An Efficient Bidirectional Propagation Method Based on Dirichlet-to-Neumann Maps

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Abstract

A new bidirectional propagation method is developed for numerical simulation of wave-guiding structures with multiple longitudinal discontinuities. It is a non-iterative method based on the Dirichlet-to-Neumann map of each uniform segment. The method is more accurate than existing bidirectional beam propagation methods and it does not require the computation of eigenmodes in each segment.

1 Introduction

Optical wave-guiding structures that are piecewise uniform along the main propagation direction are widely used in many applications. Efficient numerical methods are essential in the analysis and design of these structures. Existing methods for analyzing such structures with multiple longitudinal discontinuities include various modal methods [1, 2, 3, 4, 5], the bidirectional beam propagation method (BiBPM) [6, 7, 8, 9] and the finite difference time domain (FDTD) method.

In the modal methods, the wave field in each z-invariant segment (where z is the waveguide axis) is expanded in the eigenmodes of the transverse operator. The eigenmodes can be obtained from the eigenvalue decomposition of the matrix approximating the transverse operator [2]. When a perfectly matched layer (PML) is used to truncate the transverse variable, the matrix is complex and unsymmetric, and its eigenvalue decomposition is expensive to compute. For two-dimensional step-index structures, it is possible to compute the eigenmodes analytically by solving a nonlinear equation. Due to the presence of the PMLs, there are leaky modes and Berenger modes with complex propagation constants [10]. It is not a simple task to find all solutions of this nonlinear equation in the complex plane [4, 11, 12, 13]. The BiBPMs rely on rational approximations of a square root operator and its exponential (i.e. the one-way propagator). For

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piecewise uniform structures with large longitudinal discontinuities (as in deeply etched waveguide gratings), a correct modeling of the evanescent modes is important. This implies that the rotating branch-cut Padé approximants [14] must be used, but they do not have a high accuracy unless the degree is relatively large. The FDTD method is generally applicable, but it appears to be less efficient, especially when the medium is dispersive.

In this letter, we develop a bidirectional propagation method based on the Dirichlet-to-Neumann (DtN) map of each z-invariant segment. The DtN map is computed numerically by a Chyebyshev collocation method in the z direction for each segment. The method requires about the same number of operations as the BiBPM based on the scattering operators [8], but it is more accurate, since rational approximations for operators are mostly avoided. Compared with the method using the full eigenvalue decomposition of the transverse operator, our method is much more efficient.

2 The Dirichlet-to-Neumann map

We consider the transverse electric (TE) polarization of a two-dimensional piecewise uniform wave-guiding structure. The governing equation is

$$\partial_z^2 u + \partial_x^2 u + k_0^2 n^2(x,z)\, u = 0, \tag{1}$$

where u is the y-component of the electric field, k_0 is the free space wavenumber and $n = n(x,z)$ is the refractive index function. For a piecewise z-invariant structure, we assume that

$$n(x,z) = n_j(x) \quad \text{for} \quad z_{j-1} < z < z_j \quad \text{and} \quad j = 0, 1, ..., m+1, \tag{2}$$

where $z_{-1} = -\infty$, $z_0 < z_1 < ... < z_m$ and $z_{m+1} = \infty$. In a z-invariant segment given by $z_{j-1} < z < z_j$ for $1 \le j \le m$, we define the Dirichlet-to-Neumann (DtN) map $\mathcal{M}$ as the operator that maps u at z_{j-1} and z_j to its z-derivative there. That is

$$\mathcal{M} \begin{bmatrix} u(x, z_{j-1}) \\ u(x, z_j) \end{bmatrix} = \begin{bmatrix} \partial_z u(x, z_{j-1}) \\ \partial_z u(x, z_j) \end{bmatrix}. \tag{3}$$

When x is discretized by N points, the operator $\mathcal{M}$ is approximated by a $(2N) \times (2N)$ matrix. Let $\mathcal{M}$ be given in 2×2 blocks as

$$\mathcal{M} = \begin{bmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{bmatrix}, \tag{4}$$

it is easy to see that $\mathcal{M}_{12} = -\mathcal{M}_{21}$ and $\mathcal{M}_{22} = -\mathcal{M}_{11}$.

The transverse variable x can be truncated by the PML technique. In this case, the term $\partial_x^2 u$ is replaced by $s^{-1}\partial_x(s^{-1}\partial_x u)$, where $s = s(x)$ is a function of x and $s \ne 1$ only in the PML regions. Therefore, Eq. (1) in the segment (z_{j-1}, z_j) becomes

$$\partial_z^2 u + \mathcal{L} u = 0, \quad \mathcal{L} = \frac{1}{s(x)}\frac{\partial}{\partial x}\left(\frac{1}{s(x)}\frac{\partial}{\partial x}\right) + k_0^2 n_j^2(x). \tag{5}$$

To find $\mathcal{M}$, we need an efficient method for solving the standard Dirichlet problem: given u at z_{j-1} and z_j, find $\partial_z u$ at z_{j-1} and z_j. The matrix $\mathcal{M}$ is obtained if we repeatedly solve the Dirichlet problem N times by taking $[u(x, z_{j-1}), u(x, z_j)]^T$ as the first N columns of the $(2N) \times (2N)$ identify matrix.

In the following, we develop a Chebyshev collocation method that computes $\mathcal{M}$ in $O(qN^2)$ operations, where q is the number of points for discretizing (z_{j-1}, z_j) as

$$\xi_k = z_{j-1} + \frac{z_j - z_{j-1}}{2} \left[1 - \cos\left(\frac{k\pi}{q} \right) \right], \quad k = 0, 1, ..., q.$$

Notice that $\xi_0 = z_{j-1}$ and $\xi_q = z_j$. For a function of z, its derivative can be evaluated by multiplying the differentiation matrix C:

$$\begin{bmatrix} v'(\xi_0) \\ v'(\xi_1) \\ \vdots \\ v'(\xi_q) \end{bmatrix} = C \begin{bmatrix} v(\xi_0) \\ v(\xi_1) \\ \vdots \\ v(\xi_q) \end{bmatrix},$$

where v is an arbitrary function of z, v' is its derivative. The (k, l) entry (for k, $l = 0$, ..., q) of the matrix C is [15]

$$c_{kl} = -\frac{2}{z_j - z_{j-1}} \times \begin{cases} (2q^2+1)/6 & \text{if } k = l = 0, \\ -(2q^2+1)/6 & \text{if } k = l = q, \\ -0.5\tau_k/(1-\tau_k^2) & \text{if } 0 < k = l < q, \\ (-1)^{k+l}\sigma_k\sigma_l^{-1}/(\tau_k - \tau_l) & \text{otherwise,} \end{cases}$$

where

$$\tau_k = \cos\left(\frac{k\pi}{q} \right), \quad \sigma_k = \begin{cases} 2 & \text{if } k = 0,\, q \\ 1 & \text{if } 0 < k < q. \end{cases}$$

Similarly, the second derivative v'' at these discrete points can be evaluated by multiplying C^2. Let us write down the matrices C and C^2 as follows:

$$C = \begin{bmatrix} c_{00} & \tilde{c}_0 & c_{0q} \\ \vdots & \vdots & \vdots \\ c_{q0} & \tilde{c}_q & c_{qq} \end{bmatrix}, \quad C^2 = \begin{bmatrix} d_{00} & \cdots & d_{0q} \\ \hat{d}_0 & \hat{D} & \hat{d}_q \\ d_{q0} & \cdots & d_{qq} \end{bmatrix}, \tag{6}$$

where $\tilde{c}_0$ and $\tilde{c}_q$ are row vectors of length $q-1$, $\hat{d}_0$ and $\hat{d}_q$ are column vectors of length $q-1$, and $\hat{D}$ is a $(q-1) \times (q-1)$ matrix. Eq. (5) is assumed to be valid at ξ_k for $k = 1$, 2, ..., $q-1$. Thus

$$\hat{d}_0 u(x, z_{j-1}) + \hat{D} U + \hat{d}_q u(x, z_j) + \mathcal{L}\, U = 0, \tag{7}$$

where $U = [u(x, \xi_1), u(x, \xi_2), ..., u(x, \xi_{q-1})]^T$. We can diagonalize the matrix $\hat{D}$ as

$$\hat{D} = R \begin{bmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_{q-1} \end{bmatrix} R^{-1}.$$

Eq. (7) is then reduced to the following $q-1$ un-coupled ordinary differential equations:

$$\mathcal{L}\, w_k + \mu_k w_k = -\alpha_k u(x, z_{j-1}) - \beta_k u(x, z_j), \quad k = 1, 2, ..., q-1, \tag{8}$$

where

$$\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_{q-1} \end{bmatrix} = R^{-1} U, \quad \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{q-1} \end{bmatrix} = R^{-1} \hat{d}_0, \quad \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{q-1} \end{bmatrix} = R^{-1} \hat{d}_q.$$

If u is given at z_{j-1} and z_j, we can solve the functions $w_k(x)$ in $O(qN)$ operations. Using the first and last rows of the matrix C, we can evaluate $\partial_z u$ at z_{j-1} and z_j. Therefore

$$\partial_z u(x, z_{j-1}) = c_{00}\, u(x, z_{j-1}) + \sum_{k=1}^{q-1} \gamma_k w_k(x) + c_{0q}\, u(x, z_j), \tag{9}$$

$$\partial_z u(x, z_j) = c_{q0}\, u(x, z_{j-1}) + \sum_{k=1}^{q-1} \delta_k w_k(x) + c_{qq}\, u(x, z_j), \tag{10}$$

where

$$[\gamma_1, \gamma_2, ..., \gamma_{q-1}] = \tilde{c}_0 R, \quad [\delta_1, \delta_2, ..., \delta_{q-1}] = \tilde{c}_q R.$$

The matrix $\mathcal{M}$ is obtained in $O(qN^2)$ operations, since we have to repeatedly solve the Dirichlet problem for N times. However, we only need to compute matrices C and C^2, the eigenvalue decomposition of $\hat{D}$ and the vectors (α_k), (β_k), (γ_k) and (δ_k) once. Overall, computing the DtN map $\mathcal{M}$ is much easier than computing the eigenvalue decomposition of transverse operator $\mathcal{L}$.

3 An operator marching scheme

For the piecewise z-invariant structure specified in (2), we assume that an incident wave u^+ is given in $z < z_0$ and there are only outgoing waves for $z > z_m$. Therefore, $u = u^+ + u^-$ for $z < z_0$, where u^+ is given and u^- is the unknown reflected field. The directional wave field components satisfy one-way Helmholtz equations involving the square root operator $B_0 = \sqrt{\partial_x^2 + k_0^2 n_0^2(x)}$:

$$\partial_z u^+ = iB_0 u^+, \quad \partial_z u^- = -iB_0 u^-, \quad z < z_0.$$

The following boundary condition for u is obtained if we eliminate u^-:

$$\partial_z u + iB_0 u = 2iB_0 u^+(x, z_0-), \quad z = z_0. \tag{11}$$

For $z > z_m$, we have $u = u^+$. This leads to the boundary condition

$$\partial_z u - iB_{m+1} u = 0, \quad z = z_m, \tag{12}$$

where $B_{m+1} = \sqrt{\partial_x^2 + k_0^2 n_{m+1}^2(x)}$.

While it is unstable to solve the Helmholtz equation (1) as an initial value problem in the z direction (due to evanescent modes that grow or decay exponentially in z), it is possible to formulate stable initial value problems for a pair of operators. One possibility is to use the scattering operators. In our case, it is more convenient to use the Dirichlet-to-Neumann (DtN) map Q and Fundamental Solution (FS) operator Y [16] defined at each fixed z as

$$Q(z)u(x,z) = \partial_z u(x,z), \quad Y(z)u(x,z) = u(x,z_m), \tag{13}$$

where u is an arbitrary solution of (1) satisfying the outgoing radiation condition (12). Here, the operator Q is also a DtN map, but it follows a different definition as $\mathcal{M}$. From the boundary condition (12) and the definition of Y, we have

$$Q(z_m) = iB_{m+1}, \quad Y(z_m) = I, \tag{14}$$

where I is the identity operator. Using the DtN map $\mathcal{M}$, we can manipulate Q and Y from z_j to z_{j-1}. For $\mathcal{M}$ given in its block form (4), we write down the two equations in (3) and obtain

$$Q(z_{j-1}) = \mathcal{M}_{11} + \mathcal{M}_{12}[Q(z_j) - \mathcal{M}_{22}]^{-1}\mathcal{M}_{21}, \tag{15}$$

$$Y(z_{j-1}) = Y(z_j)[Q(z_j) - \mathcal{M}_{22}]^{-1}\mathcal{M}_{21}. \tag{16}$$

The above recursion formulas can be applied from $j = m$ to $j = 1$. Once $Q(z_0)$ is calculated, we use the boundary condition (11) and solve $u(x, z_0)$ from

$$[Q(z_0) + iB_0]\, u(x,z_0) = 2iB_0 u^+(x, z_0-). \tag{17}$$

The reflected wave is obtained from $u^-(x, z_0-) = u(x, z_0) - u^+(x, z_0-)$. The transmitted wave is obtained from the operator $Y(z_0)$, that is

$$u(x, z_m) = Y(z_0)u(x, z_0). \tag{18}$$

When x is discretized by N points, the operators B_0, B_{m+1}, Q, Y and $\mathcal{M}_{kl}$ are all approximated by $N \times N$ matrices. The square root operators B_0 and B_{m+1} are still approximated by a rotating branch-cut Padé approximant and this requires $O(pN^2)$ operations, where p is the degree of the Padé approximant. By formulas (15) and (16), the step from z_j to z_{j-1} requires $O(N^3)$ operations. Therefore, the total required number of operations is $O(mN^3)$.

4 Examples

To validate our method, we consider two examples in this section. The first example is a modeling exercise of COST 268 [17]. It is about a high-contrast optical waveguide with a deeply etched short Bragg grating. The original waveguide is formed by a Si_3N_4 layer of the thickness $0.5\mu m$ deposited onto a SiQ_2 substrate. The refractive indices of waveguide core and the substrate are frequency dependent and given in Ref. [17]. The Bragg grating is composed of 20 rectangular grooves with a grating period of $0.43\mu m$. The widths of the "tooth" and "groove" are chosen to be equal, i.e., $0.215\mu m$. This implies that $m = 39$ and $z_j - z_{j-1} = 0.215\mu m$ for $j = 1, 2, ..., m$. For the groove depth $0.125\mu m$ (the width of the waveguide core under a groove is $0.375\mu m$), we obtain the power reflectance R, the transmittance T and the loss $L = 1 - R - T$ of the fundamental transverse electric (TE) mode as shown in Fig. 1. Our numerical results are nearly identical to the earlier results

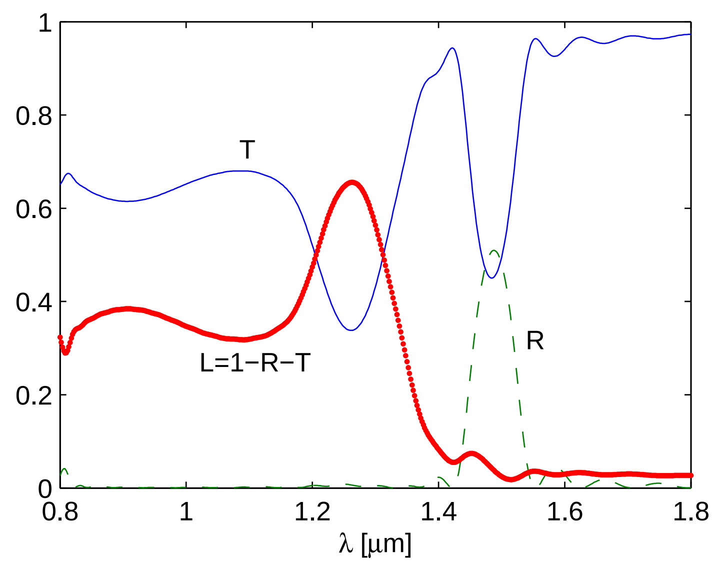

Figure 1: Reflectance, transmittance and loss of the fundamental TE mode in a high contrast optical waveguide with 20 rectangular grooves (COST 268 [17]).

reported in Ref. [17]. In our calculations, the transverse variable x is truncated to the total of $3\mu m$ with a $1.5\mu m$ substrate and a $1\mu m$ air superstrate. The transverse operator is approximated by a finite difference method using 200 grid points in x. For each end of the x interval, we use a PML with a thickness corresponding to 20 grid points. For this structure, we only have to calculate two DtN maps (for the "teeth" and the "grooves", respectively). They are obtained with $q = 10$.

For another example, we consider the segmented waveguide studied in [18]. This is a symmetric waveguide with air claddings. It corresponds to the top view of the 3-D waveguide D2 in Ref. [18]. The width and the refractive index of the waveguide core are $2.5\mu m$ and $n = 3.165$, respectively. The waveguide has a five-period grating with a defect in the middle. This is obtained by putting six air slots of thickness $0.2\mu m$ in the waveguide. The thickness of the middle segment is $1.01\mu m$ and thickness of the remaining four segments is $0.88\mu m$. This implies that $m = 11$ and

$$z_j - z_{j-1} = \begin{cases} 0.20\mu m & \text{if } j = 1, 3, 5, ..., 11, \\ 1.01\mu m & \text{if } j = 6, \\ 0.88\mu m & \text{if } j = 2, 4, 8, 10. \end{cases}$$

Our results for the power reflectance, transmittance and loss of the fundamental TE mode of this structure are shown in Fig. 2. These calculations are obtained with a truncated

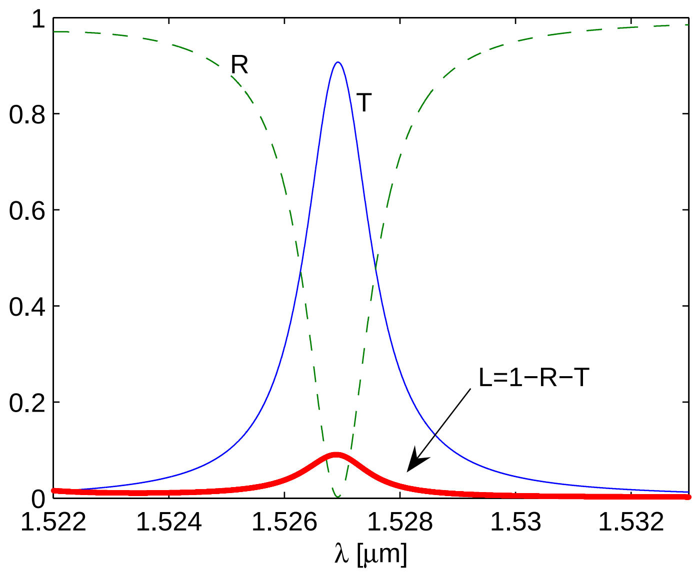

Figure 2: Reflectance, transmittance and loss of the fundamental TE mode in a segmented waveguide [18].

x interval of $5\mu m$ and they confirm the earlier results [18] using the BiBPM based on the scattering operators [8]. The transverse operator is discretized by a finite difference method with 200 grid points in x and a PML with a thickness of 20 grid points is used at each end of the x interval. The DtN maps for the large segment in the middle, the four smaller segments and the air slots are calculated with $q = 20$, $q = 16$ and $q = 8$, respectively.

5 Conclusions

We have developed a new method for analyzing two-dimensional piecewise z-invariant wave-guiding structures. The method is suitable for structures with large longitudinal discontinuities, where a correct modeling of the evanescent mode is often necessary. Compared with existing BiBPMs, our new method is more accurate, since operator rational approximations are mostly avoided, except for the square root operators at the two ends of the structure. These rational approximants cannot easily approximate both the propagating modes and evanescent modes accurately. Since a computation of the eigenmodes in each uniform segment is not needed, the method is more efficient than modal methods based on the eigenvalue decomposition of the transverse operator.

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