

# **A three-dimensional non-paraxial beam propagation method using complex Jacobi iteration**

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*A new complex Jacobi iterative technique adapted for the solution of three-dimensional (3D) non-paraxial beam propagation is presented. The beam propagation equation for analysis of optical propagation in waveguide structures is based on a novel modified Padé(1,1) approximant operator we recently proposed. The effectiveness of our new approach is demonstrated in comparison with the traditional direct matrix inversion. Our method is targeted towards large waveguide structures with a long path length.*

## **Introduction**

The Padé-approximant-based non-paraxial or wide-angle (WA) beam propagation method (BPM) has become one of the most commonly used techniques for modeling optical waveguide structures [1]. However, the method was originally limited to 2D structures due to the lack of efficient solvers. Recently, C. Ma *et al.* [2] presented a new 3D WA-BPM also based on Hoekstra's scheme. By using a technique for shifting the simulation window to reduce the dimension of the numerical equation and a threshold technique to further ensure its convergence, this approach shows accuracy and effectiveness. However, the resultant propagation scheme can be very slow if either the problem size is large or the structure or the boundary conditions are changing as the propagation proceeds, requiring frequent reinversions of the propagation matrix. Thus, it is imperative to find more efficient solution methods for 3D WA-BPM.

Recently, the complex Jacobi iterative method, a new iterative technique for solution of the indefinite Helmholtz equation, was introduced [3]. For beam propagation of wave profiles within a 2D cross section, the beam propagation equation can be cast in terms of a Helmholtz equation with source term, but that equation needs to be solved efficiently since numerous propagation steps are routinely required during the course of a problem solution. For this purpose the complex Jacobi iterative (CJI) method is proposed and shown to be highly efficient.

The beam propagation equation for analysis of optical propagation in waveguide structures is based on a modified Padé(1,1) approximant operator we recently proposed [4]. Our modified Padé approximant propagation operators allow more accurate approximation to the true Helmholtz equation. Furthermore, since the utility of the CJI technique depends mostly upon its execution speed in comparison with the direct matrix inversion (DMI) method, we also present several speed comparisons. Numerical implementations are carried out for 3D optical waveguide structures.

## **Modified Padé approximation operators**

Recently we proposed the WA-BPM algorithm based on the Padé approximation using the following recurrence relation with initial value of  $\left. \frac{\partial}{\partial z} \right|_0 = -k\beta$  ( $\beta$  is a damping parameter) [4]:

$$\left. \frac{\partial}{\partial z} \right|_{n+1} = i \frac{\frac{P}{2k}}{1 - \frac{i}{2k} \left. \frac{\partial}{\partial z} \right|_n} \quad (1)$$

where  $P = \nabla_{\perp}^2 + k_0^2(n^2 - n_{ref}^2) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + k_0^2(n^2 - n_{ref}^2)$  with  $k = k_0 n_{ref}$ ,  $n_{ref}$  the reference refractive index,  $k_0$  the vacuum wavevector. For  $\left. \frac{\partial}{\partial z} \right|_2$ , this gives us the modified Padé(1,1) approximant-based WA beam propagation formula as follows:

$$\frac{\partial H}{\partial z} \approx i \frac{\frac{P}{2k}}{1 + \frac{P}{4k^2(1 + \frac{i\beta}{2})}} H. \quad (2)$$

## WA-beam propagation formulation

### Basic equation

By using the modified Padé(1,1) approximant, the 3D semivectorial WA beam propagation equation can be written as follows:

$$(1 + \xi P)\phi^{n+1} = (1 + \xi^* P)\phi^n \quad (3)$$

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

### WA-BPM using CJI

By dividing both sides of Eq.(3) by  $\xi$ , it may be written as an inhomogeneous Helmholtz equation

$$\left( \nabla_{\perp}^2 + k_0^2(n^2 - n_{ref}^2) + \frac{1}{\xi} \right) \phi^{n+1} = \left( \frac{\xi^*}{\xi} P + \frac{1}{\xi} \right) \phi^n \quad (4)$$

or

$$\left( \nabla_{\perp}^2 + k_0^2(n^2 - n_{ref}^2) + \frac{1}{\xi} \right) \phi^{n+1} = \left( \frac{\xi^*}{\xi} P + \frac{1}{\xi} \right) \phi^n \quad (5)$$

$$4k_0^2 n_{ref}^2 \frac{1 + (1 + k^2 \beta \Delta z / 2) \beta / 2 + ik \Delta z}{(1 + k^2 \beta \Delta z / 2)^2 + k^2 \Delta z^2} \phi^{n+1} = source\ term$$

Thus the beam propagation can be cast as a 2D Helmholtz equation with source term in

$$4k_0^2 n_{ref}^2 \frac{k\Delta z}{\left(1 + k_0^2 n_{ref}^2 \beta \Delta z / 2\right)^2 + k^2 \Delta z^2}$$

an effective medium with loss of  $k\Delta z$ . This loss is high for a typical choice of  $k\Delta z$ . This is a condition that favors rapid convergence for the CJI method.

### WA-BPM using DMI

By discretizing Eq. (4), we find that

$$\begin{aligned} A_{n+1}\phi_{i+1,j}^{n+1} + B_{n+1}\phi_{i-1,j}^{n+1} + C_{n+1}\phi_{i,j}^{n+1} + D_{n+1}\phi_{i,j-1}^{n+1} + E_{n+1}\phi_{i,j+1}^{n+1} \\ = A_n\phi_{i+1,j}^n + B_n\phi_{i-1,j}^n + C_n\phi_{i,j}^n + D_n\phi_{i,j-1}^n + E_n\phi_{i,j+1}^n \end{aligned} \quad (6)$$

where

$$\begin{aligned} A_{n+1} = B_{n+1} &= \frac{1}{\Delta x^2}, & D_{n+1} = E_{n+1} &= \frac{1}{\Delta y^2}, \\ C_{n+1} &= k_o^2(n^2 - n_{ref}^2) + \frac{1}{\xi} - 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right), \\ A_n = B_n &= \frac{\xi^*}{\xi} \frac{1}{\Delta x^2}, & D_n = E_n &= \frac{\xi^*}{\xi} \frac{1}{\Delta y^2}, \\ C_n &= \frac{\xi^*}{\xi} \left( k_o^2(n^2 - n_{ref}^2) + \frac{1}{\xi^*} - 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) \right) \end{aligned} \quad (7)$$

Eq. (6) is an  $M^2$  by  $M^2$  matrix equation for an M by M mesh grid. However, each row of the coefficient matrix has no more than five non-zero values. As a result, this sparse matrix equation can be efficiently solved using various methods. In our calculations, the sparse matrix solver-UMFPACK package has been used.

### Benchmark results

We now employ the WA-BPM using the new CJI and the traditional DMI methods to perform benchmark tests on 3D optical waveguide structures. We first consider the Gaussian beam propagation in a straight rib waveguide and guided-mode propagation in a Y-branch rib waveguide [4]. The Gaussian beam with a waist radius  $w_0 = 0.3 \mu m$  has been injected into the rib waveguide at wavelength  $\lambda = 1.55 \mu m$ . Due to the large memory required for DMI, the small computational window of  $2 \times 2 \mu m$  is discretized with a grid size of  $\Delta x = \Delta y = 0.1 \mu m$ , and the short path length of  $2 \mu m$  is discretized with a propagation step size  $\Delta z = 0.1 \mu m$ . The resulting runtime of DMI is 177.9 seconds while runtime for CJI is only 4.7 seconds.

For a Y-branch, the initial rib waveguide is split into two 5-degree tilted waveguides. The longitudinal dimension is  $h_1 = 1 \mu m$ . The fundamental mode of the ridge waveguide

of width  $w = 2 \mu\text{m}$  for polarization TE mode at  $1.55 - \mu\text{m}$  wavelength is used as the excited field at  $z=0$ . The propagation step size is  $\Delta z = 0.1 \mu\text{m}$ . Due to the high effective loss in the propagation medium the complex Jacobi method performed propagation only in 5.9 seconds while DMI required an amount of 268.9 seconds.

TABLE 1  
Quantitative comparison of runtimes of the direct matrix inversion and the complex Jacobi iteration for WA beam propagation in waveguide (WG) structures

Structure	3D	
	Straight rib WG	Y-branch rib WG
DMI	177.9 s	268.9 s
CJI	4.7 s	5.9 s

Table 1 shows the performance of the two methods for the optical waveguide structures chosen here. It is clearly seen that the runtime of the iterative method is substantially faster 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.

## Conclusion

A new complex Jacobi iterative method adapted for the solution of 3D WA beam propagation has been presented. A quantitative comparison of runtimes between the traditional direct matrix inversion and the new complex Jacobi iterative method for 3D WA beam propagation demonstrates convincingly that the complex Jacobi iterative method is very competitive for demanding problems.

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