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VECTOR MODE ANALYSIS OF OPTICAL WAVEGUIDES BY QUADRATIC SPLINE COLLOCATION METHOD

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Abstract—We present an accurate, efficient numerical analysis for vector modes of dielectric optical waveguide structures with an arbitrary refractive index profile using a quadratic spline collocation method (QSCM). The unknown weights of the polynomials are determined by forcing the errors at the collocation points to be zero. Consequently, the original second order differential equation is converted to a set of algebraic equations which can be solved by matrix techniques. The proposed QSCM method demonstrates better performance than the standard finite-difference method of the same convergence rate in terms of grid size with the same degree of computational complexity.

1. INTRODUCTION

Mode analysis for optical waveguides is usually the starting point for design and simulation of guided-wave photonic devices and integrated circuits. For most practical waveguide structures, analytical or even semi-analytical methods are rather limited in applicability [1]. In the past decades, researchers have proposed and developed various numerical methods; among which the finite-difference method (FDM) and the finite element method (FEM) are two of the most popular approaches [2–11]. The finite difference method (FDM) gains its popularity owing to its simplicity and effectiveness [4–11]. On the

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other hand, the finite element method (FEM) is more adaptive for complex waveguide structures with irregular interfaces [2, 3]. Some other methods which utilize global basis functions for representing the mode solutions have been reported in the literature though they are not as popular as FDM and FEM [12, 13].

As an optical mode solver, the ability to accurately simulate the vectorial properties of the optical field is critical in dealing with those strongly guided structures. This is of particular interest in silicon photonics due to the large index contrast in SOI (Silicon on Insulator) waveguides [14, 15].

Both FDM and FEM are built on localized unknown values, which naturally possess the flexibility to tackle the interfaces. With a small enough grid size, FDM and FEM will reach a certain required accuracy. On the opposite, due to their lacking of local treatment, those numerical mode solvers built on global bases or variables generally don't work for optical waveguides with high index contrast at interfaces or corners, unless the whole domain is divided into sub-domains, each of which will be approximated by its own whole-domain basis functions and interface conditions that are later imposed across adjacent sub-domains [16].

In this paper, we present a quadratic spline collocation method (QSCM), which uses a set of localized piecewise quadratic polynomials to approximate the exact mode solution. The unknown weights of the polynomials are then determined by forcing the errors at a set of points, called collocation points, to be zero. The original second order differential equation is therefore transferred to a set of algebraic equations, which can be solved by matrix techniques. Spline collocation method is considered as one of finite element methods (FEM) [17], as it utilizes finite element, namely, localized basis functions which can become infinitely small when the grid size of the computation window is decreased. However, the spline collocation method uses the weights of the basis-functions as the undetermined values and forces the approximation functions to exactly match the unknown functions at a set of points. Such approach is quite different from the traditional FEM, which chooses element nodes as the undetermined variables that can be solved by the variational principles or the Galerkin method [13].

Though the idea of collocation is not new in optics [18–22], the spline collocation based on the piecewise polynomials is rarely examined. Most of the available collocation approaches are based on orthogonal collocation [18–22], which use global basis functions that are nonzero throughout the whole computation domain. Such global collocation methods have difficulties in dealing with dielectric interfaces where the field or the first-order derivative is discontinuous. Improvements on global collocation method have been reported when the computation domain is divided into sub-regions according to the position of the dielectric interfaces, and each sub-region is applied with global collocation, and finally, interface and boundary conditions are forced [16]. However, the increased complexity may impede its popularization.

The paper is structured as follow. We will brief the basic idea and the formulation of QSCM for boundary value problems, and will implement QSCM in the uniform region and dielectric interfaces in Section 2. In Section 3, various waveguide structures are evaluated with QSCM followed by comparison with the standard FDM result. We finally summarize our work in Section 4.

2. STRUCTURE AND WORKING PRINCIPLE

For a general two-point second-order boundary value problem, the computation domain $(a,\, b)$ is divided into M uniform intervals with a grid size h, the middle points of which τ_i $(i = 1, 2, \ldots, M)$ are chosen as the collocation points. The quadratic basis functions are chosen as [17]

$$s_i(x) \equiv \frac{2}{3}\psi\left(\frac{x-a}{h} - i + 2\right) \qquad i = 0, \ldots, M+1 \tag{1}$$

where

$$\psi(x) \equiv \begin{cases} 0 & x > 3 \text{ or } x < 0 \\ x^2 & 0 \le x \le 1 \\ -3 + 6x - 2x^2 & 1 \le x \le 2 \\ 9 - 6x + x^2 & 2 \le x \le 3 \end{cases} \tag{2}$$

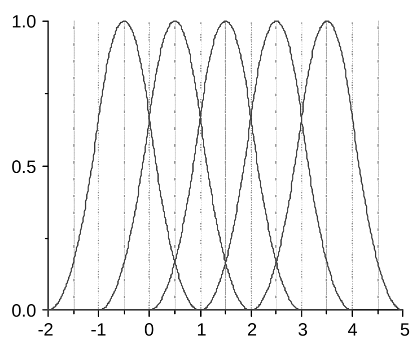

Figure 1. The quadratic spline collocation method basis functions example.

Figure 1 shows an example set of quadratic basis functions with computation domain (0, 3) and grid size 1.0. The collocation points are 0.5, 1.5, and 2.5. The boundary points are 0 and 3. Each of the piecewise quadratic basis functions have nonzero values only across three intervals as shown in Figure 1. This localization feature gives QSC flexibility for easy implementation for various boundary condition and discontinuity as discussed later.

The summation of the weighted basis functions [17]

$$\phi(x) = \sum_{i=0}^{M+1} \theta_i s_i(x) \quad i = 0, \dots, M+1, \tag{3}$$

is formed as the approximate solution with unknown weights θ_j, which are determined by substituting Eq. (3) into the second order partial differential equation and the boundary conditions. For a longitudinally invariant waveguide, the full vector governing equations in magnetic field are given by

$$n^2 \frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial H_y}{\partial x}\right) + \frac{\partial^2 H_y}{\partial y^2} + n^2 k^2 H_y - n^2 \frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial H_x}{\partial y}\right) + \frac{\partial^2 H_x}{\partial x \partial y} = \beta^2 H_y \tag{4}$$

$$n^2 \frac{\partial}{\partial y}\left(\frac{1}{n^2}\frac{\partial H_x}{\partial y}\right) + \frac{\partial^2 H_x}{\partial x^2} + n^2 k^2 H_x - n^2 \frac{\partial}{\partial y}\left(\frac{1}{n^2}\frac{\partial H_y}{\partial x}\right) + \frac{\partial^2 H_y}{\partial x \partial y} = \beta^2 H_x \tag{5}$$

The boundary conditions used in this work are given by: for the discontinuity along y direction, H_x, H_y, $d(H_y)/d_y$, $d(H_y)/d_x$ are continuous; for the discontinuity along x direction, H_y, H_x, $d(H_x)/d_x$, $d(H_x)/d_y$ are continuous. It is worthy of noting that higher order boundary conditions will improve the accuracy. However, in this letter, we were trying to start with the simple boundary conditions to show the feasibility of the QSCM in mode solvers, the improved version incorporated with the higher order boundary conditions and the related applications such as beam propagation method are in development and will be presented in future publications. Substituting Eq. (3) into the Eq. (4) and Eq. (5), we have

$$Y_1 \bar{\theta}^{H_y} + X_1 \bar{\theta}^{H_x} = B_1 \bar{\theta}^{H_y} \tag{6}$$

$$Y_2 \bar{\theta}^{H_y} + X_2 \bar{\theta}^{H_x} = B_2 \bar{\theta}^{H_X} \tag{7}$$

here

$$\begin{aligned}
Y_1 &= D_2^{x'} \otimes D_0^y + D_0^x \otimes D_2^y + k_0^2 N D_0^x \otimes D_0^y \\
B_1 &= \beta^2 D_0^x \otimes D_0^y \\
X_2 &= D_2^x \otimes D_0^y + D_0^x \otimes D_2^{y'} + k_0^2 N D_0^x \otimes D_0^y \\
Y_2 &= -D_1^{x'} \otimes D_1^y + D_1^x \otimes D_1^y \\
Y_2 &= -D_1^{x'} \otimes D_1^y + D_1^x \otimes D_1^y
\end{aligned}$$

Here N is the distribution matrix for the permittivity (n^2), and the coefficient matrix for the zero-order, the first-order, and the second-order derivatives are given by [17]:

$$D_2^{x,y} = \frac{4}{3h_{x,y}^2}\begin{pmatrix} -3 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & & \cdots & & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -3 \end{pmatrix} \tag{8}$$

$$D_1^{x,y} = \frac{2}{3h_{x,y}}\begin{pmatrix} 1 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & & & \cdots & & \\ & & & -1 & 0 & 1 \\ & & & & -1 & -1 \end{pmatrix} \tag{9}$$

$$D_0^{x,y} = \frac{1}{6}\begin{pmatrix} 5 & 1 & & & & \\ 1 & 6 & 1 & & & \\ & & & \cdots & & \\ & & & 1 & 6 & 1 \\ & & & & 1 & 5 \end{pmatrix} \tag{10}$$

$D_0^{y'}$, $D_1^{y'}$, $D_2^{y'}$ are the modified coefficient matrices for the zero-order, the first-order and the second-order derivative operators, respectively. Those modified coefficient matrices are obtained by modifying the basis function and imposing the boundary conditions. Assuming there are discontinuities at jth and $(j+1)$th points along y direction, the elements have to be modified as

$$\begin{aligned} D_0^{y'}(j,j) &= \frac{1}{6}\left(\frac{n_{j+1}^2 - n_j^2}{n_{j+1}^2 + n_j^2} + 6\right) D_0^y(j,j) \\ D_0^{y'}(j,j+1) &= \frac{2n_j^2}{n_{j+1}^2 + n_j^2} D_0^y(j,j+1) \\ D_0^{y'}(j+1,j) &= \frac{2n_{j+1}^2}{n_{j+1}^2 + n_j^2} D_0^y(j+1,j) \\ D_0^{y'}(j+1,j+1) &= \frac{1}{6}\left(\frac{n_j^2 - n_{j+1}^2}{n_{j+1}^2 + n_j^2} + 6\right) D_0^y(j+1,j+1) \end{aligned}$$

for the zero-order derivative operators, and

$$\begin{aligned} D_1^{y'}(j,j) &= \frac{n_{j+1}^2 - n_j^2}{n_{j+1}^2 + n_j^2} + D_1^y(j,j) \\ D_1^{y'}(j,j+1) &= \frac{2n_j^2}{n_{j+1}^2 + n_j^2} D_1^y(j,j+1) \end{aligned}$$

$$
\begin{aligned}
D_1^{y'}(j+1,j) &= \frac{2n_{j+1}^2}{n_{j+1}^2+n_j^2} D_1^y(j+1,j) \\
D_1^{y'}(j+1,j+1) &= -\frac{n_j^2-n_{j+1}^2}{n_{j+1}^2+n_j^2} + D_1^y(j+1,j+1)
\end{aligned}
$$

for the first-order derivative operators, and

$$
\begin{aligned}
D_2^{y'}(j,j) &= \frac{1}{2}\left(2-\frac{n_{j+1}^2-n_j^2}{n_{j+1}^2+n_j^2}\right) D_2^y(j,j) \\
D_2^{y'}(j,j+1) &= \frac{2n_j^2}{n_{j+1}^2+n_j^2} D_2^y(j,j+1) \\
D_2^{y'}(j+1,j) &= \frac{2n_{j+1}^2}{n_{j+1}^2+n_j^2} D_2^y(j+1,j) \\
D_2^{y'}(j+1,j+1) &= \frac{1}{2}\left(2-\frac{n_j^2-n_{j+1}^2}{n_{j+1}^2+n_j^2}\right) D_2^y(j+1,j+1)
\end{aligned}
$$

for the second-order derivative operators. Similarly, with the exchange of j to i and y to x, we can obtain the modified coefficient matrices $D_0^{x'}$, $D_1^{x'}$, $D_2^{x'}$, assuming there are discontinuities between ith and $(i+1)$th points along x direction. Finally we have $A\bar{\theta} = \beta^2 B\bar{\theta}$, which is a standard eigen-value problem in which the matrices are defined as

$$
A = \begin{pmatrix} Y_1 & X_1 \\ Y_2 & X_2 \end{pmatrix}, \quad B = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix} \tag{11}
$$

For a two-dimensional waveguide structure, e.g., slab waveguide structures, Eqs. (4) and (5) become decoupled for the TM and TE modes, respectively.

$$
n^2 \frac{\partial}{\partial x}\left(\frac{1}{n^2}\frac{\partial H_y}{\partial x}\right) + n^2k^2H_y = \beta_{TM}^2 H_y \tag{12a}
$$

$$
\frac{\partial^2 H_x}{\partial x^2} + n^2k^2H_x = \beta_{TE}^2 H_x \tag{12b}
$$

In matrix form, we have

$$
Y_{TM}\bar{\theta}^{H_y} = B_{TM}\bar{\theta}^{H_y} \tag{13a}
$$

$$
X_{TE}\bar{\theta}^{H_x} = B_{TE}\bar{\theta}^{H_X} \tag{13b}
$$

Here

$$
\begin{aligned}
Y_{TM} &= D_2^{x'} + k_0^2 N D_0^x \\
B_{TM} &= \beta_{TM}^2 D_0^x \\
X_{TE} &= D_2^{y'} + k_0^2 N D_0^y
\end{aligned}
$$

$$B_{TE} = \beta_{TE}^2 D_0^y$$

It should be noted that, unlike in the FDM scheme where the (unknown) function is determined at a series of discrete points, the (unknown) function in the QSCM scheme is not only determined at a set of discrete points (i.e., the collocation points), but is also smoothed out by the local quadratic functions among the collocation points. Therefore, in a homogenous region where no abrupt change can possibly happen to the (unknown) function, the QSCM should be more accurate comparing to the FDM with a same set of discrete points. At the boundary of two different homogenous materials, however, the (unknown) function can have an abrupt change that cannot be described by a finite set of smooth functions. To solve this problem, we've modified the basis functions to explicitly represent the possible discontinuity in the (unknown) function. Such induced extra degree of freedom is then utilized to force the (unknown) function to satisfy the boundary condition embedded in the Maxwell equations. Hence the accuracy of the (unknown) function is ensured, not only inside the homogenous region, but also at the boundaries.

3. VERIFICATION OF QSC METHOD

To evaluate the QSCM mode solver performance, we compare it directly with a standard $O(h^2)$ finite difference (FD) mode solver. For a same grid size, a three-point scheme FD mode solver will result in the same tri-diagonal matrix as QSC. So the computation effort is roughly the same. The first structure we investigate is a three-layer asymmetric slab waveguide with a refractive index profile ($n_{clad} = 1.0$, $n_{core} = 3.5$, $n_{substrate} = 1.5$). The waveguide width is 0.6 μm, and the wavelength is

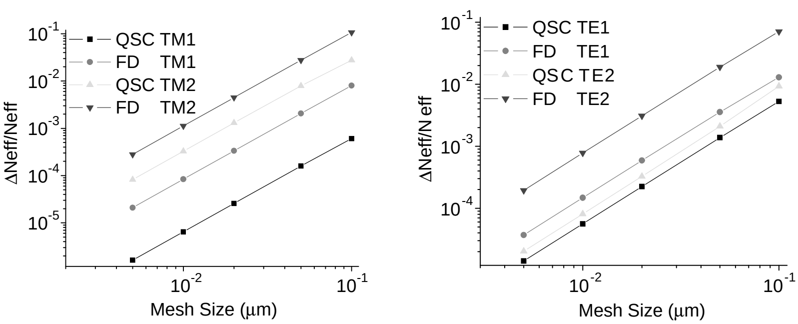

Figure 2. QSC and FD comparison with same grid size and computation effort.

1.55 μm. The slab waveguide structure is a good benchmark since it has analytical solutions. For the structure mentioned above, it supports three guided TE modes (Neff: 3.3457572/2.8514373/1.8943529) and two guided TM modes (Neff: 3.2707248/2.493801). The computation window is set to 5 micron meters and terminated with zero boundary condition. The results of the first two guided modes from FDM and QSC are shown in Figure 2 and it is observed that QSC has a better convergence rate.

Next we investigate two three-dimensional waveguides by calculating the normalized propagation constant and comparing results with those obtained by the finite difference method. For the rib waveguide in Figure 3(a), the thickness of the guiding layer d is 0.2 μm, and the height of the cladding h is 1.0 μm, the ridge width W is 2.4 μm. The other parameters have been shown in Figure 3. For purpose of comparison with the published results, we use the normalized propagation constant $B = (N_{eff}^2 - n_s^2)/(n_g^2 - n_s^2)$ for rib waveguide and the effective propagation constant for the channel waveguide.

The comparison of the current method with the published finite difference methods is shown in Figure 4. We also plot the field patterns of both rib and channel waveguide structures in Figure 5. With the decrease of the mesh size, both QSCM and FDM show the increased computation accuracy (Figure 4(a)). Since the decrease of the mesh size is equivalent to the increase of the number of the mesh points, it is reasonable that we see a convergence of the effective index with the increase of the mesh points (Figure 4(b)). Moreover, it is observed that QSCM and FDM mode solver have the same convergence rate. However, with the same grid size, namely the same amount of computation effort, QSCM mode solver is more accurate than conventional FDM mode solver [4, 5], however, it should be addressed that the current QSCM loses the advantage comparing to

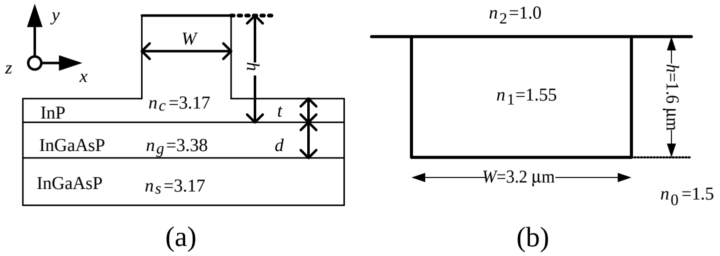

Figure 3. waveguide structures. (a) Rib waveguide [5]. (b) Channel waveguide [7].

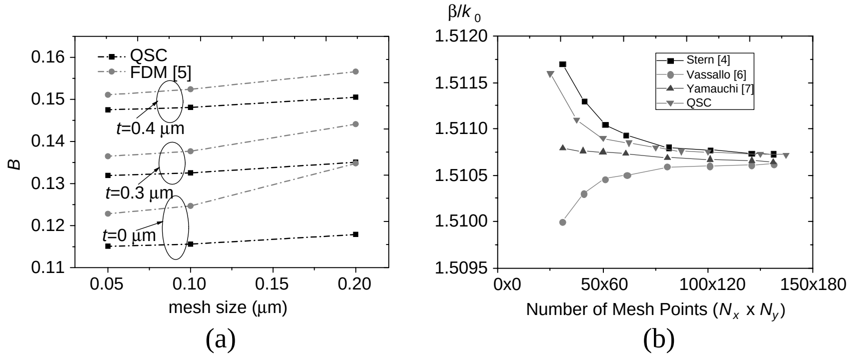

Figure 4. Comparison of QSC with finite difference method. (a) Rib waveguide. (b) Channel waveguide.

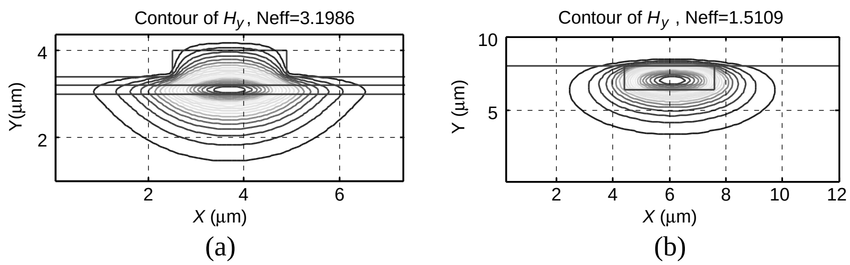

Figure 5. Field patterns calculated by QSC. (a) Rib waveguide ($t = 0.2$). (b) Channel waveguide.

the improved finite difference method [7, 10, 11] where higher order boundary conditions are applied. The improved QSCM with higher order boundary conditions will be our future work.

4. CONCLUSIONS

We have introduced a numerical mode solver based on the quadratic spline collocation method which employs piecewise second-order polynomials. The piecewise property of spline collocation method allows us to easily integrate the discontinuity of the dielectric interfaces into our formulation. The resulted QSCM mode solver performs well when it is compared with the standard finite difference method. This general method may find its applications of studying the optical characteristics of the photonic devices and applications in various eigen-modes associated methods such as beam propagation method, coupled mode theory, and mode expansion methods, etc..

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