagation through a 3D rib waveguide with and without polarization effects

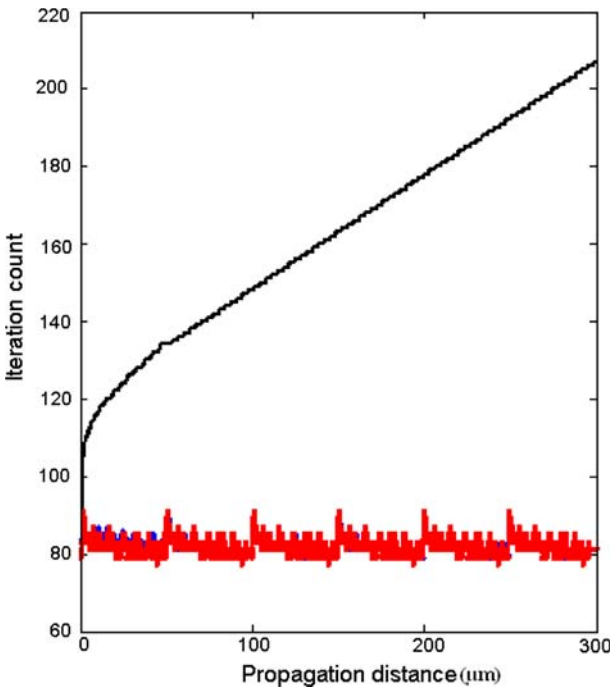


**Fig. 2** Iterations count per propagation step of the CJI method for beam propagation in a symmetric Y-branch waveguide with (blue and red lines for the iteration count of Eqs. 7 and 9 respectively) and without (*black line*) using the ICN method (color figure online)

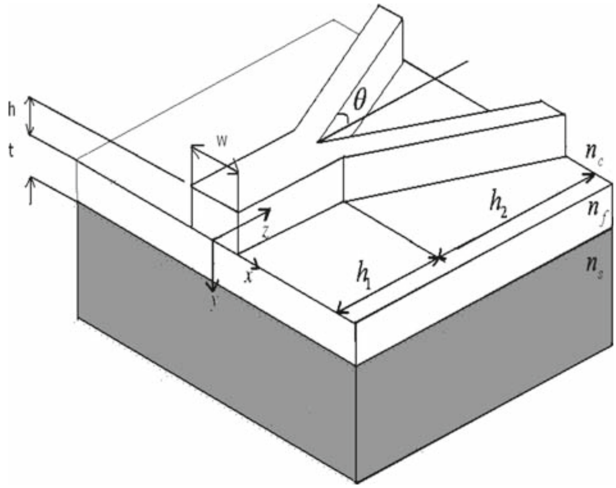


**Fig. 3** Y-branch optical rib waveguide

However, as we mentioned in previous section, besides the polarization effects affected on the convergent rate of the CJI method, varying refractive index profiles through the propagation direction leads to an increase of an iteration count between two successive cross-sections as shown in Fig. 2. In the figure, the iteration count of the CJI method for semivectorial WA-BPM with and without using the ICN method between two successive cross-sections in a Y-junction waveguide are calculated. The initial rib waveguide is split into two 5-degree tilted waveguides as shown in Fig. 3, where the longitudinal dimension is $h_1 = 1\,\mu$m, and the width and height of the straight rib waveguide are $w = 2\,\mu$m and $h = 1.1\,\mu$m. The guiding core has an index $n_f = 3.44$ and a thickness $t = 0.2\,\mu$m while the refractive index of substrate and cover is $n_s = 1.44$ and $n_c = 1$, respectively. The fundamental TE mode of the ridge waveguide of width $w = 2\,\mu$m at 1.3 $\mu$m wavelength is used as the excited field at $z = 0$. The iterations were terminated when a field-weighted residual of $10^{-7}$ was satisfied at each grid point.

For a grid size $\Delta x = \Delta y = \Delta z = 0.05\mu$m, the iteration count between two successive cross-sections required for the CJI method without using ICN increases dramatically as can be seen in Fig. 2. The same figure also shows that the iteration count of the ICN-CJI method is stable. Even though there are two ICN-CJI iterations needed per equivalent non-ICN-CJI iteration, this fact becomes quickly offset for larger propagation distances.

## 4 Conclusions

A fast semivectorial wide-angle beam propagation method based on the recently proposed modified Padé(1,1) approximant operator using the new complex Jacobi iterative method has been presented. It is obtained from an extension of the method developed earlier for scalar propagation to solve the semivectorial equation where polarization effects were taken into account. However, the semivectorial iterative method is itself unstable for propagation in high-index-contrast waveguides with refractive index profiles varying during the propagation direction. In order to overcome this problem, we have proposed the utility of the iterated Crank–Nicholson method. The resulting semivectorial method was stable and very well-suited for large structures with long path length. Through a quantitative comparison of runtimes between the traditional direct matrix inversion and the recently proposed complex Jacobi method for wide-angle beam propagation, it is demonstrated that the complex Jacobi method is very competitive for demanding problems.

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