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Some Techniques for Computing Wave Propagation in Optical Waveguides

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Abstract. Optical wave-guiding structures that are non-uniform in the propagation direction are fundamental building blocks of integrated optical circuits. Numerical simulation of lightwaves propagating in these structures is an essential tool to engineers designing photonic components. In this paper, we review recent developments in the most widely used simulation methods for frequency domain propagation problems.

Key words: Optical waveguides; operator marching method; mode matching method; beam propagation method; bidirectional propagation methods; rational approximations.

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1 Introduction

Optical waveguides [1–3] are structures that guide the propagation of light. They are fundamental building blocks of optical communications systems [4] and integrated optical circuits [5]. For a straight waveguide which is invariant along the waveguide axis (denoted by z in this paper), the basic issue is to analyze the mode structures at a fixed frequency. A propagating mode of a straight waveguide is a special solution of the Maxwell's equations that depends on z as $e^{i\beta z}$ and decays to zero as the transverse variables (x and y) tend to infinity. For a lossless medium, the propagation constant β is real. The problem of computing the modes is an eigenvalue problem where β^2 is the eigenvalue. An optical waveguide is typically an open structure, that is, its cross section is the entire xy-plane. As a result, a general wave field in a straight waveguide contains not only the propagating modes, but also a continuum (represented as an integral) of the radiation and the

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evanescent modes. A general three-dimensional optical waveguide may also have complex modes [6,7]. The propagation constants of these modes are complex and their mode profiles decay to zero at infinity. Analytic solutions of waveguides modes are only available in a few simple cases. Numerical methods [8–10] are needed for computing the modes of most practical waveguides.

Optical waveguides (or general wave-guiding structures) that are non-uniform in z are important for integrated optics [5]. For example, a bent waveguide is used to turn the propagation direction, an S-bend is used to introduce a lateral displacement, a Y-branch is used to split one waveguide into two, a taper is needed to connect two waveguides of different sizes, waveguide gratings are introduced for various purposes such as filters and reflectors. To simulate the lightwave propagation in these z-varying wave-guiding structures, accurate and efficient numerical or analytic methods are needed. The problem is more difficult since the z-variable is no longer separated, except when the structure is a bent waveguide with a constant bending curvature. In that case, the variable z can be defined along the bend and be separated again. For a general z-varying wave-guiding structure, the frequency domain propagation problem is a boundary value problem. Assuming that the structure is z-invariant for $z < 0$ and $z > a$, we can impose boundary conditions at $z = 0$ and $z = a$. The length of the structure a is usually much larger than the typical wavelength. In some cases, a may be a few millimeters, but the free space wavelength λ_0 is on the order of a micrometer. Since a certain number of grid points (or basis functions) are needed for each wavelength, standard numerical methods that discretize the whole wave-guiding structure are prohibitively expensive.

Fortunately, a number of special features are available for typical optical waveguides. Some efficient numerical and analytical methods have been developed to take advantage of these features. Firstly, although the cross section of an open optical waveguide is the entire xy-plane, the size of the waveguide core is on the order of λ_0 and it is much smaller than a. Using the powerful perfectly matched layer (PML) [11,12] technique, the transverse plane can be truncated to a relatively small region. Therefore, the propagation problem is formulated in a domain with just one direction (i.e. z) having a particularly large length. This special geometric feature gives rise to *marching methods* that reformulate (exactly or approximately) the original boundary value problem as initial value problems in z. Exact reformulations are developed for pairs of operators and they will be referred to as the operator marching methods (OMM). Secondly, many structures such as waveguide tapers, bent waveguides, S-bends and even Y-branches change with z slowly (i.e. there is little variation on the scale of a wavelength in the z direction). For these slowly varying waveguides, the beam propagation method (BPM) is widely used. These are marching methods based on approximate one-way models. Thirdly, many z-varying wave-guiding structures such as waveguide gratings, are made of piecewise z-invariant segments. The bidirectional beam propagation methods (BiBPM) are designed to take advantages of this feature. The mode matching method (MMM) is also widely used for piecewise z-invariant structures. Both BiBPM and MMM are aimed at solving the full boundary value problem while reducing unnecessary computation in each z-invariant segment. Each of these two methods have two variants depending on whether or not they are used together with an operator marching method. In the following, we present these methods after a brief introduction to the basic equations in Section 2.

2 Basic equations

For time-harmonic lightwaves propagating in a wave-guiding structure composed of linear isotropic dielectric materials, the governing equations are the frequency domain Maxwell's equations:

$$\begin{aligned} \nabla \times E &= i\omega\mu_0 H && (2.1)\\ \nabla \times H &= -i\omega\epsilon E && (2.2)\\ \nabla \cdot (\epsilon E) &= 0 && (2.3)\\ \nabla \cdot H &= 0, && (2.4) \end{aligned}$$

where ω is the angular frequency, the time dependence is $e^{-i\omega t}$, μ_0 (a constant) is the magnetic permeability, ϵ is the permittivity of the medium. Furthermore, $\epsilon = \epsilon_0 n^2$, where ϵ_0 is the permittivity of vacuum, $n = n(x, y, z)$ is the refractive index function. After eliminating the z-components of the electric and magnetic fields, we obtain a system of equations for the transverse components of the electric and magnetic fields:

$$-i\omega\epsilon_0 \frac{\partial E_t}{\partial z} = \mathcal{A} H_t, \quad -i\omega\mu_0 \frac{\partial H_t}{\partial z} = \mathcal{B} E_t, \tag{2.5}$$

where

$$E_t = \begin{bmatrix} E_x \\ E_y \end{bmatrix}, \quad H_t = \begin{bmatrix} H_y \\ -H_x \end{bmatrix},$$

E_x, E_y, H_x and H_y are the x- and y-components of E and H, $\mathcal{A}$ and $\mathcal{B}$ are matrix operators given by

$$\mathcal{A} = k_0^2 I + \begin{bmatrix} \partial_x(n^{-2}\partial_x\cdot) & \partial_x(n^{-2}\partial_y\cdot) \\ \partial_y(n^{-2}\partial_x\cdot) & \partial_y(n^{-2}\partial_y\cdot) \end{bmatrix}, \quad \mathcal{B} = k_0^2 n^2 I + \begin{bmatrix} \partial_y^2 & -\partial_{yx}^2 \\ -\partial_{xy}^2 & \partial_x^2 \end{bmatrix}, \tag{2.6}$$

and $k_0 = \omega\sqrt{\mu_0\epsilon_0}$ is the free-space wavenumber. Formally, we can write down separate equations for the electric or magnetic transverse components using the inverses of $\mathcal{A}$ and $\mathcal{B}$. We have

$$\mathcal{A}\frac{\partial}{\partial z}\left(\mathcal{A}^{-1}\frac{\partial E_t}{\partial z}\right) + \mathcal{L} E_t = 0 \tag{2.7}$$

$$\mathcal{B}\frac{\partial}{\partial z}\left(\mathcal{B}^{-1}\frac{\partial H_t}{\partial z}\right) + \mathcal{M} H_t = 0, \tag{2.8}$$

where $\mathcal{L}$ and $\mathcal{M}$ are operators defined as

$$\mathcal{L} = \frac{1}{k_0^2}\mathcal{A}\mathcal{B}, \qquad \mathcal{M} = \frac{1}{k_0^2}\mathcal{B}\mathcal{A}.$$

After some simplifications, we have

$$\mathcal{L}\begin{bmatrix} f \\ g \end{bmatrix} = \begin{bmatrix} k_0^2 n^2 f + \partial_y^2 f - \partial_{xy}^2 g + \partial_x[n^{-2}\partial_x(n^2 f)] + \partial_x[n^{-2}\partial_y(n^2 g)] \\ k_0^2 n^2 g + \partial_x^2 g - \partial_{yx}^2 f + \partial_y[n^{-2}\partial_y(n^2 g)] + \partial_y[n^{-2}\partial_x(n^2 f)] \end{bmatrix}, \tag{2.9}$$

$$\mathcal{M}\begin{bmatrix} f \\ g \end{bmatrix} = \begin{bmatrix} k_0^2 n^2 f + \partial_y^2 f - \partial_{yx}^2 g + n^2\partial_x(n^{-2}\partial_x f) + n^2\partial_x(n^{-2}\partial_y g) \\ k_0^2 n^2 g + \partial_x^2 g - \partial_{xy}^2 f + n^2\partial_y(n^{-2}\partial_x f) + n^2\partial_y(n^{-2}\partial_y g) \end{bmatrix}, \tag{2.10}$$

for any given functions f and g.

In a z-invariant section of the structure, the refractive index function n and the operators $\mathcal{A}$ and $\mathcal{B}$ are independent of z, equations (2.7) and (2.8) are reduced to

$$\frac{\partial^2 E_t}{\partial z^2} + \mathcal{L}E_t = 0, \tag{2.11}$$

$$\frac{\partial^2 H_t}{\partial z^2} + \mathcal{M}H_t = 0, \tag{2.12}$$

and the wave fields can be decomposed. For example, the transverse electric field can be written as

$$E_t = E_t^+ + E_t^-,$$

where E_t^+ represents waves propagating in the increasing z direction or evanescent waves that decay in the increasing z direction. With a suitable definition of the square root operator $\sqrt{\mathcal{L}}$, we have

$$\partial_z E_t^+ = i\sqrt{\mathcal{L}}\,E_t^+, \quad \partial_z E_t^- = -i\sqrt{\mathcal{L}}\,E_t^-.$$

The square root of $\mathcal{L}$ is a linear operator and it can be defined based on the spectral decomposition [68–70] of the operator $\mathcal{L}$. Let Φ and λ satisfy $\mathcal{L}\Phi = \lambda\Phi$, then $\sqrt{\mathcal{L}}\Phi = \beta\Phi$, where $\beta = \sqrt{\lambda}$ is chosen to have $\mathrm{Im}(\beta) \geq 0$ and $\mathrm{Re}(\beta) \geq 0$ if $\mathrm{Im}(\beta) = 0$. This ensures that $\Phi e^{i\beta z}$ either decays exponentially as z increases or propagates in the increasing z direction.

We consider a structure that is z-invariant for $z < 0$ and $z > a$. Let $n = n_0(x, y)$ and $n = n_\infty(x, y)$ for $z < 0$ and $z > a$, respectively. The operator $\mathcal{L}$ corresponding to these two cases are denoted by $\mathcal{L}_0$ and $\mathcal{L}_\infty$ respectively. For $z < 0$, we assume that an incident wave $E_t^{(i)}$ is given and we look for the reflected wave $E_t^{(r)}$. Since $E_t^{(i)}$ and $E_t^{(r)}$ correspond to E_t^+ and E_t^- respectively, we have the following boundary condition:

$$\partial_z E_t + i\sqrt{\mathcal{L}_0}E_t = 2i\sqrt{\mathcal{L}_0}E_t^{(i)}, \quad z = 0-. \tag{2.13}$$

For $z > a$, we assume that there exist only outgoing waves and evanescent waves that decay to zero as $z \to \infty$. This gives rise to the following condition:

$$\partial_z E_t = i\sqrt{\mathcal{L}_\infty}\,E_t, \quad z = a+. \tag{2.14}$$

The boundary conditions for H_t are similar.

For the 2-D cases, we have a refractive index n that is independent of y. Under the assumption that E and H are also independent of y, the Maxwell's equations can be reduced to scalar Helmholtz equations. We have

$$\partial_z^2 E_y + \partial_x^2 E_y + k_0^2 n^2(x,z) E_y = 0 \tag{2.15}$$

for the transverse electric (TE) polarization and

$$\partial_z(n^{-2}\partial_z H_y) + \partial_x(n^{-2}\partial_x H_y) + k_0^2 H_y = 0 \tag{2.16}$$

for the transverse magnetic (TM) polarization. Boundary conditions at $z = 0-$ and $z = a+$ can be similarly posed using square root operators.

3 Operator marching method

For waveguide problems, it is possible to reformulate the boundary value problems of the frequency-domain Maxwell's equations (or Helmholtz equations for the 2-D cases) described in the previous section as "initial" value problems for pairs of operators. These initial value problems are solved by marching in the z direction. For this reason, we name this class of methods the operator marching method (OMM). One advantage of the OMM is that its required computer memory is independent of the total length of the non-uniform part of the waveguide, i.e., a. Compared with other methods that solves the boundary value problem directly, the required computer memory of an OMM is much smaller.

The formulation based on a pair of scattering operators has been known for many years. For simplicity, we consider the 2-D Helmholtz equation (2.15) for the TE polarization and denote E_y by u in the following. As in Section 2, we assume that the structure is z-invariant for $z < 0$ and $z > a$, and there are only outgoing or exponentially decaying waves for $z > a$. First, we consider the case where the wave-guiding structure is piecewise uniform in z. We have

$$0 = z_0 < z_1 < \dots < z_m = a, \tag{3.1}$$

such that $n(x,z) = n_j(x)$ for $z_{j-1} < z < z_j$. This is valid even for $j = 0$ and $j = m$, if we define $z_{-1} = -\infty$, $z_{m+1} = \infty$ and $n_{m+1} = n_\infty$. In the segment (z_{j-1}, z_j), we can decompose the wave field as $u = u^+ + u^-$, such that

$$\frac{\partial u^+}{\partial z} = i\Lambda_j u^+, \quad \frac{\partial u^-}{\partial z} = -i\Lambda_j u^-, \tag{3.2}$$

for

$$\Lambda_j = \sqrt{\partial_x^2 + k_0^2 n_j^2(x)}. \tag{3.3}$$

For any z which is not a longitudinal discontinuity, i.e., $z \neq z_j$ for $j = 0, 1, \dots, m$, we can define the reflection operator $R(z)$ and transmission operator $T(z)$ by

$$R(z)u^+(x,z) = u^-(x,z), \quad T(z)u^+(x,z) = u^+(x,a+). \tag{3.4}$$

At a discontinuity z_j, the operators R and T are discontinuous there. The outgoing wave condition for $z > a$ gives rise to $R(a+) = 0$, and it is obvious that $T(a+) = I$ where I is the identity operator. These two operators can be easily solved from $z = a+$ to $z = 0-$ in a sequence of steps. To pass through the discontinuity z_j, i.e., from z_j+ to z_j-, we have the following formulas

$$\begin{aligned} C &= \Lambda_j^{-1}\Lambda_{j+1}[I - R(z_j+)][I + R(z_j+)]^{-1}, && (3.5)\\ R(z_j-) &= (I + C)^{-1}(I - C), && (3.6)\\ T(z_j-) &= T(z_j+)[I + R(z_j+)]^{-1}[I + R(z_j-)]. && (3.7) \end{aligned}$$

To march through a z-independent segment from z_j- to $z_{j-1}+$, we have

$$\begin{aligned} P_j &= \exp(i(z_j - z_{j-1})\Lambda_j), && (3.8)\\ R(z_{j-1}+) &= P_j R(z_j-) P_j, && (3.9)\\ T(z_{j-1}+) &= T(z_j-) P_j. && (3.10) \end{aligned}$$

In a different version, we define z_0, z_1, ..., z_m at continuous points of the refractive index function. For each z_j, we further assume that there is a small neighborhood in which the refractive index n is z-independent. This allows us to have a wave field decomposition and define the operators T and R in the neighborhood of z_j. On the other hand, n is allowed to vary with z away from these small neighborhoods. Given the two operators at z_j, we can calculate these two operators at z_{j-1} by making use of the four scattering operators $r^\pm$ and $t^\pm$ of the segment. For the segment (z_{j-1}, z_j), an incident wave at z_{j-1}, say v, gives rise to a reflected wave at z_{j-1} and a transmitted wave at z_j and they are r^+v and t^+v, respectively. Similarly, an incident wave w at $z = z_j$ (coming from $z = +\infty$) gives rise to the reflected wave r^-w at z_j and transmitted wave t^-w at z_{j-1}. Then, the operators R and T at z_{j-1} are given by

$$\begin{aligned} R(z_{j-1}) &= [I - t^- R(z_j) r^-]^{-1}[r^+ + t^- R(z_j) t^+], && (3.11)\\ T(z_{j-1}) &= T(z_j)[t^+ + r^- R(z_{j-1})]. && (3.12) \end{aligned}$$

The continuous formulation of the scattering operators was developed by Fishman [13] based on the wave field decomposition

$$u = u^+ + u^-, \quad \frac{\partial u}{\partial z} = i\Lambda(z)[u^+ - u^-], \tag{3.13}$$

and the same definitions of R and T as before. It was found that u^+ and u^- satisfy the following system:

$$\frac{\partial}{\partial z}\begin{bmatrix} u^+ \\ u^- \end{bmatrix} = \begin{bmatrix} i\Lambda(z) - \alpha(z) & \alpha(z) \\ \alpha(z) & -i\Lambda(z) - \alpha(z) \end{bmatrix}\begin{bmatrix} u^+ \\ u^- \end{bmatrix}, \tag{3.14}$$

where $\alpha(z) = \Lambda^{-1}(z)\Lambda'(z)/2$, and R and T satisfy

$$\frac{dR}{dz} = \alpha(z) - [i\Lambda(z) + \alpha(z)]\ R - R\ [i\Lambda(z) - \alpha(z)] - R\alpha(z)R, \tag{3.15}$$

$$\frac{dT}{dz} = -T\left[i\Lambda(z) - \alpha(z)(I - R(z))\right]. \tag{3.16}$$

A different operator marching scheme is based on the Dirichlet-to-Neumann (DtN) map Q and the Fundamental Solution (FS) operator Y [14]. These two operators are defined at a fixed z by

$$Q(z)u(\cdot, z) = \partial_z u(\cdot, z), \quad Y(z)u(\cdot, z) = u(\cdot, a), \tag{3.17}$$

for all solutions of the Helmholtz equation (2.15) (with $u = E_y$) satisfying the outgoing wave condition for $z > a$. Therefore, we have

$$Q(a) = i\sqrt{\partial_x^2 + k_0^2 n^2(x, a+)}, \quad Y(a) = I. \tag{3.18}$$

For a piecewise z-invariant structure described earlier, we have the following marching formulas from z_j to z_{j-1} [15]:

$$\Lambda_j = \sqrt{\partial_x^2 + k_0^2 n_j^2(x)}, \qquad P_j = \exp(i(z_j - z_{j-1})\Lambda_j), \tag{3.19}$$

$$C = [i\Lambda_j + Q(z_j)]^{-1}[i\Lambda_j - Q(z_j)], \qquad D = P_j C P_j, \tag{3.20}$$

$$Q(z_{j-1}) = i\Lambda_j (I - D)(I + D)^{-1}, \qquad Y(z_{j-1}) = Y(z_j)(I + C)P_j(I + D)^{-1}. \tag{3.21}$$

In a more general setting, we may allow the refractive index n to vary with z for $z_{j-1} < z < z_j$. In that case, we can find the marching formulas using a solution operator for this segment. If the Helmholtz equation has a unique solution in $z \in (z_{j-1}, z_j)$ for any given Dirichlet boundary conditions at $z = z_{j-1}$ and $z = z_j$, then we can find the Dirichlet-to-Neumann map M of this segment, such that

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

If the operator M is partitioned as 2×2 blocks, we can easily derive the following

$$Q(z_{j-1}) = M_{11} + M_{12}[Q(z_j) - M_{22}]^{-1} M_{21}, \tag{3.22}$$

$$Y(z_{j-1}) = Y(z_j)[Q(z_j) - M_{22}]^{-1} M_{21}. \tag{3.23}$$

The continuous formulation based on the DtN and FS operators was developed in [14]. We have the following differential equations for Q and Y:

$$\frac{dQ}{dz} = -Q^2 - [\partial_x^2 + k_0^2 n^2(x, z)], \tag{3.24}$$

$$\frac{dY}{dz} = -YQ. \tag{3.25}$$

The operators Q and Y may fail to exist at some particular values of z. In that case, we can use the Neumann-to-Dirichlet map or the more general Robin-to-Dirichlet (RtD) map J. For a constant α, the RtD map is defined by

$$J\left(\frac{\partial u}{\partial z} - \alpha u\right) = u$$

for all solutions of the Helmholtz equation satisfying the outgoing wave condition for $z > a$. Similar to the operator Y, we need the operator W given by

$$W\left(\frac{\partial u}{\partial z} - \alpha u\right) = u|_{z=a}.$$

The marching formulas for J and W can be similarly derived. There are also simple formulas that switches between (Q, Y) and (J, W).

In a practical implementation, the operators must be represented by matrices. If we discretize the transverse operators by a finite difference or a finite element method, we obtain matrix approximations of the operators. However, these matrices tend to be very large. On the other hand, it is often much more efficient when the operator marching schemes are used with a local eigenfunction expansion.

4 Local eigenfunction expansion

One of the most widely used methods for modeling optical waveguides is the mode matching method [16–18]. The method is particularly suitable for 2-D piecewise z-invariant wave-guiding structures. Consider the TE case and the piecewise uniform structure defined in Section 3. For $z_{j-1} < z < z_j$, the wave field can be decomposed as forward and backward components and expanded in the eigenfunctions of the transverse operator, i.e., $\partial_x^2 + k_0^2 n_j^2(x)$, with unknown coefficients. The method completely avoids a discretization of z in the interval (z_{j-1}, z_j). A set of equations for the coefficients in all z-invariant segments can be established by the continuities of u and u_z (again for (2.15)) and the boundary conditions at $z = 0-$ and $z = a+$. For a continuously z-varying structure, a discretization in z is necessary. If z_0, z_1, ..., z_m are the discretization points, we can approximate the refractive index in each segment by its midpoint value:

$$n(x, z) \approx n\left(x, \frac{z_{j-1} + z_j}{2}\right) = n_j(x), \quad z_{j-1} < z < z_j. \tag{4.1}$$

For a slowly varying waveguide, n varies with z slowly, the grid size in z can be relatively large.

For open waveguides where the transverse variables are unbounded, the PML technique has been applied to the mode matching method [20]. When the transverse variable x is terminated by a PML [19, 20], the set of eigenfunctions of the transverse operator is discrete. A number of methods are available to compute the eigenmodes in the presence of a PML [21–26]. If the wave-guiding structure has a large length in the propagation direction (i.e. a large a), the operator marching techniques are useful. Earlier mode matching methods [17, 18] for optical waveguides are developed based on the "transfer matrix" operator and they suffer from numerical instability. Stable mode matching schemes can be developed in connection with a scattering operator [19] or a DtN-FS formalism [14, 15]. Consider a z-invariant segment $z_{j-1} < z < z_j$, let $\{\phi_k^{(j)},\ k = 1, 2, ...\}$ be the eigenfunctions of the transverse operator modified by the PML, we can expand the function $R(z)\phi_k^{(j)}$, where $R(z)$ is the reflection operator, as

$$R(z)\,\phi_k^{(j)} = \sum_{l=1}^{\infty} r_{lk}\,\phi_l^{(j)}.$$

The matrix (r_{lk}) can be truncated and used to represent the operator R. For the transmission operator, we have

$$T(z)\,\phi_k^{(j)} = \sum_{l=1}^{\infty} t_{lk}\,\phi_l^{(m+1)},$$

where $\phi_l^{(m+1)}$ $(k = 1,\ 2,\ ...)$ are the eigenfunctions of the transverse operator for $z > a$. Matrix representations of Q and Y are similarly defined.

The mode matching method is particularly advantageous for 2-D waveguides with a piecewise constant refractive index profile. In that case, the eigenfunctions have piecewise analytic formulas while the eigenvalues can be solved from a single nonlinear equation. Unfortunately, for 3-D waveguides without rotation symmetry, analytic solutions are not available. A large number of modes are often needed in the mode expansion method, but computing the eigenmodes in each segment becomes a prohibitive task. Nevertheless, the mode matching method can still be useful if many of the segments are identical.

5 One-way models

One-way models are widely used for modeling wave propagation in slowly varying waveguides. They are derived as approximations to the original governing equations and they involve only first order derivatives in the propagation direction z and can be efficiently solved as "initial value problems" by marching forward in z. For underwater acoustics, the first one-way model was introduced by Tappert [27] in the 70's. At about the same time, a similar model was introduced by Feit and Fleck [28] for optical waveguides. A more accurate one-way model was introduced later by Clarebout [29] for geophysical applications and Greene [30] for underwater acoustics. These one-way models for field propagation are actually closely related to the one-way operator introduced by Engquist and Majda [31,32] for terminating unbounded domains. The higher order one-way models based on the diagonal Padé approximants of the square root operator were developed by Zhang [33] and Bamberger et al [34]. They were applied to underwater acoustics by Collins [35] and to optics by Hadley [36]. For historical reasons, the one-way modeling techniques are called Parabolic Equation (PE) method and Beam Propagation Method (BPM) in acoustics and optics, respectively.

We consider the Helmholtz equation (2.15) for the TE polarization. If the waveguide is z-invariant, we have a decomposition $u = u^+ + u^-$, where $u = E_y$. The forward component u^+ satisfy $\partial_z u^+ = i\Lambda u^+$ exactly, where $\Lambda = \sqrt{\partial_x^2 + k_0^2 n^2}$ is the square root operator. For a slowly varying waveguide, $n = n(x, z)$ changes with z slowly. If we are interested in waves that propagate in the positive z direction, we approximate the original Helmholtz equation (2.15) by the following ideal one-way model:

$$\partial_z u = i\Lambda\, u. \tag{5.1}$$

The above is often called the one-way Helmholtz equation. Since n depends on z, so does the operator Λ. Compared with the original Helmholtz equation (2.15), the ideal one-way equation (5.1) is easier to solve, because it gives rise to an "initial value problem" in z. This is true, especially when the square root operator is properly approximated.

For the transverse magnetic polarization, the ideal one-way model can also be written as (5.1), if we let

$$u = H_y, \quad \Lambda = \sqrt{n^2\partial_x(n^{-2}\partial_x\cdot) + k_0^2 n^2}. \tag{5.2}$$

For 3-D waveguides, we can use the transverse components of the electric or magnetic fields. If the transverse components of E are used, we have the one-way equation (5.1) with

$$u = E_t, \quad \Lambda = \sqrt{\mathcal{L}}, \tag{5.3}$$

where $\mathcal{L}$ is given in (2.9). Similarly, if we use the transverse magnetic components, we need to define

$$u = H_t, \quad \Lambda = \sqrt{\mathcal{M}}, \tag{5.4}$$

for $\mathcal{M}$ given in (2.10). One-way models based on (5.1) and (5.3) or (5.4) give rise to the full-vectorial beam propagation methods [50].

For practical numerical implementations, it is expensive to evaluate Λ rigorously using its definition by the spectral decomposition. Instead, we use various approximations. Consider the 2-D TE case again, we introduce a reference refractive index n_*, such that

$$\partial_x^2 + k_0^2 n^2(x, z) = k_0^2 n_*^2 (1 + X), \quad X = \frac{1}{k_0^2 n_*^2}\partial_x^2 + \frac{n^2}{n_*^2} - 1. \tag{5.5}$$

Therefore, $\Lambda = k_0 n_* \sqrt{1 + X}$. If can let $u = v e^{ik_0 n_* z}$, then

$$\frac{\partial v}{\partial z} = ik_0 n_* (\sqrt{1 + X} - 1)\, v. \tag{5.6}$$

The simplest approximation is

$$\sqrt{1 + X} - 1 \approx \frac{X}{2}. \tag{5.7}$$

This is the paraxial approximation which gives rise to the early one-way models [27, 28]. More accurate one-way models are derived from the $[p/p]$ Padé approximants:

$$\sqrt{1+X}-1 \approx \sum_{l=1}^{p} \frac{a_l X}{1+b_l X}, \tag{5.8}$$

where p is a positive integer and a_l, b_l are given explicitly as follows:

$$a_l = \frac{2}{2p+1}\sin^2\theta_l, \quad b_l = \cos^2\theta_l \quad \text{for} \quad \theta_l = \frac{l\pi}{2p+1}. \tag{5.9}$$

The case $p=1$ was first proposed by Claerbout [29]. The general case corresponds to the higher order one-way models developed in [33–36].

While we can insert (5.8) into (5.1) and try to solve the resulting equation by operator-splitting and Crank-Nicolson's method, Collins [37] realized that it is more efficient to approximate the one-way propagator directly. Consider the step from z_0 to $z_1 = z_0 + \Delta z$ (of course, the other steps are similar), we can formally solve (5.6) by

$$v_1 = P\, v_0, \quad P = P(X) = e^{is(\sqrt{1+X}-1)} \quad \text{for} \quad s = k_0 n_* \Delta z, \tag{5.10}$$

where $P(X)$ is the one-way propagator (exponential of the square root operator) and X is evaluated at $z = z_{1/2} = z_0 + \Delta z/2$. Collins' idea is to approximate $P(X)$ directly by a rational function of X. For example, if we have

$$P(X) \approx c_0 + \sum_{l=1}^{p} \frac{c_l}{X+d_l} \tag{5.11}$$

(the coefficients depend on s and an integer p), then

$$v_1 = c_0 v_0 + \sum_{l=1}^{p} c_l w_l, \tag{5.12}$$

where w_l can be solved from

$$(X+d_l) w_l = v_0. \tag{5.13}$$

For 2-D waveguides (both TE and TM cases), solving w_l from (5.13) is extremely simple. Since the operator X involves derivatives only in x, its discretization leads to a simple banded matrix. For the full-vectorial BPM, X is a 2×2 operator matrix involving partial derivatives in both x and y and it becomes expensive to solve w_l from (5.13). One possibility is to use the iterative ADI (alternating direction implicit) method developed in [53]. On the other hand, the full-vectorial paraxial model can be efficiently solved with a non-iterative ADI scheme [51, 52]. For this reason, the paraxial full vector BPM is still widely used.

In a z-invariant waveguide, the evanescent waves (corresponding to eigenvalues of X that are less than -1) should decay as z increases. However, in the paraxial approximation (5.7) or a diagonal Padé approximation of $\sqrt{1+X}$, the evanescent waves will be incorrectly propagated. Since the coefficients in (5.9) are real, $\sqrt{1+\mu}$, for $\mu < -1$, will be approximated by a real number using (5.8). For slowly varying waveguides, the evanescent waves are not very important, but they should certainly be damped. This issue, first realized by Wetton and Brooke [38], becomes more serious for one-way modeling using the elastic wave equations [38] and the full vector Maxwell's equations [50]. For example, the operators $\mathcal{L}$ and $\mathcal{M}$ are not self-adjoint and there may be pairs of complex conjugate eigenvalues [6]. Using the paraxial or the diagonal Padé approximants, one of the complex eigenvalues will always increase exponentially in z and this leads to instability. To damp the evanescent waves, we can develop complex coefficient rational approximants of $\sqrt{1+X}$. A rotating branch-cut procedure was developed in [39], but it does not always give rise to stable one-way models. A modified Padé procedure that gives rise to truly stable one-way models was developed in [40].

For the propagator-based one-way models (5.11), (5.12), (5.13), we also have the difficulty with the evanescent waves. If we use a diagonal Padé approximant of $P(X)$, the evanescent waves will again be incorrectly propagated. For elastic wave equations and the full-vectorial Maxwell's equations, the complex modes give rise to instabilities. Since the propagator-based one-way models are more efficient, it is important to develop stable rational approximants of P that are accurate for the forward propagating waves, but can also suppress the evanescent waves and complex modes. Yevick [41] developed some approximants of $P(X)$ in connection with the approximants of $\sqrt{1+X}$ in [39] and [40]. In [42], it is shown that we can use the $[(p-1)/p]$ Padé approximants of $P(X)$. To avoid too much damping (especially when p is small), it was proposed in [43] to use a rational approximation that connects the $[(p-1)/p]$ and $[p/p]$ Padé approximants. Similar to the θ-method (for the heat equation) which combines the backward Euler method with the Crank-Nicolson method, a parameter θ is introduced for connecting the two rational approximants of $P(X)$. More precisely, let $R_{p-1,p}$ and $R_{p,p}$ be the $[(p-1)/p]$ and $[p/p]$ Padé approximants of $P = e^{is(\sqrt{1+X}-1)}$ given by

$$R_{p,p}(X) = \frac{F_p(X)}{G_p(X)}, \quad R_{p-1,p}(X) = \frac{S_{p-1}(X)}{T_p(X)}, \tag{5.14}$$

where S_{p-1} is a polynomial of degree $p-1$, F_p, G_p and T_p are polynomials of degree p. We assume that the four polynomials are scaled such that they all equal 1 at $X = 0$. Then, we approximate $P(X)$ by the following rational function of X:

$$R_p(X;\theta) = \frac{(1-\theta)S_{p-1}(X) + \theta F_p(X)}{(1-\theta)T_p(X) + \theta G_p(X)}. \tag{5.15}$$

For practical use, we re-write $R_p(X;\theta)$ as the right hand side of (5.11) with suitable coefficients.

Notice that the one-way Helmholtz equation (5.1) is only an approximation of the Helmholtz equation (2.15) when n varies with z slowly. It is desirable to develop one-way models that are more accurate than (5.1), but are still easy to solve. To understand the limitation of (5.1), we consider the simplest 1-D model. Let the exact equation be the 1-D Helmholtz equation

$$\frac{d^2u}{dz^2} + k_0^2 n^2(z) u = 0, \tag{5.16}$$

then, the one-way Helmholtz equation corresponds to the following first order ODE:

$$\frac{du}{dz} = ik_0 n(z) u. \tag{5.17}$$

The exact solution of the above is

$$u(z) = u(0) e^{ik_0 \int_0^z n(\xi) d\xi}.$$

For Eq. (5.16), we do not have a general expression for its solutions, but a WKB analysis gives rise to the following approximate solution:

$$u(z) \approx u(0) \sqrt{\frac{n(0)}{n(z)}} e^{ik_0 \int_0^z n(\xi) d\xi}.$$

Notice that

$$|u(z)| \approx |u(0)| \sqrt{\frac{n(0)}{n(z)}}.$$

This is very different from the solution of (5.17) which satisfies $|u(z)| = |u(0)|$.

To improve the accuracy of BPM, two different approaches can be used. The first is to use the so-called energy-conserving improvement [44–47]. The idea is to solve

$$\phi = \sqrt[4]{\partial_x^2 + k_0^2 n^2(x,z)}\, u$$

assuming that ϕ satisfies the one-way Helmholtz equation

$$\partial_z \phi = i\Lambda\, \phi.$$

In terms of the original function u, we have

$$\partial_z u = \left(i\Lambda - \Lambda^{-1/2} \frac{d\sqrt{\Lambda}}{dz} \right) u. \tag{5.18}$$

Another approach is to use the single scatter approximation. The original idea of single scatter approximation was introduced for 1-D Helmholtz equation by Bremmer in the 50's. It has been used in a discrete form by some authors to improve the BPM. A continuous version of the single scatter approximation has been developed [48, 49]. This implies that we solve u from

$$\partial_z u = \left[i\Lambda(z) - \frac{1}{2}\Lambda^{-1}(z)\Lambda'(z) \right] \; u. \tag{5.19}$$

Although it does not look very simple, this equation can be discretized with a suitable operator rational approximation. The improved one-way models are also available for the TM case. Unfortunately, they are not available for full-vectorial cases.

6 Bidirectional beam propagation method

Optical wave-guiding structures that are piecewise uniform in z are important, because they correspond to actual fabricated photonic devices, such as waveguide gratings. Due to the discontinuity of the refractive index function at multiple values of z, reflections are important for these structures and the traditional BPM one-way models that ignore reflections are not suitable. The mode matching method [17–19] is a good choice for such a structure, but the bidirectional beam propagation method (BiBPM) is often more efficient.

Let us first consider a single waveguide discontinuity at $z = 0$ for TE polarized waves. Such a discontinuity can be the end facet of an optical waveguide or the junction between two different waveguides. We assume $n(x,z) = n_0(x)$ for $z < 0$ and $n(x,z) = n_1(x)$ for $z > 0$. If the mode matching method is used, the eigenmodes of the transverse operator (modified with a PML) must be calculated. On the other hand, BiBPM applies rational approximation techniques developed for traditional BPM in an iterative scheme for solving the reflection and transmission at the discontinuity. If an incident wave $u^{(i)}$ is given for $z < 0$, the reflected wave and the transmitted wave satisfy

$$(\Lambda_0 + \Lambda_1)u^{(r)}|_{z=0-} = (\Lambda_0 - \Lambda_1)u^{(i)}|_{z=0-}, \tag{6.1}$$

$$(\Lambda_0 + \Lambda_1)u^{(t)}|_{z=0+} = 2\Lambda_0 u^{(i)}|_{z=0-}. \tag{6.2}$$

When x is discretized, say by N points, the transverse operator $\partial_x^2 + k_0^2 n_j^2$ is approximated by a sparse matrix, but the square root operator Λ_j can only be approximated by a dense matrix. With an eigenvalue decomposition of the transverse operator, a matrix approximation of the square root operator Λ_j can actually be written down, but the computation is expensive, since the required number of operations is $\mathcal{O}(N^3)$. A much more efficient approach is to use rational approximations for the square root operator as in the beam propagation method. For a reference refractive index n_*, we write Λ_j as $\Lambda_j = k_0 n_* \sqrt{1 + X_j}$ for an operator X_j, then approximate $\sqrt{1 + X_j}$ by a rational function of X_j. This leads to

$$\Lambda_j \approx S_j = k_0 n_* a_0 \prod_{k=1}^{p} \frac{1 + c_k X_j}{1 + b_k X_j}.$$

The coefficients a_0, b_k, c_k above depend on the degree p and other parameters. Therefore, the equation for $u^{(r)}|_{z=0-}$ can be approximated by

$$(S_0 + S_1)u^{(r)} = (S_0 - S_1)u^{(i)}. \tag{6.3}$$

Since X_j is approximated by a sparse matrix, the action of S_j or S_j^{-1} on a given function of x can be efficiently evaluated. A number of iterative schemes are developed in [54], [55] and [56]. To speed up the convergence, we can multiply (6.3) by S_0^{-1} or S_1^{-1} or $S_{1/2}^{-1}$, then use a Krylov subspace iterative method [57]. Here, $S_{1/2}$ is a rational approximant of $\sqrt{\partial_x^2 + k_0^2 n_{1/2}^2}$ for $n_{1/2}^2 = (n_0^2 + n_1^2)/2$.

Consider a piecewise z-invariant structure given by $0 = z_0 < z_1 < ... < z_m = a$, where z_j is a longitudinal discontinuity of the refractive index function. The BiBPMs are designed to take advantage of the z-independence in each segment by using operator rational approximations as in the traditional BPM. BiBPMs are first proposed based on the transfer matrix operator [58, 59], but these methods are numerically unstable, unless the evanescent modes are intentionally treated incorrectly. However, the evanescent modes are excited at the longitudinal discontinuities and a correct modeling of these modes is essential to the accuracy of the simulation results. A stable BiBPM [60, 61] was developed based on the scattering operators. The idea is to use rational approximants of the square root operators Λ_j and Λ_{j+1} to speed up the computation of operator C in (3.5), and similarly, to use a rational approximant of one-way propagator P_j in (3.8) to speed up the calculations of $R(z_{j-1}+)$ and $T(z_{j-1}+)$ in (3.9) and (3.10). Stable rational approximants for the square root operator and the one-way propagator that suppress the evanescent modes can be used. Although the method still requires manipulations of matrices representing the scattering operators, it is much more efficient than a direct method that computes the square root operator and the one-way propagator by an eigenvalue decomposition of the transverse operator. Compared with the mode matching method, the scattering operator BiBPM is highly competitive. Another BiBPM [62] was developed based on iteratively solving a linear system for wave field components at the longitudinal discontinuities. At a discontinuity z_j, we have four unknown functions $u^+(\cdot, z_j+)$, $u^+(\cdot, z_j-)$, $u^-(\cdot, z_j+)$ and $u^-(\cdot, z_j-)$. It turns out that we can eliminate two of them and setup a system for $u^+(\cdot, z_j-)$ and $u^-(\cdot, z_j+)$ at all longitudinal discontinuities. The coefficient matrix is sparse and its non-zero entries are related to the square root operators Λ_j and the one-way propagator P_j, but these operators need not be explicitly formed. If a Krylov subspace method is used to solve this system, we only need to find the multiplication of the coefficient matrix with a given vector in each iteration. This can be reduced to the actions of P_j and $(\Lambda_j + \Lambda_{j+1})^{-1}$ on given functions. The action of P_j can be efficiently evaluated by its rational approximant. The action of $(\Lambda_j + \Lambda_{j+1})^{-1}$ is closely related to the scattering problem at a single waveguide discontinuity and it can also be efficiently evaluated using the iterative method described earlier in this section. This iterative BiBPM can be very efficient if the structure does not vary too much between different segments. Unfortunately, the method may fail to converge if the refractive index profiles of segments are very different.

More efforts are needed for 3-D wave-guiding structures with longitudinal discontinuities. Even for a single waveguide discontinuity, an efficient and rigorous 3-D full-vectorial treatment is not available.

7 Higher order operator marching methods

As we have seen in Section 3, it is possible to reformulate the propagation problem in waveguides as initial value problems for a pair of operators. Marching formulas for the scattering operators R and T, or the DtN map Q and FS operator Y are given in Section 3. In this section, we present some higher order marching formulas for slowly varying waveguides.

For structures such as a taper, a Y-branch, a S-bend and waveguide couplers, the refractive index varies with z continuously (at least in part of the structure). In this case, it is necessary to approximate the z-varying structure by a piecewise z-invariant structure. In the segment from z_j to $z_{j+1} = z_j + \Delta z$, the refractive index profile $n(x,z)$ is usually replaced by its profile at the midpoint. That is, $n(x,z) \approx n_{j+1/2}(x) = n(x, z_{j+1/2})$, where $z_{j+1/2} = z_j + \Delta z/2$. This introduces a second order error in the solution. Therefore, it is necessary to use a relatively small Δz to maintain the overall accuracy of the solution. Notice that the second order error of the piecewise z-invariant approximation is very different from the error in a second order finite difference (or finite element) method for solving the Helmholtz equation directly. In the latter case, the error exists even when the structure is actually z-invariant. A number of fourth order (in z) methods have been developed based on the DtN and FS formalism. These fourth order methods have a similar advantage as the second order piecewise uniform approximation, namely, the errors are small when the variation in z is weak.

Consider the Helmholtz equation for the TE polarization, it can be written as a first order system

$$\frac{\partial}{\partial z}\begin{bmatrix} u \\ \partial_z u \end{bmatrix} = A(z)\begin{bmatrix} u \\ \partial_z u \end{bmatrix}, \quad A(z) = \begin{bmatrix} 0 & 1 \\ -\partial_x^2 - k_0^2 n^2(x,z) & 0 \end{bmatrix}, \tag{7.1}$$

where $u = E_y$ is the y-component of the electric field. Although the above system is unstable if it is solved as an initial value problem in z, we can use it to derive relationships between the Q and Y operators at z_j and z_{j-1}, and then propagate the operators from $z = a+$ to $z = 0-$. In fact, the second order marching formulas (3.19-3.21) are related to the following second order mid-point exponential method for (7.1):

$$\begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_j} = e^{\Delta z\, A_{j-1/2}} \begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_{j-1}}, \tag{7.2}$$

where $A_{j-1/2} = A(z_{j-1/2})$. Now, instead of (7.2), we can use other higher order exponential methods [63]. The fourth order operator marching scheme developed in [15] was derived from the following fourth order exponential method:

$$\begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_j} = Q^{-1}PQ \begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_{j-1}}, \quad P = e^{\Delta z\, A_{j-1/2} + \frac{\Delta z^3}{24} A''_{j-1/2}}, \; Q = e^{-\frac{\Delta z^2}{12} A'_{j-1/2}}, \tag{7.3}$$

where $A'_{j-1/2} = A'(z_{j-1/2})$, etc. The derivatives A' and A'' can also be avoided [64]. Another possibility is to use an approximate Magnus method [65]. The operator marching method in [66] was derived from the following fourth order Magnus method [67]:

$$\begin{aligned} \begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_j} &= e^{\Omega_j} \begin{bmatrix} u \\ \partial_z u \end{bmatrix}_{z=z_{j-1}}, \\ \Omega_j &= \frac{\Delta z}{2}(A_{j,1} + A_{j,2}) + \frac{\sqrt{3}\Delta z^2}{12}(A_{j,2}A_{j,1} - A_{j,1}A_{j,2}), \end{aligned} \tag{7.4}$$

where

$$A_{j,k} = A(z_{j-1} + c_k \Delta z) \quad \text{for} \quad k = 1,2 \quad \text{and} \quad c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \quad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}.$$

In [15] and [66], the fourth order operator marching methods are implemented with a local eigenfunction expansion and they give more accurate solutions with very little computing overhead. These methods are suitable for continuously z-varying waveguides.

8 Concluding remarks

For modeling and simulation of lightwaves propagating in optical wave-guiding structures, we have identified three key ideas. The first is to reformulate the boundary value problem (of the frequency domain propagation problem) as initial value problems for a pair of operators and march these operators along the waveguide axis. The second is to approximate the square root operator or the exponential of the square root operator by rational functions of the transverse differential operator for efficient propagation of one-way wave field components. The third idea is to use a local eigenfunction expansion for writing down the wave fields in each z-invariant segments. These ideas give rise to some powerful methods for simulating waves propagating in slowly varying waveguides and piecewise z-invariant structures. However, much work is still needed for 3-D wave-guiding structures. In the 3-D case, the wide-angle full-vectorial BPM is relatively inefficient and improved one-way models have not been developed yet. For a 3-D waveguide discontinuity, an efficient full-vectorial treatment is still lacking and the mode matching method becomes much too expensive. Since 3-D waveguides are the fundamental building blocks of integrated photonic circuits, it is clearly important to develop more efficient simulation tools for lightwave propagation in these structures.

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