A Unified Mode Solver for Optical Waveguides Based on Mapped Barycentric Rational Chebyshev Differentiation Matrix

Jianxin Zhu, Xuecang Zhang, and Rencheng Song

***Abstract*—A unified high-accuracy mode solver is proposed to compute the modes of planar optical waveguides. The advantage of this solver is composed of three aspects. The first is the high accuracy of mapped barycentric rational Chebyshev differentiation matrix (MBRCDM) for approximating differential operator. The second is the high efficiency of multidirectional Newton iteration for root finding on complex plane. The third is the outstanding performance of perfectly matched layer (PML) as an absorbing boundary condition (BC). Specifically, MBRCDM method is accurate enough to compute as many modes as necessary for waveguides bounded with regular Robin BCs. MBRCDM-PML method, where PML is used to truncate an unbounded waveguide followed by the MBRCDM method, performs very well. MBRCDM-Newton method, where multidirectional Newton iteration for a dispersion equation is implemented with some initial values obtained by MBRCDM method, is more efficient. By this combined solver, a large number of accurate modes can be easily calculated. This solver is particularly essential for the computing of high index modes.**

***Index Terms*—Leaky modes, Newton iteration, optical waveguide, perfectly matched layer (PML), propagation constant, spectral differentiation matrix.**

I. Introduction

THE determination of a large number of propagation constants (or modes), especially the high-index complex propagation constants, plays an important role in many wave propagation analysis. More detail discussions about this subject refer to [1]–[5] and the references therein. For some waveguides, there are algebraic dispersion relations of the form $f(\beta) = 0$, where β is the propagation constant. But, it is usually impossible to get an explicit analytic formula of β. And the common root solvers are inefficient for the complex β. For other waveguides, there are even no such dispersion equations. Thus, the development of numerical methods for the computation of propagation constants is essentially important. In fact, the accurate and efficient calculation of high modes is still an open issue. [4].

Manuscript received December 20, 2009; revised March 31, 2010; accepted April 04, 2010. Date of publication April 22, 2010; date of current version May 31, 2010. This work was supported by the Natural Science Foundation of China under Grant 10571162 and in part by the Natural Science Foundation of Zhejiang Province under Grant Y605181.

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Digital Object Identifier 10.1109/JLT.2010.2048891

Most numerical methods can be classified into two sets. The first set are based on the dispersion equations. It usually starts with a valid initial guess followed by the iterative procedure [4], [6], [7] or the noniterative procedure [8]–[13]. Asymptotic approximations, such as asymptotic expansion, Wentzel–Kramers–Brillouin method, etc. [2], [4], [14], [16], are preferable methods to get a good initial guess. For some waveguides, even the asymptotic expansion is accurate enough to approximate some high modes [16]. But their validation is limited to some special structures where an asymptotic analysis works. The Newton iteration is very inefficient for root finding on complex domain. Even worse is that the numerical evaluation of $f(\beta)$ may be unstable due to its sophisticated mathematical structure.

The second set are of course the dispersion equations independent. They are more straightforward numerical methods, which discretize the original governing differential eigenvalue equation into a matrix eigenvalue problem. Three mainstream of them are finite difference (FD), finite element (FE), and spectral methods [5], [18]–[23]. FD and FE have a long history in the numerical analysis of waveguides. They construct generalized matrix eigenvalue problem with low-order accuracy. Due to their low-order accuracy, a very large matrix or a multiple iteration technique [24], [25] is needed to achieve a given precision. This is very time consuming. Even if we can find all the accurate eigenvalues of this large generalized matrix eigenvalue problem, most of them are actually not the modes of the original problem. In fact, only the low-index eigenvalues are the corresponding modes of the waveguide; the higher index eigenvalues are totally way off. It is known as the spurious modes phenomenon of these low-order accuracy methods [26]. A spurious mode is the kind of eigenvalue, which is accurate for matrix eigenvalue problem but not a physically meaningful mode. Spectral methods, known for their high accuracy in discretizing differential equation, come to be preferable for approximating the modes of differential operator [18], [22], [27]–[29]. These pseudospectral methods produce higher accuracy results than FD and FE methods. But as we will show, they still produce a few meaningless spurious modes. They are still not so accurate and efficient.

In this paper, we propose two methods based on spectral differentiation matrix to unify the merits of the existing methods. Spectral differentiation matrix is the discrete approximation of differential operator by spectral methods. The accuracy of this approximation is mainly determined by which spectral method we use and how we handle the boundary conditions (BCs). The

state-of-the-art pseudospectral method we will use is first proposed for boundary value problem by Berrut *et al.* [30]–[33] and further developed for the time-dependent problem in [34]. In this new pseudospectral method, the conformal mapping technique is employed to redistribute the collocation points, and the barycentric rational interpolation is used to replace the Lagrange interpolation. Consequently, a better conditioned differentiation matrix with higher accuracy is obtained to approximate a differential operator on finite domain. Furthermore, if the BCs are regular Robin type, then they can also be easily discretized by this pseudospectral method without additional treatment. Combining the discretized differential equation and BCs, we get a final spectral differentiation matrix to approximate the differential operator. We will call it the mapped barycentric rational Chebyshev differentiation matrix (MBRCDM).

But most waveguides are open. That is, their BCs are regular Robin type at the infinite or the nonlinear radiation BCs on finite domain. MBRCDM method cannot be directly used for both cases to get a standard matrix eigenvalue problem. Two new methods, MBRCDM-Newton and MBRCDM-perfectly matched layer (PML), are proposed to solve this kind of problems. These two methods are corresponding to the two sets of the existing methods we have mentioned. MBRCDM-Newton method uses MBRCDM of a simplified problem to get rough initial values for multidirectional newton iteration. It is dispersion equation dependent. MBRCDM-PML method uses PMLs to truncate the unbounded domain into a finite computational domain. Then MBRCDM method is employed.

For multilayered waveguide problems with strongly discontinuous refractive index profile (RIP) interfaces, domain decomposition method is suggested [21], [35], [37]. In each layer, the MBRCDM method is used with a proper treatment of interface conditions, just like the handling of regular BCs. The MBRCDMs of each layer can be finally combined into a overall spectral differentiation matrix, which approximates the differential operator of the multilayered waveguide problem.

This paper is organized as follows. In Section II, the basic ideas of the direct MBRCDM, MBRCDM-Newton, and MBRCDM-PML methods are discussed in details. In Section III, extensive numerical examples are given to validate the high efficiency, high accuracy, and simplicity of the proposed methods. The last section will be the conclusion.

II. Formulas and Methods

A. Mathematical Model of Waveguide

We consider a single-layer planar waveguide with x as the transverse direction and z as the propagating direction, specified by RIP $n(x,z)$. The frequency domain Maxwell equations governing the time harmonic (time dependent by $e^{-i\omega t}$) wave propagation in this dielectric planar waveguide can be reduced to the following 2-D Helmholtz equation

$$\rho\frac{\partial E}{\partial x}\left(\frac{1}{\rho}\frac{\partial E}{\partial x}\right)+\rho\frac{\partial E}{\partial z}\left(\frac{1}{\rho}\frac{\partial E}{\partial z}\right)+k_0^2n^2(x,z)E=0 \quad (1)$$

where k_0 is free-space wavenumber. For the TE polarization, E is the y-component of electric field and $\rho=1$. For the TM polarization, E is the y-component of magnetic field and $\rho=n^2$. For simplicity, we focus on TE case. The idea is similar in TM case. RIP is usually z-independent in waveguide. According to continuous translational symmetry in the z-direction, the general solution of (1) has the form

$$E=u(x)e^{i\beta z} \quad (2)$$

where β is the propagation constant. Substitute (2) into (1), we get

$$Lu=\left[\frac{d^2}{dx^2}+k_0^2n^2(x)\right]u(x)=\beta^2u(x). \quad (3)$$

This equation, subject to specific BCs in x-direction, is the general eigenvalue problem in waveguide. Both β and $u(x)$ need to be determined. For multilayered waveguide, the governing equation in the interior of each layer is the same as (3). On the interface, specific interface conditions are satisfied.

B. Mapped Barycentric Rational Chebyshev Differentiation Matrix

Consider (3) with $x\in[-1,1]$ and imposed the following regular Robin BCs:

$$a_1u(-1)+b_1u'(-1)=0 \quad (4)$$

$$a_2u(1)+b_2u'(1)=0 \quad (5)$$

where a_i,b_i $(i=1,2)$ are constant. Using pseudospectral method [27], [28], we expand the solution $u(x)$ of (3), (4), and (5) into an infinite series of Chebyshev polynomials, then truncate it into N terms

$$u_N(x)=\sum_{k=0}^{N}\hat{u}_kT_k(x) \quad (6)$$

where $T_k(x)=\cos(k\cos^{-1}x), k=0,1,2,\ldots,N$, is the first kind Chebyshev polynomial of degree k. The expansion coefficients $\hat{u}_k, k=0,\ldots,N$ are determined by asking $u_N(x)$ to coincide with $u(x)$ at the Chebyshev--Gauss--Lobatto (CGL) collocation points $x_i=\cos\pi i/N, i=0,\ldots,N$. Therefore, the polynomial of degree N defined by (6) is just the Lagrange interpolation polynomial based on CGL points. Hence, an equivalent form of (6) is

$$u_N(x)=\sum_{k=0}^{N}L_k(x)u(x_k) \quad (7)$$

with $u_N(x_k)=u(x_k)$, and $L_k(x)$ is the Lagrange basis polynomial of degree *N* defined by

$$L_k(x)=\frac{(-1)^{k+1}(1-x^2)T_N'(x)}{\bar{c}_kN^2(x-x_k)} \quad (8)$$

where $\bar{c}_0=\bar{c}_N=2,\bar{c}_k=1$ for $1\le k\le N-1$, and $L_k(x_l)=\delta_{kl},\delta_{kl}$ is the Kronecker delta. In the context of (7),

which does not involve the expansion coefficients $\hat{u}_k$, the unknowns are the grid values $u(x_k)$. Differentiate both sides of (7) at CGL points and use the properties of Chebyshev polynomial. We can express the derivatives at CGL points in terms of the grid values $u(x_i)$. That is, the pth derivatives

$$u_N^{(p)}(x_i) = \sum_{j=0}^{N} d_{i,j}^{(p)} u_N(x_j), \qquad i = 0, \ldots, N \tag{9}$$

where the coefficients $d_{i,j}^{(p)} = L_j^{(p)}(x_i)$, which can be evaluated explicitly from expression (8). Very efficient MATLAB programs for this evaluation have been developed by Weideman and Reddy[38] and Trefethen *et al.*[41]. Comparing to the existing ways of treating pseudospectral methods for waveguide eigenvalue problem [18], [22], [29], we use a more elaborate way by the notation of differentiation matrix [27], [28]. Define the pth-order Chebyshev differentiation matrix (CDM) $D^{(p)}$ as

$$D^{(p)} = \left(d_{i,j}^{(p)}\right). \tag{10}$$

Let $D = D^{(1)}$, it is easy to see $D^{(p)} = D^p$. In vector notation, (9) may be expressed as

$$U^{(p)} = D^p U \tag{11}$$

where $U^{(p)} = (u_N^{(p)}(x_0), \ldots, u_N^{(p)}(x_N))^T, U = U^{(0)}$. Now, we can discretize (3) into matrix-vector form

$$\left[D^2 + k_0^2 \mathtt{diag}(n^2(x_0), \ldots, n^2(x_N))\right] U = \beta^2 U. \tag{12}$$

An alternative and numerically better way to obtain CDM is using the following barycentric rational interpolation to replace Lagrange interpolation in (7)

$$u_N(x) = \frac{\sum_{k=0}^{N} \frac{\omega_k}{x - x_k} u(x_k)}{\sum_{k=0}^{N} \frac{\omega_k}{x - x_k}} \tag{13}$$

where $\omega_0, \omega_1, \ldots, \omega_N$ are called barycentric weights. For every set of collocation points x_k, there is a unique set of barycentric weights ω_k [39] to ensure (13) is theoretically equivalent to (7). For CGL points, $\omega_0 = c/2, \omega_k = (-1)^k c, k = 1, \ldots, N-1$, and $\omega_N = (-1)^N c/2$ for some nonzero constant c. Following the same way in previous paragraph, the same CDM in (10) can be derived from (13) [33], [34]. Unlike the Lagrange interpolation in (7), this barycentric rational form can interpolate at any set of grid points without the drawback of the Runge phenomenon. Even if the barycentric weights are taken randomly, (13) still interpolates the data as a rational function.

For the consideration of accuracy, the BCs (4) and (5) must be imposed into the CDM as accurate as possible. There are several ways to discretize the BCs [28], [37]. A natural way is substituting the first and the last equations of (9) with $p = 1$ into (4) and (5) to eliminate $u_n(x_0), u_N(x_N)$ in (12), i.e., from the following equations

$$a_1 u_N(x_N) + b_1 \sum_{j=0}^{N} d_{N,j}^1 u_N(x_j) = 0 \tag{14}$$

$$a_2 u_N(x_0) + b_2 \sum_{j=0}^{N} d_{0,j}^1 u_N(x_j) = 0 \tag{15}$$

we can eliminate $u_n(x_0), u_N(x_N)$. Then the size of CDM in (12) is reduced from $(N+1) \times (N+1)$ to $(N-1) \times (N-1)$. Only by this way, the discrete form of (3), (4), and (5) can be formulated into standard matrix eigenvalue problem.

$$AU = \beta^2 U. \tag{16}$$

In MATLAB notation, let

$$M = D^2 + k_0^2 \mathtt{diag}(n^2(x_0), \ldots, n^2(x_N))$$
$$B = m_1(\beta_1 d_2 - \alpha_1 d_1) + m_2(\beta_2 d_1 - \alpha_2 d_2)$$

where $m_1 = M(2:N,1), d_1 = D(1,2:N), m_2 = M(2:N, N+1), d_2 = D(N+1, 2:N)$, and when $b_i \neq 0 (i = 1,2)$, $\alpha_1 = (a_1 + b_1 d_{N,N}^1)/\gamma$, $\beta_1 = b_2 d_{0,N}^1/\gamma$, $\alpha_2 = (a_2 + b_2 d_{0,0}^1)/\gamma, \beta_2 = b_1 d_{N,0}^1/\gamma, \gamma = (a_2 + b_2 d_{0,0}^1)(a_1 + b_1 d_{N,N}^1) - b_1 b_2 d_{0,N}^1 d_{N,0}^1$; when $b_i = 0 (i = 1,2)$, $\alpha_i = \beta_i = 0$. Then

$$A = M(2:N, 2:N) + B. \tag{17}$$

To demonstrate that the accuracy and efficiency of direct CDM method is superior to low-order method, we consider a simple model of general problem (3), (4), and (5)

$$-\frac{d^2}{dx^2} u(x) = \lambda u(x), \qquad 0 < x < \pi \tag{18}$$
$$u(0) = 0 \tag{19}$$
$$u(\pi) = 0. \tag{20}$$

The exact eigenvalues of this problem are $\lambda = n^2, n \in \mathbb{Z}$. We use CDM and Numerov's fourth-order FD method [42] to discretize this equation. The resulting matrix eigenvalue problems are solved by the same MATLAB eigenvalue solver. Some results are compared in Table I. Because of the near-optimal property of Chebyshev approximation for smooth function, a much smaller CDM easily achieves machine precision. Whereas a much larger Numerov matrix only gets high precision for the first few eigenvalues. In fact, about 60% of the eigenvalues obtained by CDM are in high accuracy (the accurate 70th eigenvalue in Table I is computed by MBRCDM, not by CDM), whereas less than 10% are in good precision by FD or FE methods. More discussions about the accuracy of pseudospectral method refer to [27] and[28]. It is apparent that CDM is much better than the fourth-order FD method in the sense of both accuracy and efficiency, not to mention the traditionally preferred second-order central difference.

But we can see from the results that there are still some spurious modes in CDM method (e.g., the *italic* one in Table I), though the number of them is much less than that of FD. If we want more accurate modes, a larger CDM can be used. A powerful MATLAB package, which can automatically do this has been developed by Trefethen *et al.* [41]. In this package, the matrix size is automatically increased to ensure the accuracy. For a differentiation matrix with a fixed size, the conformal map

TABLE I
COMPARISON OF CDM AND NUMEROV METHOD FOR MODEL PROBLEM

Method	n	$\lambda_n = n^2$	Matrix Size	CPU (s)
CDM	1	1.0000000000	100	0.1
	2	4.0000000000		
	3	8.9999999999		
	4	15.999999999		
	5	24.999999999		
	48	2303.9999998		
	49	2401.0000005		
	50	2500.0000023		
	51	2600.9999949		
	70	*5333.3407191*		
	(70)	4899.9999995		
Numerov	1	1.0000000000	1000	42.9
	2	3.9999999999		
	3	8.9999999996		
	4	15.999999998		
	5	24.999999993		
	48	2303.9950115		
	49	2400.9943543		
	50	2499.9936265		
	51	2600.9928222		
	70	4899.9519663		

technique [40] can be used to improve the accuracy. This technique is based on redistributing the original CGL points to resolve the coefficients and eigenfunctions. For example, the following function map the unequal distance CGL points to almost equal distance points.

$$y = g(x, \alpha) = \frac{\sin^{-1}(\alpha x)}{\sin^{-1}\alpha} \tag{21}$$

where $0 < \alpha < 1$. It has been studied that if $\alpha = \operatorname{sech}(|\ln \epsilon|/N)$, where ϵ is the machine precision, then the roundoff error introduced by this map is guaranteed to be harmless. In two limit cases, $\alpha \to 0$ keeps the CGL points unchanged, whereas $\alpha \to 1$ maps them to be equidistant [40]. For waveguide problems, equal distance points is usually better, but not always. Generally, more points should be distributed in the area where the modal profiles change a lot. After the conformal map, we can get a new differentiation matrix with respect to the new points.

$$\hat{D} = GD \tag{22}$$

where G is a diagonal matrix with elements $G_{ii} = 1/g'(x_i, \alpha)$. We will call this new differentiation matrix the mapped CDM (MCDM).

Based on barycentric rational interpolation (13), there is a more stable way to get the mapped differentiation matrix. In (13), we still keep the CGL weights unchanged while CGL points is mapped to almost equal distance points. Then with the barycentric weights of CGL points and mapped points, new differentiation matrix can be derived from (13). We call it MBRCDM.

In Fig. 1, we compare the spurious modes of the Numerov's fourth-order FD, the CDM, the MCDM, and the MBRCDM methods with the same matrix size for the model problem. We

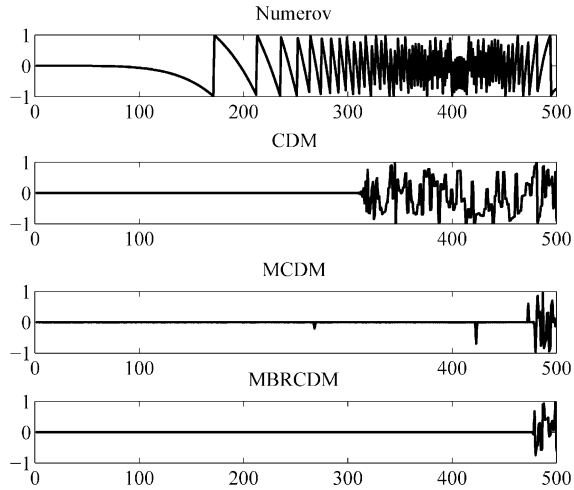

Fig. 1. Comparison of the spurious modes of Numerov, CDM, MCDM, MBRCDM method for the first 500 modes of model problem. The oscillation parts present the spurious modes. It is obvious MBRCDM method produces the smallest number of spurious modes.

define the relative error of the nth eigenvalue as $r(n) = (\sqrt{\lambda_n} - \texttt{round}(\sqrt{\lambda_n}))/0.5$, where λ_n is the nth eigenvalue of differentiation matrix, $\texttt{round}(x)$ presents the nearest integer to x. The relative error of all 500 eigenvalues of different differentiation matrix are plotted. It is apparent that the conformal map technique eliminates significantly much more spurious modes than the traditional pseudospectral method. The MBRCDM method is more stable and in higher accuracy than other existing methods. It is definitely the method of choice. So far as the waveguide eigenvalue problems with regular BCs (4) and (5) are considered, MBRCDM method can solve them very accurately and efficiently. And it is particularly competitive when a large number of eigenvalues need to be computed.

C. MBRCDM-Based Newton and PML Technique

Consider an open slab waveguide with profile $n(x) = n_1$ for $x < 0$, $n(x) = n_2$ for $x > d$, $n(x) = n_0$ for $0 < x < d$. The governing equation in each layer of this waveguide is (3) with the following nonlinearly β-dependent radiation BCs at the interface

$$\frac{du}{dx} = -i\sqrt{k_0^2 n_1^2 - \beta^2}\,u, \qquad \text{at } x = 0 \tag{23}$$

$$\frac{du}{dx} = i\sqrt{k_0^2 n_2^2 - \beta^2}\,u, \qquad \text{at } x = d. \tag{24}$$

From nonlinear eigenvalue problem (3), (23), and (24), the following dispersion algebraic equation can be easily derived

$$f(\beta) = \tan(\gamma_0 d)(\gamma_0^2 + \gamma_1\gamma_2) - i\gamma_0(\gamma_1 + \gamma_2) = 0 \tag{25}$$

where $\gamma_i = \sqrt{k_0^2 n_i^2 - \beta^2}, i = 0, 1, 2$.

For this open slab waveguide, direct MBRCDM method proposed in previous section encounters a serious difficulty. The nonlinear BCs (23) and (24) cannot be properly imposed into differentiation matrix to get a linear matrix eigenvalue problem. A noniterative method is proposed in [5], where FD is used to construct differentiation matrix and a nonlinear matrix eigenvalue problem has to be solved. In [20], Mur's absorbing BCs are used to approximate the exact BCs and a nonlinear matrix

eigenvalue problem also need to be solved. The solution of nonlinear matrix eigenvalue problem is inefficient. More stable and accurate methods for this kind of problems are using asymptotic analysis to get a good starting value followed by a Newton iteration for dispersion (25) [2], [4], [13], [16].

In this section, two methods based on direct MBRCDM method are provided to handle this kind of problems. In terms we call them MBRCDM-Newton method and MBRCDM-PML method.

1) MBRCDM-Multidirectional Newton Iteration: Instead of traditional asymptotic analysis method in getting initial value for Newton iteration, we use the MBRCDM method to compute the initial values. Specifically, we simplify nonlinear BCs (23) and (24) to β independent by giving an initial guess to β. Then use MBRCDM method to calculate the eigenvalues of this simplified problem as the initial values of the multidirectional Newton iteration for (25).

In each step of traditional root finding techniques (e.g., Newton--Raphson or Muller's iteration), only one direction is searched with one starting point on complex plane and only one root may be found. Here we introduce the multidirectional Newton iteration method, which has been programmed by Matt Fig in very high level vectorized MATLAB Mfile (NEWTZERO). The program can be found in MATLAB File-Exchange Central. The main idea of this algorithm is extending single searching direction of Newton-Raphson iteration to multidirection searching on complex plane. For $f(\beta)=0$, find the tangent line (numerically replaced by a secant nearby if $f'(\beta)$ is complicated) of $f(\beta)$ at starting point, then generate an initial vector of k lines at different angles to the tangent line. At the k intercept of each line (including the initial guess) the earlier process is repeated to give the Newton--Raphson method k^2 initial guesses. Since all these are vectorized, the process is fast. Given one starting value, NEWTZERO may find more than one root, even if the initial guess is way off. It is particularly powerful when a large number of roots must be found. For example, if we use this method to find the zeros of Bessel function $J_0(x)$ with the initial guess $x = 1,35$ roots around origin will be found immediately. In practical use, this MBRCDM-Newton method can work like a prediction-correction procedure. The initial guess of β for simplifying BCs can be properly adjusted.

2) MBRCDM-PML Technique: In [21] and [29], spectral collocation methods based on Hermite or Laguerre polynomials are used to deal with unbounded waveguide problems. But convergence problem may be suffered in these methods. PML absorbing BCs have been widely used to truncate an unbounded domain to a finite computational domain [14], [44]. PML usually performs better than the other absorbing BCs, such as the Mur's type [20]. Owe to the perfect absorbing property of PML, nonlinear BCs on two sides of the waveguide can be replaced by homogenous Dirichlet BCs on PML boundary. With PML of thickness h, the waveguide problem (3), (23), and (24) is stretched to $[-h, d+h]$ from $[0, d]$

$$\frac{1}{s(x)}\frac{d}{dx}\left(\frac{1}{s(x)}\frac{du}{dx}\right)+k_0^2n^2(x)u(x)=\beta^2u(x) \tag{26}$$

$$u(-h)=0 \tag{27}$$

$$u(d+h)=0 \tag{28}$$

where $s(x)=1+i\sigma(x)$, the real function $\sigma(x)$ is the PML profile, $\sigma(x)=0$ for $0\le x\le d, \sigma(x)>0$ for the other domains. In this paper, we take the following C^∞ smooth $\sigma(x)$:

$$\sigma(x)=\begin{cases}\sigma_0 e^{1-\frac{h^p}{(-h-x)^p}}, & \text{if } -h<x<0\\ 0, & \text{if } 0<x<d\\ \sigma_0 e^{1-\frac{h^p}{(x-d)^p}}, & \text{if } d<x<d+h\end{cases} \tag{29}$$

where σ_0, p are constant. Apparently problem (26), (27), and (28) can be solved straightforwardly by MBRCDM method. In fact, the MBRCDM of this equation is just

$$A=\mathrm{PDPD}+K \tag{30}$$

where P is a diagonal matrix with $(1)/(s(x_i))$ as the ith diagonal element. K is also a diagonal matrix with diagonal element $k_0^2n^2(x_i)$. D is the MBRCDM for first-order derivative operator. The homogenous Dirichlet BC is imposed by deleting the first and last row of A, correspondingly the first and last column.

D. Discontinuous Interface Treatment

For multilayered waveguide problems with strong discontinuity on the interface, the interface condition must be taken into account. In fact, (26) is not strictly satisfied on the interface $x=0$ and $x=d$. Only interface conditions are satisfied. That is, modal field $u(x)$ and its derivatives are continuous on the interface, e.g., at $x=0$:

$$u(x^-)=u(x^+) \tag{31}$$

$$\frac{1}{\rho^-}\frac{du(x^-)}{dx^-}=\frac{1}{\rho^+}\frac{du(x^+)}{dx^+}. \tag{32}$$

We provide two strategies to deal with the interface conditions. The first one is the traditionally used domain decomposition technique [18]–[22], [35], [37]. The computational domain is naturally decomposed into subdomains by the discontinuous interfaces (in multilayered waveguide, each layer is just one subdomain). In each subdomain, MBRCDM method is used, then MBRCDMs from each layer are patched into a single-larger MBRCDM. The patching method in this paper is just like the imposing of BCs. The unknowns on the interface are eliminated by interface conditions. If there are many interfaces, this patching method could be tedious.

The second strategy is to avoid it lazily. If there is no grid point on the interface, then the interface conditions are automatically avoided by MBRCDM method. This can be easily done by a microadjustment of the matrix size. Because of the high accuracy of MBRCDM, this lazy but simple method still preserves the merits of MBRCDM.

III. Numerical Examples

In this section, we study several waveguide examples to validate the methods proposed in the previous section. The algorithms are easily programmed based on Differentiation Matrix Suite or Chebfun system. They are all implemented in MATLAB 2007b on a personal computer with Intel(R) Core(TM)2 Duo CPU 2.33 GHz RAM 2 GB.

TABLE II
PARAMETERS OF THREE LAYERS OPEN SLAB WAVEGUIDES

Example	n_0	n_1	n_2	d (μm)	λ (μm)
1	3.3	3.17	1.0	0.8	1.55
2	3.3	3.17	3.17	0.2	1.55

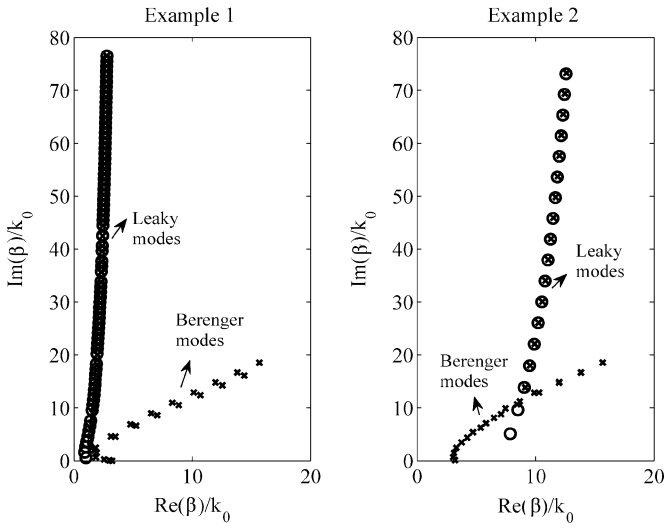

Fig. 2. Guided, leaky, and Berenger modes of slab waveguide computed by MBRCDM-Newton and MBRCDM-PML methods. Exact values, which are obtained by MBRCDM-Newton iteration with tolerance error 1E-13, are denoted by "$\circ$." The modes computed by MBRCDM-PML method are denoted by "$\times$." The results of two methods coincide very well, except an additional branch (Berenger modes) arises in MBRCDM-PML method.

A. MBRCDM-Newton and MBRCDM-PML Methods for Slab Waveguide

We first consider the open slab waveguide as a benchmark problem to test the MBRCDM-Newton and MBRCDM-PML algorithms. This kind of waveguides have been widely studied in [13] and [16], and some accurate results have been obtained. We study exactly the same two examples as in [16] to compare the results. The waveguide parameters are shown in Table II. The first example is an unsymmetrical slab waveguide, and the second is a symmetric slab waveguide. The free-space wavelength is assumed to be $\lambda = 1.55$ μm.

We calculate exact modes by MBRCDM-Newton method. The tolerance error in the MBRCDM-Newton iteration procedure is taken to be 10^{-14}, i.e., if $|f(\beta)| < 10^{-14}$, then β is taken as an exact root. Results obtained under this error bound are much more accurate than those in [16], where the exact values are actually not accurate enough. In fact, the residual $|f(\beta)|$ with the "exact" β in [16] is just only the order of $O(1)$ in Example 1, and the order of $O(10^{-4})$ in Example 2. However the error bound is cruel, MBRCDM-Newton is still very fast. It costs only several seconds to get hundreds of roots. Whereas if we use multi-Rayleigh iterative method based on low-order FD method, it may take hours to get worse results for the same problem [24].

To implement MBRCDM-PML method, we choose the following PML parameters in (29): $\sigma_0 = 10, p = 5, h = 0.2$ μm. The original slab waveguide is truncated into finite thickness on both sides by two PMLs. The nonlinear radiative BCs are reduced to homogenous Dirichlet type. Then the problem can be easily and accurately solved by direct MBRCDM method. Because the imposing of PML, a new branch of modes arises. This new branch modes, which only depend on PML parameters, are known as Berenger modes. Results of MBRCDM-Newton (exact) and MBRCDM-PML are illustrated in Fig. 2. We can see that leaky modes calculated by two methods are quite coincident. This means that the noniterative MBRCDM-PML method is also very accurate. In MBRCDM-PML, the knowledge of dispersion equation will be unnecessary. For many structures, of which dispersion equations are very cumbersome or even impossible to be derived, this dispersion relation independent noniterative MBRCDM-PML method is essential.

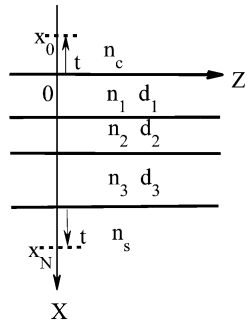

Fig. 3. Sketch of high-loss-multilayered planar waveguide. The computational domain is $[\boldsymbol{x_0}, \mathbf{x_N}]$.

B. MBRCDM-PML Method for Lossy Multilayered Waveguide

In this section, we study a high-loss multilayered planar waveguide depicted in Fig. 3, which is the same example as in [5]. The waveguide structure parameters are: $n_c = 1.0, n_1 = 3.591 - i0.084, d_1 = 1.502$ μm, $n_2 = 3.211, d_2 = 0.74$ μm, $n_3 = 3.166, d_3 = 3.5$ μm, $n_s = 3.15$. The free-space wavelength is $\lambda = 1.55$ μm. For comparison, the same computational domain as in [5] is used. Both direct MBRCDM method imposed Dirichlet zero BC and MBRCDM-PML technique can be implemented for this problem. But the results by MBRCDM-PML are more accurate. Compared to [5], where lower order FD is used and a nonlinear matrix eigenvalue problem must be solved, MBRCDM-PML method is more straightforward, simpler, and much more accurate, and also noniterative. In Table III, we show some comparison results. The parameter $t = 1$ μm and the grid size $N = 200$ are used in both methods. More accurate results can be obtained by MBRCDM-PML method combined with domain decomposition.

C. Chebop for Gaussian RIP Waveguide

We consider a planar waveguide with variable Gaussian RIP $n^2(x) = n_s^2 + 2n_s c\exp(-(x^2/t)^2) + c^2(\exp(-(x/t)^2))^2$, as depicted in Fig. 4, $n_s = 1.512, c = 0.0833, t = 2.66$ μm, $\lambda = 0.6328$ μm. The computational domain is $[-L, L]$.

For this continuous RIP problem, we briefly introduce Chebfun and Chebop system. This is a state-of-the-art object-oriented MATLAB package using Chebyshev series and interpolants for numerical computation. More details about this system can be found in [41], [43], [45]. Based on this powerful system, the implementation of CDM method for this

TABLE III
TE COMPLEX PROPAGATION CONSTANTS OF THE LOSSY MULTILAYERED WAVEGUIDE

TE_i	Ref. [5]	MBRCDM
0	$3.5627 - i0.8401(-1)$	$3.5626 - i0.8402(-1)$
1	$3.4776 - i0.8374(-1)$	$3.4768 - i0.8378(-1)$
2	$3.3359 - i0.8135(-1)$	$3.3334 - i0.8137(-1)$
3	$3.1631 - i0.5281(-2)$	$3.1648 - i0.5909(-2)$
4	$3.1594 - i0.3513(-2)$	$3.1593 - i0.2189(-2)$

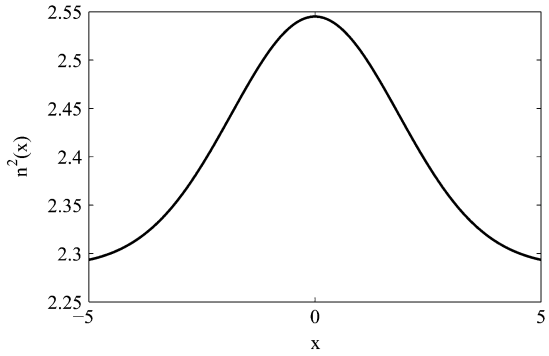

Fig. 4. Continuous Gaussian RIP.

TABLE IV
EXACT PROPAGATION CONSTANTS OF GAUSSIAN RIP WAVEGUIDE

TE_i	Ref. [29]	Chebop
0	1.58935	1.589348472403796
1	1.57775	1.577748079556395
2	1.56682	1.566820828828896
3	1,55661	1.556611470916948
4	1.54717	1.547171852429019
5	1.53856	1.538563704779744
6	1.53086	1.530863314813039
7	1.52417	1.524170056262246
8	1.51862	1.518624073487937
9	1.51444	1.514451267495924

eigenvalue problem can be extraordinarily simple and convenient in MATLAB code, and the high accuracy of results are automatically preserved. In Table IV, the first several TE modes accurate up to machine precision are obtained by implementing CDM based on Chebop, setting computational window $L = 20$ and homogeneous Dirichlet conditions on the boundary. The convergence behavior of the first mode with respect to the change of computational window is shown in Table V. The efficiency of Chebop is also very surprising.

D. Discontinuous RIP Waveguide

As a final example, we consider a planar waveguide with strongly discontinuous RIP to compare the two strategies of handling the interface conditions. This structure has been studied in [22] and[29]. The RIP is $n^2(x) = 1$ if $x < 0$, $n^2(x) = n_s^2 + 2n_s c\exp(-(x^2/t)^2) + c^2(\exp(-(x/t)^2))^2$ if $x > 0$, where $n_s = 1.512$, $c = 0.0833$, $t = 2.66$ μm, $\lambda = 0.6328$ μm, as depicted in Fig. 5. We take the symmetrical computational domain $[-L, L]$. If the number of grid point is odd, then the center grid point happens to be on the interface, the direct CDM

TABLE V
CONVERGENCE OF THE FIRST TE MODE OF GAUSSIAN RIP WAVEGUIDE

Computational Window L	TE_0
1	1.585971583951386
3	1.589348451219056
5	1.589348472403794
10	1.589348472403795
20	1.589348472403796
50	1.589348472403798

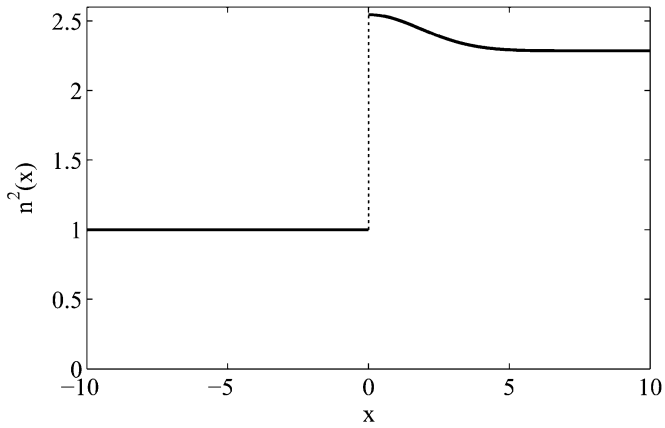

Fig. 5. Discontinuous RIP.

TABLE VI
CONVERGENCE BEHAVIOR OF DIFFERENT METHODS IN HANDLING DISCONTINUOUS INTERFACE

Matrix Size	CDM	MBRCDM	Multidomain CDM
50	1.579561	1.579468	1.579106
51	1.580963	1.580700	1.579106
100	1.579237	1.579187	1.579106
101	1.579972	1.579758	1.579106
300	1.579122	1.579114	1.579106
301	1.579373	1.579286	1.579106
500	1.579112	1.579109	1.579106
501	1.579263	1.579210	1.579106
Benchmark value	1.57911		

without considering the interface conditions will fail to converge. If we take an even number of points, there is not any grid point on the interface. The interface conditions can be reasonably avoided. Then the results are convergent. Since the RIP changes a lot near the interface, the coarsest grid near the center cannot properly resolve the RIP variation. Using the mapping technique can speed up the convergence. These views are verified in Table VI, the computational window is $L = 3$ μm. The results imply that domain decomposition MBRCDM method is the most stable and efficient in handling discontinuous interface. But when several interfaces are involved, the domain decomposition MBRCDM method becomes a little cumbersome. In this circumstance, the single MBRCDM method is a lazy but simple choice.

IV. CONCLUSION

A unified solver for computing a large number of propagation constants has been proposed. And its high accuracy

and high efficiency have been extensively verified by computing the modes of several waveguide structures. This solver contains two main methods—the MBRCDM-Newton and MBRCDM-PML. MBRCDM-Newton method is useful for waveguides with simple dispersion equations. MBRCDM-PML method is adaptable to all kinds of waveguides and produces much less physically meaningless spurious modes than any other similar methods ever used. Both methods are easy to implement and achieve almost the same accuracy as long as the numerical evaluation of dispersion equation is stable. In this stable case, MBRCDM-Newton is usually faster. This solver indeed unifies the merits of existing methods. It is essential when we want to compute a large number of modes, especially the leaky modes or other high index modes.

This paper is concerned with the planar waveguides with z-independent RIP. But the MBRCDM-PML method is not limited to this kind of waveguides. With the idea of mode matching or mode coupling, it can be easily used for other practically useful 2-D waveguides, such as the piecewise waveguides and weakly varying waveguides, whose RIPs are varying in the propagation direction. It also can be generalized to some 3-D waveguides by the coordinate transformation and tensor product techniques.

ACKNOWLEDGMENT

The authors would like to thank the editor and reviewers for their patience and valuable comments.

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