

# High-Accuracy Waveguide Leaky-Mode Analysis Using a Multidomain Pseudospectral Frequency-Domain Method Incorporated With Stretched Coordinate PML

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**Abstract**—A recently developed pseudospectral frequency-domain (PSFD) method employing a penalty scheme is further incorporated with stretched coordinate perfectly matched layers (PMLs) in order to solve waveguide leaky modes. Several standard leaky-mode slab and circular waveguides, including the W-type and M-type ones, are examined first by solving their complex effective indexes and field profiles, showing that the PSFD method achieves computational accuracy on the order of  $10^{-15}$ . Then, this high-accuracy solver is used to analyze waveguide structures with more complicated geometries, such as the leaky six-air-hole fiber, for which self convergence of accuracy in calculated effective indexes is demonstrated to be on the orders of  $10^{-14}$ , and two rectilinear waveguides with sharp corners, i.e., the rib waveguide and the photonic wire. Comparison of the PSFD method obtained results for these more complicated waveguide structures with those from other methods in the literature is presented and discussed.

**Index Terms**—Leaky waveguide modes, optical waveguide analysis, pseudospectral frequency domain (PSFD) method.

## I. INTRODUCTION

GENERALLY, optical wave-guiding mechanisms based on total internal reflection [1], photonic band gap effect [2]–[4], and antiresonant reflection [5]–[7] have been mostly adopted. However, imperfect field confinement in the guiding region might occur in certain waveguide structures functioned

by these mechanisms, resulting in leaky modes with confinement losses. Physically, leaky modes are known not members of a complete set of orthogonal basis functions, and behave analogy to the tunneling effect in quantum physics [8], [9] that most wave powers are longitudinally guided inside the core but portions are laterally propagating in the outermost layer. The most specific characteristics of the leaky mode are therefore its complex propagation constant and infinite field magnitude at the infinite transverse spatial limit [9], because longitudinal decay would lead to increase of fields in the transverse direction according to the relationship between wavenumber and propagation constant [10]. Therefore, an accurate computational method implemented with well-functioning absorbing mechanism such as using the perfectly matched layers (PMLs) [11] is essential for solving waveguide leaky modes with such field profiles.

In analyzing waveguides, modal characteristics including field profiles, propagation constants, effective indexes, modal (confinement) losses, and dispersion curve are mainly concerned, and the effective index which is defined as the propagation constant divided by the free-space wavenumber is usually chosen as an indicator for assessing the computation accuracy of a method. Optical waveguide leaky-mode solvers have been developed, in particular after the invention of holey fibers or photonic crystal fibers [2]–[4], based on different numerical methods, such as the finite difference method [12]–[14], the finite element method [15], [16], the multipole method [17], [18], the boundary integral equation method [19], the pseudospectral frequency-domain (PSFD) method [20], [21], etc. This paper concerns further development of the pseudospectral method which is based on the high-order Legendre or Chebyshev interpolation basis and can then provide exponentially converged computation accuracy with respect to the grid resolution [22], [23]. Prior PSFD mode solvers have been formulated using second-order Helmholtz equations [20]–[23] and demonstrated to provide excellent numerical accuracy in eigenmode analysis.

Recently, an alternate PSFD method with a penalty scheme was developed [24], which shows  $10^{-15}$  accuracy in solving the modal effective indexes for standard metallic and fiber waveguides. Different from above-mentioned Helmholtz equations-based methods, this newly reported PSFD method is formulated on the first-order differential equations written from both curl and divergence laws in Maxwell equations

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[26]. Besides, the multidomain scheme is employed in the formulation, with which the computational domain is divided into suitable number of curvilinear sub-domains [25] such that the shapes of the waveguide structure interfaces can fit the sub-domain boundaries, facilitating accurate fulfillment of the field continuity conditions across the interfaces. In this paper, this new method is adopted and implemented with the stretched coordinate PML [27], [28], which is quite suitable for first-order equations, for solving waveguide leaky modes with high accuracy. We will show in the numerical examples that the inclusion of the stretched coordinate PML still maintains high accuracy of the PSFD method, and the position where the PML region is placed has negligible effect on the computation accuracy, even for waveguides with no need in effective indexes of the PML like the fiber waveguide. It will be shown that this PSFD solver can achieve  $10^{-15}$ – $10^{-14}$  numerical accuracy for solving leaky-mode waveguide structures without singular-field corners. In comparison of our PSFD solution for a leaky six-air-hole fiber [17] with that from a recently reported new high-order boundary-integral-equation (BIE) method [19] which was shown to achieve exponential convergence and extremely high accuracy, it is found that the agreement in the calculated effective index is to the order of  $10^{-13}$  for both the real and imaginary parts. The PSFD analysis will then be applied to the conventional rib waveguide [29] and the more complicated photonic wire [30] for which the application of the BIE method would become more difficult.

The rest of this paper is organized as follows. The governing Maxwell's equations with the penalty scheme, the implementation of the stretched coordinate PML, and the eigenmode solver formulation are described in Section II. The Legendre pseudospectral method is introduced in Section III. Then, numerical examples are given and discussed in Section IV, where several one-dimensional (1-D) (slab) and 2-D (circular) leaky-mode waveguides, including W-type [9], [31] and M-type [5], [6] waveguides, are analyzed first, followed by the examination of the more complicated 2-D structures such as the six-air-hole fiber and the photonic wire. The conclusion is drawn in Section V.

## II. PHYSICAL EQUATIONS, PML, AND PENALTY-SCHEME FORMULATION

In a source-free and linear isotropic medium with permittivity  $\varepsilon$  and permeability  $\mu$ , the time-harmonic Maxwell's curl and divergent equations for frequency-domain computation are written as

$$\nabla \times \mathbf{E} = -j\omega \mu \mathbf{H} \quad (1a)$$

$$\nabla \times \mathbf{H} = j\omega \varepsilon \mathbf{E} \quad (1b)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = 0 \quad (1c)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad (1d)$$

where  $\omega$  is the angular frequency. Without loss of generality, waves are considered to propagate along the  $z$ -axis in the waveguide, i.e., no structural variations along the  $z$  direction. Therefore, spatial derivative with respect to  $z$  becomes  $\partial/\partial z = -j\beta$ ,

where  $\beta$  is the modal propagation constant. For convenience, we normalize the magnetic field  $\mathbf{H}$  to  $\sqrt{\varepsilon_0/\mu_0}\mathbf{H}$ .

Traditionally, waveguide modes are solved by second order Helmholtz equations, like in [23]. A new PSFD method has been recently developed in [24] using first order formulations instead, which we adopt in this paper as well. In brief, two of the eight equations in (1) without  $j\beta$  terms are removed, i.e.,

$$-jk_0 H_y + \frac{\partial E_z}{\partial x} = j\beta E_x \quad (2a)$$

$$jk_0 H_x + \frac{\partial E_z}{\partial y} = j\beta E_y \quad (2b)$$

$$-\frac{\partial E_x}{\partial x} - \frac{\partial E_y}{\partial y} = j\beta E_z \quad (2c)$$

$$jk_0 \varepsilon_r E_y + \frac{\partial H_z}{\partial x} = j\beta H_x \quad (2d)$$

$$-jk_0 \varepsilon_r E_x + \frac{\partial H_z}{\partial y} = j\beta H_y \quad (2e)$$

$$-\frac{\partial H_x}{\partial x} - \frac{\partial H_y}{\partial y} = j\beta H_z. \quad (2f)$$

These six equations lead to an eigen-problem in the form,  $\tilde{A}\tilde{x} = \lambda\tilde{x}$ , for solving waveguide modes, with  $\tilde{A}$  containing the differential operators, the eigenvalue  $\lambda$  equal to  $j\beta$  to be searched, and the eigenvector  $\tilde{x}$  composed of the electric and magnetic fields of the corresponding mode. This eigen-problem can be solved using efficient iterative algorithms such as the bi-conjugate gradient (BiCG) method along with the shifted inverse power method (SIPM).

For handling boundary conditions between materials, the penalty scheme as utilized in [24] is also adopted here. First, (2) can be rewritten as

$$jk_0 Mq + A_x \frac{\partial q}{\partial x} + A_y \frac{\partial q}{\partial y} = j\beta A_z q \quad (3)$$

where  $k_0 = \omega\sqrt{\varepsilon_0\mu_0}$ ,  $q = [\varepsilon_r E_x, \varepsilon_r E_y, E_z, H_x, H_y, H_z]^T$ ,  $A_z = \text{diag}[1/\varepsilon_r, 1/\varepsilon_r, -\varepsilon_r, 1, 1, -1]^T$ , and the elements of the matrices  $M$ ,  $A_x$ , and  $A_y$  are simply 0, 1, and  $-1$  depending on the presence of fields in (2). Next, the penalty term  $P = [\delta/(2\omega_0)]S(n)\Lambda[R(n) - R^{BC}(n)]$  is added into (2). The diagonal matrix  $\Lambda$  is composed of the eigenvalues of the matrix  $A(n)$ , the matrix  $S(n)$  is composed of the eigenvectors of  $A(n)$ , with  $A(n) = n_x A_x + n_y A_y$ , in which  $n_x$  and  $n_y$  are defined below, and the characteristic state vectors  $R(n)$  are defined as  $R(n) = S^T(n)q = [R_1, R_2, R_3, R_4, R_5, R_6]^T$  as in [24]. Considering boundary conditions at the interface between two adjacent sub-domains  $I$  and  $II$  in the multidomain approach, with the unit normal vector  $\hat{n} = n_x \hat{x} + n_y \hat{y}$  perpendicular to the interface with the relationship  $\hat{n} = \hat{n}^I = -\hat{n}^{II}$ , where the superscripts  $I$  and  $II$  specify the sub-domains where the vectors are defined at the interface, we add  $R_2^{II}$  to  $R_1^I$  and add  $R_6^{II}$  to  $R_5^I$  with the aids of physical boundary conditions [24] and obtain

$$R_1^I + R_2^{II} = \frac{1}{\sqrt{2}}[\hat{n} \cdot (\varepsilon_r^I \bar{E}_t^I - \varepsilon_r^{II} \bar{E}_t^{II}) - (E_z^I - E_z^{II})] = 0 \quad (4a)$$

$$R_5^I + R_6^{II} = \frac{1}{\sqrt{2}}[\hat{n} \cdot (\bar{H}_t^I - \bar{H}_t^{II}) + (H_z^I - H_z^{II})] = 0. \quad (4b)$$

Equations (4a) and (4b) lead to  $R_1^I = -R_2^{II}$  and  $R_5^I = -R_6^{II}$ , respectively, i.e.,  $R_1^{BC} = -R_2^{II}$  and  $R_2^{BC} = -R_1^{II}$ , which means that if we want to add considerations of physical boundary conditions into (2) or (3) at material interfaces of two adjacent sub-domains, we can simply place characteristic state vectors of (4) into the penalty terms. Then, after matrix multiplications of  $S(n)$ ,  $\Lambda$ , and  $[R(n) - R^{BC}(n)]$  in the penalty term  $P$ , the six first-order Maxwell's equations in (2) for sub-domain  $I$ , with the added  $P$  and straightforward manipulations, will become

$$-jk_0 H_y^I + \frac{\partial E_z^I}{\partial x} - \frac{\delta n_x^I}{2\omega_0} (E_z^I - E_z^{II}) = j\beta E_x^I \quad (5a)$$

$$jk_0 H_x^I + \frac{\partial E_z^I}{\partial y} - \frac{\delta n_y^I}{2\omega_0} (E_z^I - E_z^{II}) = j\beta E_y^I \quad (5b)$$

$$-\frac{\partial E_x^I}{\partial x} - \frac{\partial E_y^I}{\partial y} + \frac{\delta}{2\omega_0} \left[ n_x^I \left( E_x^I - \frac{\varepsilon_r^{II}}{\varepsilon_r^I} E_x^{II} \right) + n_y^I \left( E_y^I - \frac{\varepsilon_r^{II}}{\varepsilon_r^I} E_y^{II} \right) \right] = j\beta E_z^I \quad (5c)$$

$$jk_0 \varepsilon_r^I E_y^I + \frac{\partial H_z^I}{\partial x} - \frac{\delta n_x^I}{2\omega_0} (H_z^I - H_z^{II}) = j\beta H_x^I \quad (5d)$$

$$-jk_0 \varepsilon_r^I E_x^I + \frac{\partial H_z^I}{\partial y} - \frac{\delta n_y^I}{2\omega_0} (H_z^I - H_z^{II}) = j\beta H_y^I \quad (5e)$$

$$-\frac{\partial H_x^I}{\partial x} - \frac{\partial H_y^I}{\partial y} + \frac{\delta}{2\omega_0} \left[ n_x^I (H_x^I - H_x^{II}) + n_y^I (H_y^I - H_y^{II}) \right] = j\beta H_z^I \quad (5f)$$

where  $\delta$  is unity when the grid point is at the boundary edge, and is zero otherwise, and  $\omega_0$  is the quadrature weight on the interface which will be defined in the next section.

For solving waveguide leaky modes, a suitable perfectly matched layer (PML) [11] is required to be implemented. The stretched coordinate PML [27], [28] is chosen in this paper because of its ease of implementation on first order equations and its outstanding ability of absorbing outward propagating waves. According to [27] and [28], the stretched coordinate PML can be implemented by simply changing partial derivatives as  $\partial/\partial\tilde{x} = (1/s_x)\partial/\partial x$  and  $\partial/\partial\tilde{y} = (1/s_y)\partial/\partial y$ . Similarly, the vector differential operator  $\tilde{\nabla}$  in the stretched coordinate becomes  $\tilde{\nabla} = \tilde{x}(1/s_x)\partial/\partial x + \tilde{y}(1/s_y)\partial/\partial y$ . The absorptive variables  $s_x$  and  $s_y$  are defined as  $s_x = 1 + (\sigma_x)/(j\omega\varepsilon)$  and  $s_y = 1 + (\sigma_y)/(j\omega\varepsilon)$  [27], [28], where  $\sigma_x$  and  $\sigma_y$  are the electric conductivities. To reduce possible undesired reflection waves, we choose suitable profiles for  $\sigma_x$  and  $\sigma_y$  such as, for example,  $\sigma_x(x_i) = c(|x_i - x_0|/(L_{PML}))^m$  along the  $x$ -axis, with the parameters  $c$  and  $m$  being free variables for adjusting performance of the PML,  $|x_i - x_0|$  is the distance of the  $i$ th grid point away from the innermost interface of the PML, and  $L_{PML}$  is the length of the PML region. This is a gradually growing profile and thus its strength of absorption as the grids get deeper into the PML region. Therefore, in the PML region, (5) will become

$$-jk_0 H_y^I + \frac{1}{s_x} \frac{\partial E_z^I}{\partial x} - \frac{\delta}{2\omega_0} \frac{n_x^I}{s_x} (E_z^I - E_z^{II}) = j\beta E_x^I \quad (6a)$$

$$jk_0 H_x^I + \frac{1}{s_y} \frac{\partial E_z^I}{\partial y} - \frac{\delta}{2\omega_0} \frac{n_y^I}{s_y} (E_z^I - E_z^{II}) = j\beta E_y^I \quad (6b)$$

$$-\frac{1}{s_x} \frac{\partial E_x^I}{\partial x} - \frac{1}{s_y} \frac{\partial E_y^I}{\partial y} + \frac{\delta}{2\omega_0} \left[ \frac{n_x^I}{s_x} \left( E_x^I - \frac{\varepsilon_r^{II}}{\varepsilon_r^I} E_x^{II} \right) + \frac{n_y^I}{s_y} \left( E_y^I - \frac{\varepsilon_r^{II}}{\varepsilon_r^I} E_y^{II} \right) \right] = j\beta E_z^I \quad (6c)$$

$$jk_0 \varepsilon_r^I E_y^I + \frac{1}{s_x} \frac{\partial H_z^I}{\partial x} - \frac{\delta}{2\omega_0} \frac{n_x^I}{s_x} (H_z^I - H_z^{II}) = j\beta H_x^I \quad (6d)$$

$$-jk_0 \varepsilon_r^I E_x^I + \frac{1}{s_y} \frac{\partial H_z^I}{\partial y} - \frac{\delta}{2\omega_0} \frac{n_y^I}{s_y} (H_z^I - H_z^{II}) = j\beta H_y^I \quad (6e)$$

$$-\frac{1}{s_x} \frac{\partial H_x^I}{\partial x} - \frac{1}{s_y} \frac{\partial H_y^I}{\partial y} + \frac{\delta}{2\omega_0} \left[ \frac{n_x^I}{s_x} (H_x^I - H_x^{II}) + \frac{n_y^I}{s_y} (H_y^I - H_y^{II}) \right] = j\beta H_z^I \quad (6f)$$

Generally, the PML is designed to absorb waves in a single direction, therefore similar  $\sigma_y$  profile along the  $y$  direction is used by replacing the variable  $x$  with  $y$  in  $\sigma_x(x_i)$ , and both  $\sigma_x$  and  $\sigma_y$  will be needed at the corner region of the PML.

### III. THE LEGENDRE PSEUDOSPECTRAL METHOD FORMULATION

Now we discuss the Legendre pseudospectral method for numerically treating the spatial derivatives in the above governing equations. Under the multidomain scheme, each curvilinear quadrilateral sub-domain region in Cartesian coordinates  $(x, y)$  can be mapped onto a square region  $[-1, 1] \times [-1, 1]$  in curvilinear coordinates  $(\xi, \eta)$  by using the transfinite blending function described in [25] to construct  $\xi = \xi(x, y)$  and  $\eta = \eta(x, y)$ . Applying the chain rule, derivatives of a 2-D function  $f(x, y)$  will then become

$$\frac{\partial f(x, y)}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial f(x, y)}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial f(x, y)}{\partial \eta} \quad (7a)$$

$$\frac{\partial f(x, y)}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial f(x, y)}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial f(x, y)}{\partial \eta} \quad (7b)$$

Some properties of Legendre polynomials, which we use as the basis for the interpolation of a function, will be given below.

In the Legendre pseudospectral method, spatial arrangement of grid points is defined by the Legendre-Gauss-Lobatto (LGL) quadrature points  $\xi_i$  arranged in the interval  $[-1, 1]$ , which are the roots of the polynomial  $(1 - \xi^2)P'_N(\xi)$  [23], [24] with the prime denoting derivative and  $P_N$  being the Legendre polynomial of degree  $N$  defined by

$$P_N(\xi) = \frac{1}{2^N N!} \frac{d^N}{d\xi^N} (\xi^2 - 1)^N \quad (8)$$

Associated with these LGL quadrature points are a set of quadrature weights  $\omega_i$  for  $i = 0, 1, 2, \dots, N$ . If  $f(\xi)$  is a polynomial of degree at most  $2N + 1$ , we have the quadrature rule [23], [24]

$$\sum_{i=0}^N f(\xi_i) \omega_i = \int_{-1}^1 f(\xi) d\xi \quad (9)$$

where the quadrature weights are defined by

$$\omega_i = \begin{cases} \frac{2}{N(N+1)}, & i = 0, N \\ -\frac{2}{(N+1)} \frac{1}{P_N(\xi_i)P'_{N-1}(\xi_i)}, & \text{otherwise.} \end{cases} \quad (10)$$

Based on these LGL collocation points, one can use the degree- $N$  Lagrange interpolation polynomials  $l_j(\xi)$  as the bases to approximate an arbitrary function  $f(\xi)$  such that

$$f(\xi) \approx \sum_{j=0}^N f(\xi_j) l_j(\xi) \quad (11)$$

where

$$l_j(\xi) = -\frac{(1 - \xi^2)P'_N(\xi)}{N(N+1)(\xi - \xi_j)P_N(\xi_j)}. \quad (12)$$

Then, the derivative of the function  $f(\xi)$  at the LGL quadrature point  $\xi_i$  can also be approximated as

$$\frac{df(\xi_i)}{d\xi} \approx \sum_{j=0}^N \frac{dl_j(\xi_i)}{d\xi} f(\xi_j) = \sum_{j=0}^N D_{ij} f(\xi_j). \quad (13)$$

The differential coefficient  $D_{ij}$  is defined in [23] and [24] by

$$D_{ij} = \begin{cases} -\frac{N(N+1)}{4}, & i = j = 0 \\ \frac{N(N+1)}{4}, & i = j = N \\ 0, & 0 < (i = j) < N \\ \frac{P_N(\xi_i)}{P_N(\xi_j)} \frac{1}{\xi_i - \xi_j}, & i \neq j \end{cases} \quad (14)$$

The so-called differential matrix operator with  $D_{ij}$  elements can thus be substituted into the spatial derivative in (13) as

$$\frac{\partial}{\partial \xi} = \begin{bmatrix} D_{00} & D_{01} & \cdots & D_{0N} \\ D_{10} & D_{11} & \cdots & D_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ D_{N0} & D_{N1} & \cdots & D_{NN} \end{bmatrix}. \quad (15)$$

This is the key feature of the Legendre PSFD method, i.e., for the 1-D example, the derivative of  $f(\xi)$  at an LGL point  $\xi_i$  in the region  $[-1, 1]$  can be approximated in terms of  $f(\xi)$  values at the  $N + 1$  LGL points in the same region. Therefore, spatial derivatives of fields in (5) and (6) can be simply replaced by this differential matrix operator  $D_{ij}$  in the  $\tilde{A}\tilde{x} = \lambda\tilde{x}$  eigen-problem system, and the resultant eigen-problem becomes a sparse matrix having penalty, PML, and repeatedly appearing  $D_{ij}$  terms in the  $\tilde{A}$  matrix. Note that matrix sparsity will give better computational behavior, including less memory usage and faster computation. Besides, for solving huge computations of matrix multiplication by parallel computations, we adopt hardware acceleration using the graphic processing unit (GPU) that each of multi-processors can handel one row of matrix multiplication at the same time.

In the 2-D waveguide structures to be discussed in the next section, the grid meshes based on the LGL points in each sub-domain will be plotted for a given  $N = 12$ . In the figures, the curved structure and the whole computational region can be seen being partitioned into curvilinear sub-domains, and  $(N +$

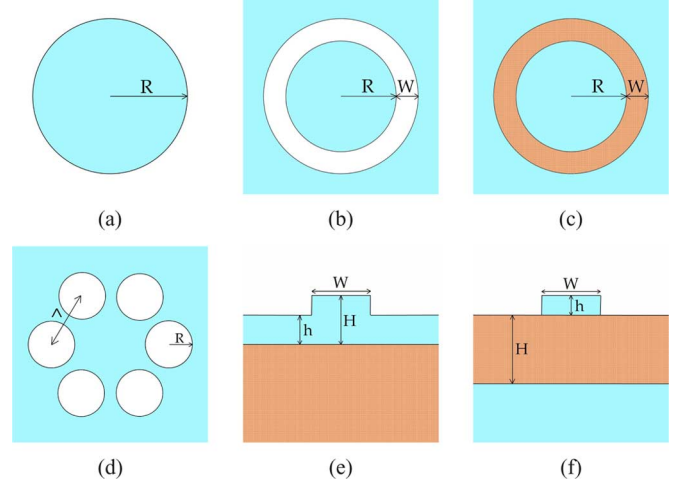


Fig. 1. 2-D waveguide geometries. (a) Circular fiber. (b) W-type fiber. (c) M-type fiber. (d) Six-air-hole fiber. (e) Rib waveguide. (f) Photonic wire.

$1) \times (N + 1)$  LGL grid points are not uniformly distributed but somewhat following the outline of the domain edges. Please note that the LGL grid points at each edge side of a sub-domain are co-located with the LGL grid points at one edge side of its adjacent sub-domain. These co-located grid points are counted as distinct sets of points, and the penalty scheme is applied on the two sets for exchanging information of boundary conditions.

#### IV. NUMERICAL RESULTS

In this section, we will apply our PSFD method with stretched coordinate PML to solve several standard optical waveguides. 1-D slab waveguides will be examined first, and then their corresponding 2-D fiber structures, which have circular symmetries, will be analyzed. Next, optical waveguides with more complicated structures will be analyzed, including the six-air-hole fiber [17], [18], the rib waveguide [29], and the photonic wire waveguide [30]. The latter two are with sharp dielectric corners at which electric-field singularities might exist, and how such sharp corners would affect the accuracy of computation will be discussed. The cross-sections of the 2-D structures to be discussed in this section are depicted in Fig. 1.

##### A. W-Type Slab Waveguide

In traditional slab waveguide with higher-index core squeezed by lower-index cladding layers, optical fields can be well guided inside the core region and exponentially decay outside. The propagation constant  $\beta$  is valued between the wavenumbers of the structure, i.e.,  $k_{clad} < \beta < k_{core}$ , where  $k_{clad}$  and  $k_{core}$  are the wavenumbers of the cladding and the core, respectively. Under this restriction of physics, waves are not allowed to propagate laterally in the cladding layers, because their transverse propagation constant  $\alpha = (k_{clad}^2 - \beta^2)^{1/2}$  is imaginary. Therefore, a simplest leaky-mode waveguide can be constructed by simply introducing a secondary (infinite) cladding region, outside the inner finite-thickness cladding layer, with structural wavenumber higher than  $\beta$ , forming the so-called W-type waveguide [9], [31], with its refractive-index profile shown in Fig. 2(a). This structure can, therefore, support

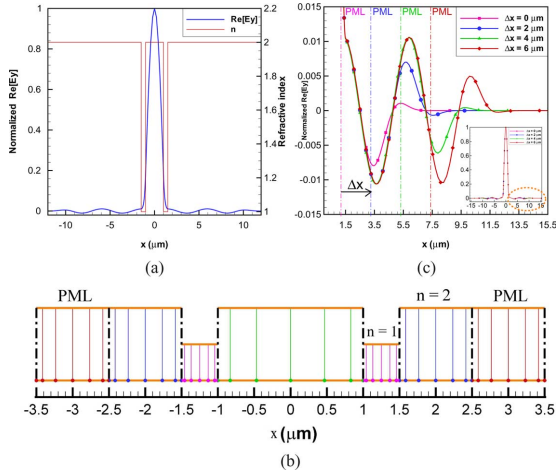


Fig. 2. (a) Structural refractive-index profile and  $\text{Re}[E_y]$  distribution showing leaky-wave characteristic for the W-type slab waveguide. (b) Domain partition (dashed lines for sub-domain edges) and LGL grid distributions (solid circles) for  $N = 6$ . (c)  $E_y$  field and leaky wave with the structural refractive index. (b) Absorption characteristics of  $\text{Re}[E_y]$  in the outer cladding layer for different distances,  $\Delta x = 0, 2, 4$ , and  $6 \mu\text{m}$ , from PML to the inner cladding layer.

waves evanescently decaying in the inner cladding layer and sinusoidally propagating in the outer cladding layer. This behavior is similar to the tunneling effect of a finite-width energy barrier in quantum physics [8], [9].

The W-type waveguide of Fig. 2(a) is structured by  $2\text{-}\mu\text{m}$ -thick core with refractive index  $n = 2$  and  $0.5\text{-}\mu\text{m}$ -thick inner cladding layer with  $n = 1$ . For supporting leaky waves, the material of the outer cladding layer is chosen to be the same as the core layer. This W-type leaky mode can be solved analytically [9], [31], and the obtained exact complex effective index of the fundamental transverse-electric (TE) mode on the given structure is  $n_{\text{eff}} = 1.972708918684279 + j0.000003930939117$ , when the operating wavelength is  $\lambda = 1.5 \mu\text{m}$ . Table I lists the PSFD computed complex effective indexes for different grid resolution or  $N$ s, which apparently shows that the accuracy in  $n_{\text{eff}}$  reaches  $10^{-15}$  as  $N = 14$  is used. The sub-domain partitioning and unevenly distributed LGL mesh grids are illustrated in Fig. 2(b) for  $N = 6$ , where seven sub-domains are depicted including the PML ones. Only one PML sub-domain on each side is shown in Fig. 2(b) although each PML region has been actually composed of three sub-domains in the modeling. The loss of this W-type structure is about  $143.02 \text{ dB/m}$ , which can be further reduced by simply increasing the width of the inner cladding layer, where the fields exponentially decay.

Wave absorption in the PML region can be observed in Fig. 2(a), in which the  $\text{Re}[E_y]$  distribution is plotted. For better view of the magnitudes of the main field and the leaky field, we normalize the maximum field value in Fig. 2(a) to 1.0. The PML is placed in the regions  $|x| \geq 7.5 \mu\text{m}$ , where the absorption coefficient of the PML material is growing with increasing  $|x|$ . Transversely propagating leaky waves can be found in the outer cladding layers, and they become weaker as going deeper into the PML region, which will finally become zero as shown. To examine the effect of the PML position on the accuracy and the field profile, we take the W-type structure mentioned with  $N = 14$  as an example and change the width

TABLE I  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL TE MODE OF THE M-TYPE SLAB WAVEGUIDE

$N$	$\text{Re}[n_{\text{eff}}]$	$\text{Im}[n_{\text{eff}}]$
4	1.959859883981541	0.000277972081040
6	1.972708918750655	0.000003930221217
8	1.972708918991630	0.000003930754473
10	1.972708918685354	0.000003930937988
12	1.972708918684282	0.000003930939124
14 ( $\Delta x = 6 \mu\text{m}$ )	1.972708918684277	0.000003930939117
14 ( $\Delta x = 4 \mu\text{m}$ )	1.972708918684279	0.000003930939116
14 ( $\Delta x = 2 \mu\text{m}$ )	1.972708918684279	0.000003930939117
14 ( $\Delta x = 0 \mu\text{m}$ )	1.972708918684279	0.000003930939118

of the outer cladding layer, that is, vary the distance  $\Delta x$  from PML to the inner cladding layer as shown in Fig. 2(c). Four distances,  $\Delta x = 0, 2, 4$ , and  $6 \mu\text{m}$ , are tested, and the resultant  $\text{Re}[E_y]$  profiles in the outer cladding layer and PML region are shown in the figure. Note that the PML widths are fixed with  $8 \mu\text{m}$ , and the vertical dashed lines indicate the start points of the PML region for different  $\Delta x$ 's. The PSFD computed complex effective indexes of these four cases with  $N = 14$  are listed in Table I and all of them are seen to be with accuracy on the order of  $10^{-15}$ , which means that the position where the PML is placed has negligible effects on the computational accuracy.

#### B. M-Type Anti-Resonant Reflecting Optical Waveguide (ARROW)

In addition to guiding by the principle of total internal reflection (TIR), anti-resonance in a Fabry-Perot layer was also known to be capable of being utilized as wave-guiding mechanism [5]–[7]. It is well known that a layer of Fabry-Perot structure can be used as a cavity of wave transmission such that waves can be highly transmitted at resonance or reflected at anti-resonance. Taking advantage of high reflection at anti-resonance, two face-to-face Fabry-Perot layers operated under the anti-resonance condition can support wave-guiding in between, resulting in the so-called anti-resonant reflecting optical waveguide (ARROW). From the transmission spectrum of a Fabry-Perot layer, we know that portion of waves will penetrate the Fabry-Perot layers and outward propagate because the reflectivity  $R$  of each dielectric Fabry-Perot layer cannot reach 100%. Therefore, the ARROW is a leaky waveguide as well. Besides, since the Fabry-Perot layers have higher refractive index than the core and the outer cladding layers, as shown in Fig. 3, this ARROW can also be regarded as an M-type structure, compared to the W-type waveguide in Fig. 2(a).

Two proposed ARROW structures are analyzed here to examine the ability and accuracy of the PSFD method treating such kind of leaky-mode waveguide with multiple interference mechanism. The first M-type structure, case-A, is the one considered in [5]. The core and the outer cladding layers are made of  $\text{SiO}_2$  with  $n = 1.46$ , and the Fabry-Perot layers are made of  $\text{TiO}_2$  with higher index  $n = 2.3$ . The operating wavelength is  $\lambda = 0.6328 \mu\text{m}$ , and the waveguide widths of the core and the Fabry-Perot layers are  $4 \mu\text{m}$  and  $0.089 \mu\text{m}$ , respectively.



TABLE II  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL TE MODE OF THE M-TYPE SLAB WAVEGUIDE

$N$	$\text{Re}[n_{eff}]$ (Case-A)	$\text{Im}[n_{eff}]$ (Case-A)	$\text{Re}[n_{eff}]$ (Case-B)	$\text{Im}[n_{eff}]$ (Case-B)
4	1.457855466583192	0.000005587298538	0.9978547439568767	0.000013218898690
6	1.45785585136149	0.000005398702142	0.9978604800321252	0.000014578997356
8	1.457855851231652	0.000005400603918	0.9978605202336727	0.000014581325891
10	1.457855851273043	0.000005400595700	0.9978605202602324	0.000014581278856
12	1.457855851272849	0.000005400596676	0.9978605202596181	0.000014581278387
14	1.457855851272856	0.000005400596683	0.9978605202596357	0.000014581278392
16	1.457855851272856	0.000005400596683	0.9978605202596358	0.000014581278392

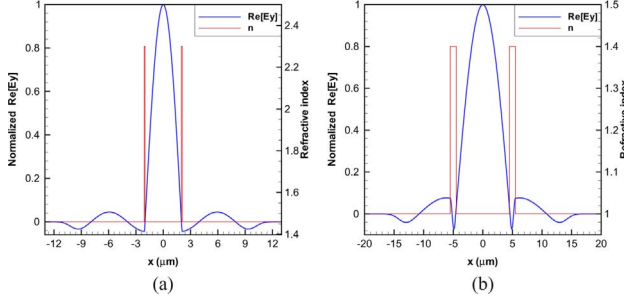


Fig. 3. Structural refractive-index profiles and  $\text{Re}[E_y]$  profiles showing leaky-wave characteristic for the M-type slab waveguide. (a) case-A. (b) case-B.

The second structure, case-B, was proposed in [6], which is an air-core pipe waveguide. Here we consider its 1-D slab structure version first, and the circular structure will be discussed in Subsection IV.E., which has  $n = 1.0$  for the core and the outer cladding layers, and  $n = 1.4$  for the Fabry-Perot layers. The widths for the core and the Fabry-Perot layer are  $9 \mu\text{m}$  and  $1 \mu\text{m}$ , respectively, and the operating wavelength is  $\lambda = 1.2 \mu\text{m}$ .

The PSFD calculated complex effective indexes for the fundamental TE mode for both cases are shown in Table II for different  $N$ s. The leaky modes on this M-type waveguide can also be solved analytically [9], [31], and the obtained exact complex effective indexes for the case-A and case-B structures are  $n_{eff} = 1.457855851272856 + j0.0000054005966836$  and  $0.997860520259636 + j0.000014581278392$ , respectively. Apparently, the PSFD accuracy reaches the order of  $10^{-15}$  for both cases. The  $\text{Re}[E_y]$  profiles for case-A and case-B are shown in Fig. 3(a) and (b), respectively, along with their refractive-index profiles. The modal fields are seen to be mainly distributed between the two Fabry-Perot layers, with those in the outer claddings laterally propagating to both ends. In case-A, the PML regions are defined to be  $|x| \geq 8.089 \mu\text{m}$ , within which the propagating waves gradually decay to zero as shown in Fig. 3(a). Similarly, the PML regions for case-B are taken to be  $|x| \geq 11.5 \mu\text{m}$ , and the laterally going waves are seen to be well absorbed in Fig. 3(b). Notice that the maximum of  $\text{Re}[E_y]$  is normalized to 1.0 in both figures.

### C. Circular Fiber Waveguide

We have shown above that the PSFD method with stretched coordinate PML can accurately solve 1-D leaky waveguide modes with the mechanism of total internal reflection or anti-resonance. We shall then discuss the application of this PSFD method to solve 2-D waveguides. Before studying leaky

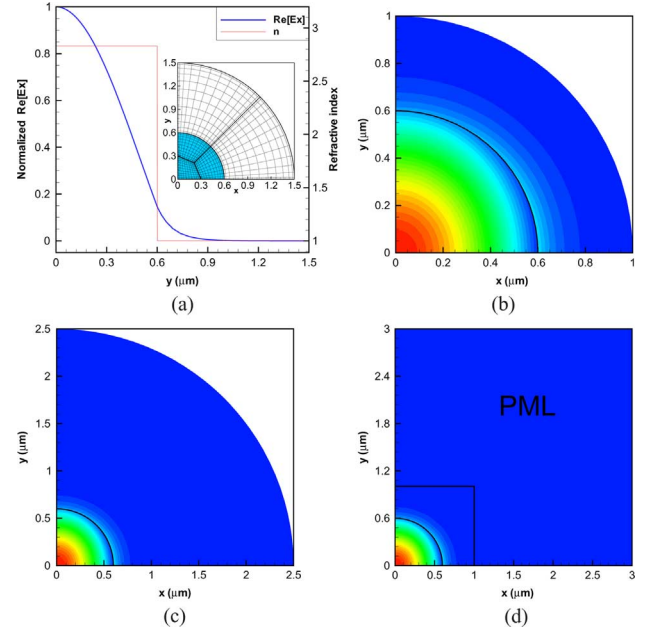


Fig. 4. Electric-field distributions of the  $\text{HE}_{11}$  mode of the circular fiber waveguide. (a)  $\text{Re}[E_x]$  profile along the  $y$ -axis, structural refractive-index profile, and in the inset sub-domain division and grid mesh. (b)  $|E_x|$  profile for the case with  $0.4\text{-}\mu\text{m}$ -radius cladding layer. (c)  $|E_x|$  profile for the case with  $1.9\text{-}\mu\text{m}$ -radius cladding layer. (d)  $|E_x|$  profile for the case with  $0.4\text{-}\mu\text{m}$ -cladding layer and PML.

waveguides, the accuracy of the PSFD analysis of 2-D structures and the effect of PML will be examined first. Circular fiber is a suitable example for examination, and an air-cladded fiber with core radius of  $0.6 \mu\text{m}$  and  $n = \sqrt{8}$  is considered. Because of its structural symmetry, we can analyze just one quarter of the whole structure for acceleration of computation, as shown in the inset of Fig. 4(a), with perfect electric conductor (PEC) or perfect magnetic conductor (PMC) placed at the left and bottom edges, respectively. The inset shows the mesh division using  $N = 12$  and the one-quarter computational domain is partitioned into curvilinear sub-domains, with the shape of the material interface being well fitted with the boundaries of corresponding sub-domains. For this fiber, the analytical effective index for the fundamental  $\text{HE}_{11}$  mode is  $n_{eff} = 2.684019321609156$  when the operating wavelength is  $\lambda = 1.5 \mu\text{m}$  [1].

Three structures are examined. The first one has an air cladding layer of  $0.4\text{-}\mu\text{m}$  thickness as shown in Fig. 4(b), the second one has air cladding layer of  $1.9\text{-}\mu\text{m}$  thickness as depicted in Fig. 4(c), and the third one is similar to the first

TABLE III  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE HE<sub>11</sub> MODE OF THE CIRCULAR FIBER (THE ANALYTICAL  $n_{eff} = 2.684019321609156$ )

$N$	$n_{eff}$ (0.4- $\mu\text{m}$ cladding)	$n_{eff}$ (1.9- $\mu\text{m}$ cladding)	$\text{Re}[n_{eff}]$ (with PML)	$\text{Im}[n_{eff}]$ (with PML)
4	2.684028578565857	2.684817661481339	2.684165820553023	0.000000003635876
6	2.684013318320761	2.684034764094687	2.684021278395971	0.000000000357849
8	2.684013297283687	2.684019429341273	2.684019331653940	0.000000000004183
10	2.684013297272886	2.684019322034613	2.684019321645284	0.000000000000089
12	2.684013297272882	2.684019321610760	2.684019321609498	0.000000000000002
14	2.684013297272882	2.684019321609156	2.684019321609159	0.000000000000001

one but with PML layers added as shown in Fig. 4(d). Note that PEC boundary condition is placed at the outermost edge of the cladding layer, where mode fields are supposed to decay to almost zero there. The PSFD calculated effective indexes with  $N$  varied from 4 to 14 are shown in Table III for these three structures. Apparently, the first case with air cladding layer of 0.4- $\mu\text{m}$  thickness is seem to have only  $10^{-6}$  accuracy, but the second case with air cladding layer of 1.9- $\mu\text{m}$  thickness has  $10^{-15}$  accuracy, instead. This is because the fields exponentially decay in the cladding layer, but not quite close to zero at the outer PEC for the first case since the cladding layer is not thick enough. For the third structure, which is designed with additional PML layers added outside the air cladding of the first case, the accuracy of the PSFD computed effective index is achieved, again, on the order of  $10^{-15}$  when  $N = 14$ . This result reveals that although the PML is placed close to the core-cladding interface with the mode fields not yet decaying to zero at  $x = y = 1 \mu\text{m}$ , such PML arrangement is found to have negligible effects on the calculation accuracy, just like those tests done for the 1-D W-type waveguide in Fig. 2(b). Notice that the imaginary parts of  $n_{eff}$  in the third case in Table III come from the introduction of PML. These non-zero values are not physically meaningful since they are comparatively much smaller than the values of the real parts and can be considered as computation noises. They actually become almost zero as  $N$  is large enough, as seen in Table III.

The  $|E_x|$  profiles are shown in Fig. 4(b), (c), and (d) for the three cases, and the  $\text{Re}[E_x]$  versus  $y$  curve of Fig. 4(c) is shown in Fig. 4(a) along with the structural refractive-index profile. Here we show the 1-D  $E_x$  field along the  $y$ -axis, because it maintains tangential continuity across different materials. The field profiles, in the format of either the absolute value or the real part, shown in the following are all normalized to 1.0, and the profiles of Fig. 4(b), (c), and (d) should be indistinguishable since the field solution differences among them are on the order of  $10^{-6}$ .

#### D. W-Type Circular Waveguide

The first 2-D leaky-mode waveguide to be discussed here is, again, the simplest W-type structure, which has the same guiding mechanism as the 1-D ones. This 2-D W-type waveguide has a circularly symmetric index profile with its radially dependent profile the same as the profile of the 1-D W-type structure in Fig. 2(a), as shown in Fig. 5(a). That is, the core has a radius of  $1 \mu\text{m}$  and  $n = 2.0$ , and the lower-index inner cladding layer has 0.5- $\mu\text{m}$  thickness with  $n = 1.0$ , and the outer cladding layer is of the same material as the core for supporting wave

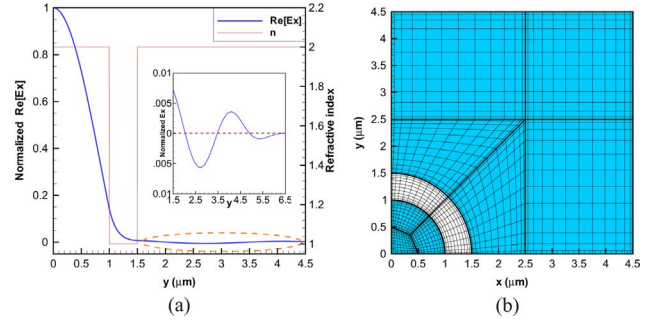


Fig. 5. (a) Structural refractive-index profile and  $\text{Re}[E_x]$  of the HE<sub>11</sub> mode versus  $y$  distribution for the W-type circular waveguide with the enlarged  $\text{Re}[E_x]$  profile for  $1.5 \mu\text{m} < y < 6.5 \mu\text{m}$  in the inset showing the leaky-wave characteristic. (b) Sub-domain arrangement and grid mesh in the computational region.

TABLE IV  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE HE<sub>11</sub> MODE OF THE W-TYPE CIRCULAR WAVEGUIDE

$N$	$\text{Re}[n_{eff}]$	$\text{Im}[n_{eff}]$
4	1.927955256717321	0.000010232110091
6	1.927952220566292	0.000009664157400
8	1.927952222316175	0.000009664102005
10	1.927952222319007	0.000009664102159
12	1.927952222319014	0.000009664102146
14	1.927952222319016	0.000009664102145

leakage. The sub-domain division in one quarter of the structural cross-section is illustrated in Fig. 5(b) for  $N = 12$ . The absorptive PML region is set at  $x \geq 2.5 \mu\text{m}$  and  $y \geq 2.5 \mu\text{m}$ , occupying the three rectangular sub-domains in Fig. 5(b). The PSFD computed complex effective indexes for the fundamental HE<sub>11</sub> mode for different  $N$ s are listed in Table IV, which shows  $10^{-15}$  self-converged accuracy as well. The obtained loss is about 351.6 dB/m, which is larger than that of the 1-D structure and can be reduced by increasing the width of the inner cladding layer.

The  $\text{Re}[E_x]$  profile along the  $y$ -axis is depicted in Fig. 5(a), which shows wave-guiding in the core region, exponentially decaying in the inner cladding layer, sinusoidally propagating in the outer cladding layer, and being absorbed in the PML region. The leaky waves can be seen to be well absorbed in the PML region in the expanded plot shown in the inset of Fig. 5(a). We have found that the position of the PML region has negligible effect on the numerical accuracy. The PSFD computed electric and magnetic mode-field distributions are shown in Fig. 6(a)–(f). It shows that the  $|E_x|$  and  $|H_y|$  profiles are similar, and so are the  $|E_y|$  and  $|H_x|$  profiles, while the  $|E_z|$

TABLE V  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE  $HE_{11}$  MODE OF THE M-TYPE FIBER WAVEGUIDE

$N$	$\text{Re}[n_{eff}]$ (Case-A)	$\text{Im}[n_{eff}]$ (Case-A)	$\text{Re}[n_{eff}]$ (Case-B)	$\text{Im}[n_{eff}]$ (Case-B)
4	1.454972011590725	0.000067964021055	0.995046857892952	0.000107811869149
6	1.454972795382911	0.000067384270784	0.995074543892952	0.000119190084682
8	1.454972795546622	0.000067382511442	0.995074815513635	0.000119172594021
10	1.454972795544452	0.000067382509617	0.995074815411661	0.000119172090879
12	1.454972795544450	0.000067382509619	0.995074815411650	0.000119172090790
14	1.454972795544450	0.000067382509619	0.995074815411650	0.000119172090790

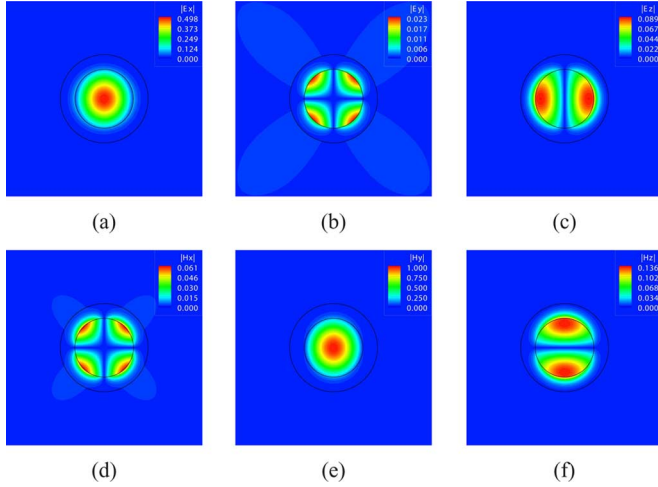


Fig. 6. Field profiles of the  $HE_{11}$  mode of the W-type fiber waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

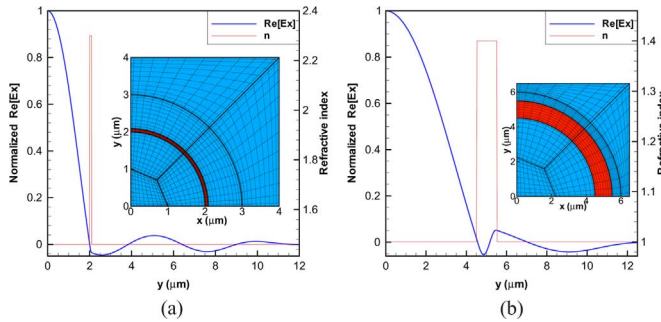


Fig. 7. Structural refractive-index profile and  $\text{Re}[E_x]$  of the  $HE_{11}$  mode versus  $y$  distribution for the M-type circular waveguide with the inset showing the sub-domain arrangement and the grid mesh. (a) case-A. (b) case-B.

and  $|H_z|$  profiles have rotated similarity. Comparing with the standard fiber waveguide, the field patterns are almost similar, except the W-type fiber possesses leaky waves in the outer cladding layer.

#### E. M-Type Circular Waveguide (ARROW Structure)

As in the 1-D case, the 2-D M-type waveguide is an ARROW structure. Again, we consider two circularly symmetric index profiles with their radially dependent profiles the same as those of the 1-D ARROWs plotted in Fig. 3(a) (case-A) and (b) (case-B), respectively, as shown in Fig. 7(a) and (b). In the case-A structure, both the core and the outer cladding are with  $n = 1.46$ , the core radius is  $2 \mu\text{m}$ , and the Fabry-Perot layer is with  $n = 2.3$  and  $0.089\text{-}\mu\text{m}$  thickness. The case-B structure is a pipe waveguide studied in [6] with the following parameters:

core radius of  $9 \mu\text{m}$ , Fabry-Perot layer of thickness  $1 \mu\text{m}$  and  $n = 1.4$ , and the core and the cladding are simply air. The field confinement and leakage property of the 2-D ARROW depends critically on the operating wavelength due to the Fabry-Perot resonant condition. Take case-B as an example, the relationship between the attenuation constant and the operating frequency can be seen in [6], which correlates with the Fabry-Perot wave transmission/reflection spectrum. Here, we choose  $\lambda = 1.2 \mu\text{m}$  at which a Fabry-Perot-layer transmission minimum or an anti-resonance occurs, resulting in better field confinement in the waveguide.

The computational sub-domain partitioning and grid meshes for both cases are shown in the insets of Fig. 7(a) and (b), respectively. The PMLs, not shown in the insets, are located in the region ( $x \geq 6 \mu\text{m}$  and  $y \geq 6 \mu\text{m}$ ) for the case-A structure in Fig. 7(a) and in the region ( $x \geq 6.5 \mu\text{m}$  and  $y \geq 6.5 \mu\text{m}$ ) for the case-B structure in Fig. 7(b). The PSFD computed complex refractive indexes for the fundamental  $HE_{11}$  mode for both structures are listed in Table V for different  $N$ s, which shows self-convergence of accuracy on the order of  $10^{-15}$  in both ones. To examine the wave leakage and PML absorption, we plot in Figs. 7(a) and (b) the respective  $\text{Re}[E_x]$  profiles along the  $y$ -axis. Apparently, the leaky waves can be well absorbed in both cases since it is seen the fields decrease gradually in the PML region and approach zero at the edge of the computational domain.

The PSFD computed electric and magnetic mode-field distributions are shown in Fig. 8(a)–(f) for case-A and in Fig. 9(a)–(f) for case-B, respectively, for comparison. From Table V, we see that  $\text{Im}[n_{eff}]$  for case-B at the considered wavelength is larger than that for case-A, as can be understood from the field distributions in Figs. 8 and 9. The loss of case-B can become smaller if it is operated at other dips in the higher frequency range [6]. The case-B structure has the advantage of avoiding material loss in the core since the guiding core is simply an air region in addition to its simple pipe geometry which can make the manufacturing very easy.

#### F. Microstructured Six-Air-Hole Fiber Waveguide

So far, we have examined the accuracy of the PSFD method with the PML by analyzing several standard 1-D and 2-D W-type and M-type leaky waveguides, and the resultant accuracy has been demonstrated to be on the order of  $10^{-15}$  for all cases. Now, we will apply this PSFD method to solve waveguides with more complicated structures.

First, we consider the popularly studied microstructured six-air-hole fiber [17]–[19], [21], as shown in Fig. 1(d). With the



TABLE VI  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL MODE OF THE SIX-AIR-HOLE WAVEGUIDE FOR THE  $p = 1$  AND  $p = 3$  MODES

$N$	$\text{Re}[n_{eff}] (p = 1)$	$\text{Im}[n_{eff}] (p = 1)$	$\text{Re}[n_{eff}] (p = 3)$	$\text{Im}[n_{eff}] (p = 3)$
4	1.438367658633584	0.000001321295554	1.445395882102650	0.000000042017309
6	1.438364943632872	0.000001432990316	1.445395236589104	0.000000031910666
8	1.438364934410756	0.000001416728792	1.445395232274384	0.000000031944327
10	1.438364934183757	0.000001416477217	1.445395232151004	0.000000031945254
12	1.438364934178938	0.000001416475936	1.445395232149312	0.000000031945250
14	1.438364934178881	0.000001416475992	1.445395232149294	0.000000031945250
16	1.438364934178884	0.000001416475997	1.445395232149295	0.000000031945250

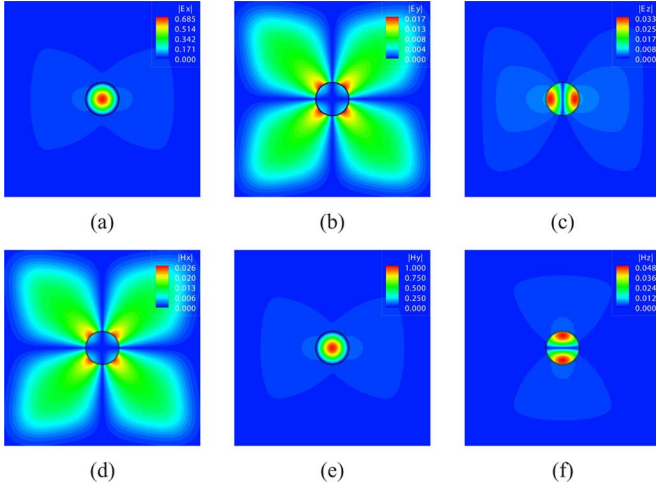


Fig. 8. Field profiles of the  $\text{HE}_{1,1}$  mode of the case-A M-type fiber waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

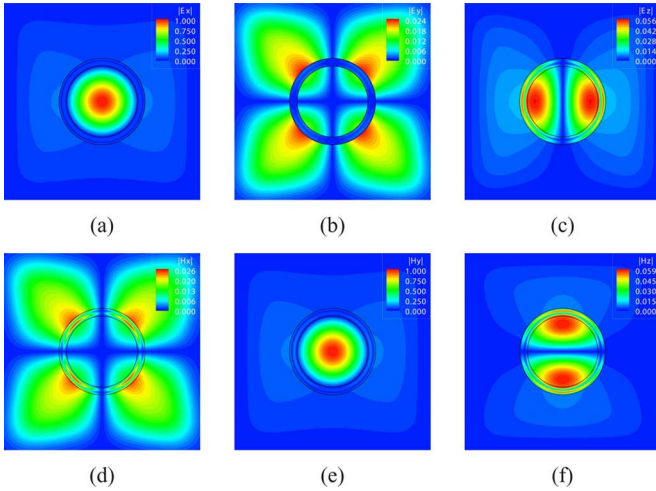


Fig. 9. Field profiles of the  $\text{HE}_{1,1}$  mode of the case-B M-type fiber waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

structural symmetry, we can again treat only one quarter of the waveguide cross-section, as we have done in the previous three circular waveguide structures. According to [17]–[19], and [21], six holes are hexagonally arranged, and the hole pitch, i.e., the center-to-center distance of adjacent holes, is  $\Lambda = 6.75 \mu\text{m}$ . The radius of each hole is  $R = 2.5 \mu\text{m}$ , and the refractive indexes for the fiber and the hole are  $n = 1.45$  and  $1.0$ , respectively. With the cladding extended to infinity, this structure possesses a similar characteristic as the W-type fiber since the six air-holes create an equivalent lower-index ring structure,

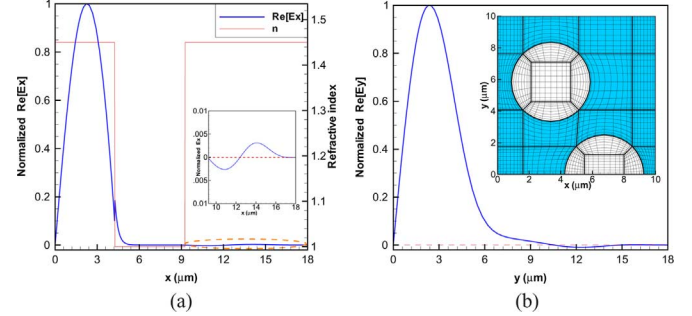


Fig. 10. (a) Structural refractive-index profile along the  $y$ -axis and  $\text{Re}[E_x]$  of the fundamental mode versus  $x$  distribution for the six-air-hole waveguide with the enlarged  $\text{Re}[E_x]$  profile for  $9 \mu\text{m} < x < 18 \mu\text{m}$  in the inset showing the leaky-wave characteristic. (b)  $\text{Re}[E_y]$  versus  $y$  distribution with the inset showing the sub-domain arrangement and grid mesh.

making the structure to support leaky modes with complex effective indexes.

The  $p = 1$  and  $p = 3$  modes, as defined in [17] and [18], are considered here at  $\lambda = 1.45 \mu\text{m}$ . The PSFD computed complex effective indexes for these two modes are listed in Table VI for different  $N$ s. Accuracy of self-convergence on the order of  $10^{-14}$  is observed for this complicated structure. According to the result of the multipole method proposed in [18], the computed effective index for this  $p = 1$  mode was  $n_{eff} = 1.43836493424529 + j0.00000141647574$ , which agrees well with our results to  $10^{-9}$  for the real part and to  $10^{-12}$  for the imaginary part. On the other hand, as mentioned in the Introduction, a new high-order boundary-integral-equation (BIE) method was reported recently and shown to achieve exponential convergence and extremely high accuracy [19]. The computed effective index for the  $p = 3$  mode provided in [19] is  $n_{eff} = 1.4453952321493 + j0.00000003194529$ , which agrees with our results to the order of  $10^{-13}$  for both the real and imaginary parts.

To observe the leaky waves and their attenuations in the PML layer,  $\text{Re}[E_x]$  versus  $x$  and  $\text{Re}[E_y]$  versus  $y$  profiles are shown in Fig. 10(a) and (b), respectively. Since scanning of  $E_x$  along the  $x$ -axis will pass through the air-hole, discontinuity of  $\text{Re}[E_x]$  would occur, as can be seen in Fig. 10(a). Domain partitioning and grid meshes in the computation are shown in the inset of Fig. 10(b). Again, one quarter the waveguide cross-section is treated and the PML, not shown in Fig. 10(b), is designed to be in the region ( $x \geq 10 \mu\text{m}$  and  $y \geq 10 \mu\text{m}$ ). From the inset in Fig. 10(a), the field can be seen well absorbed in the PML region and approaching zero eventually.

The PSFD computed electric and magnetic mode-field distributions are shown in Fig. 11(a)–(f) for the  $p = 1$  mode and in

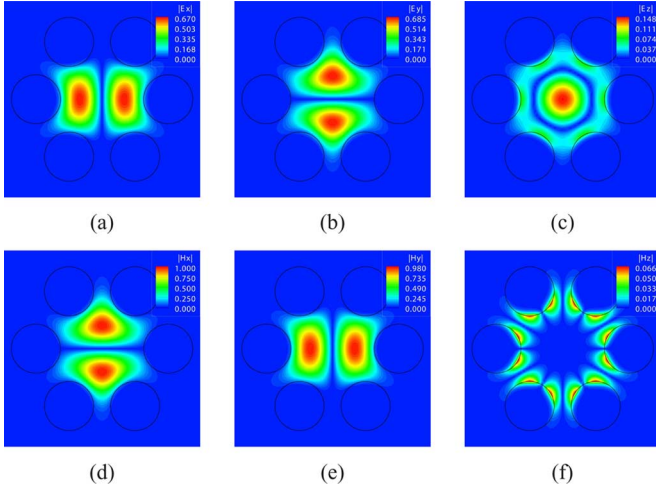


Fig. 11. Field profiles of the  $p = 1$  mode of the six-air-hole fiber waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

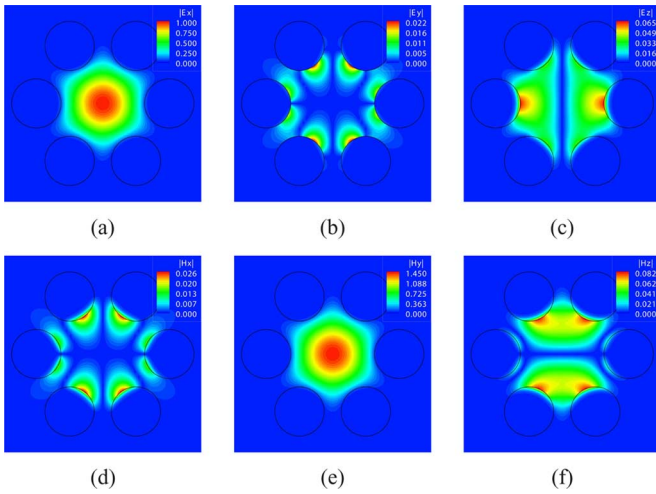


Fig. 12. Field profiles of the  $p = 3$  mode of the six-air-hole fiber waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

Fig. 12(a)–(f) for the  $p = 3$  mode, which are similar to those presented in [17] and [21]. Similar to the standard circular fibers, the  $|E_x|$  and  $|H_y|$  profiles are alike, and so are the  $|E_y|$  and  $|H_x|$  profiles.

Up to now we have analyzed four kinds of 2-D waveguides with round material interfaces, and the PSFD computed effective indexes are listed in Tables III, IV, V, and VI, respectively. Based on the data in the tables, as a useful summary, we calculate and plot the errors of  $n_{eff}$  versus  $N$  in Fig. 13(a)–(d) to show the respective characteristics of numerical convergence of the developed PSFD mode solver. For each  $N$ , the error of  $n_{eff}$  is defined as the absolute value of the difference between the calculated  $n_{eff}$  and an accurate reference  $n_{eff}$ . Fig. 13 is presented in logarithmic scales, and exponential convergence of computational accuracy is observed in all four cases, which means that numerical errors can be fast reduced by a relatively small increase in the number of grid points. Note that the calculated errors in Fig. 13(a) are based on the data assuming the air cladding layer is of  $1.9 \mu\text{m}$  thickness and the reference  $n_{eff}$  being the analytical solution, while the reference  $n_{eff}$ s for Fig. 13(b)–(d) are respectively those  $n_{eff}$ s corresponding

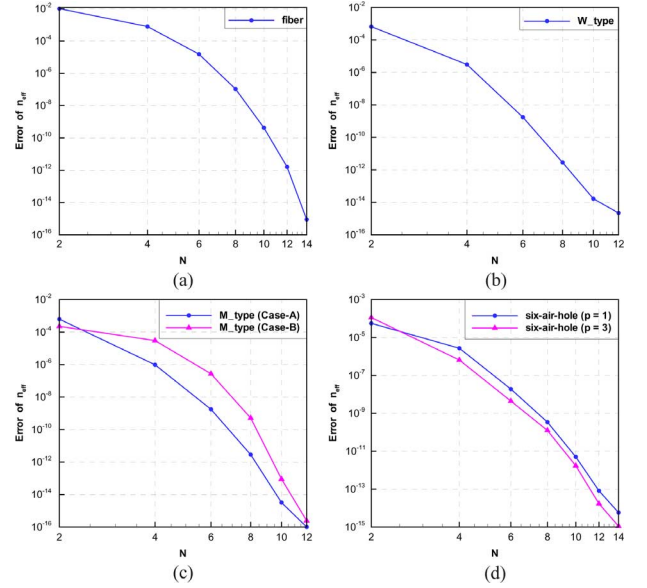


Fig. 13. Exponential convergence characteristics of the error of  $n_{eff}$  versus  $N$ . (a) The circular fiber. (b) The W-type circular fiber. (c) The M-type circular fiber. (d) The six-air-hole fiber waveguide.

to the respective maximum  $N$  value in Tables IV, V, and VI. Regarding computer resources used, we provide the following data for the case of the circular fiber obtained using one core on a 2.66-GHz Intel® Core™ i7-920 PC machine. With  $N = 4, 6, 8, 10, 12$ , and  $14$ , the corresponding computation times are 4.14 s, 20.4 s, 68.11 s, 212.38 s, 443.58 s, and 783.13 s, respectively, the matrix sizes are 1050, 2058, 3402, 5082, 7098, and 9450, respectively, and the memories taken are 1864 kB, 2112 kB, 2356 kB, 2676 kB, 3120 kB, and 3588 kB, respectively. It can be seen our program uses small memories. Fig. 13(a) reveals that with  $N = 8$  the error of  $n_{eff}$  already goes down to the practically impressive order of  $10^{-7}$ .

### G. RIB Waveguide

We have analyzed several leaky-mode waveguides with circular interfaces, and the PSFD method is shown to give  $10^{-15}$  accuracy through self-convergence tests. It has been shown in [24] that using the PSFD method for analyzing (nonleaky) dielectric channel waveguides with sharp dielectric corners can provide only  $10^{-8}$  accuracy in the effective index with  $N = 10$ ; with  $N = 16, 24$ , and  $40$ , the accuracy improves to  $10^{-9}$ ,  $10^{-10}$ , and  $10^{-11}$ , respectively. The convergence characteristic is not an exponential one as in the 2-D waveguides without corners discussed so far but more with a first-order convergent rate. This is due to that the sharp dielectric corners are associated with electric-field singular points, which ruins the computation [24].

Below, we will consider two rectilinear waveguides, the rib waveguide and the photonic wire waveguide, as shown in Fig. 1(e) and (f), respectively. First, in this subsection, the rib waveguide is examined. The waveguide structure is the same as that studied in [29]. Referring to Fig. 1(e), the thicknesses in the rib region are  $H = 1.0 \mu\text{m}$  and  $h = 0.5 \mu\text{m}$ , the rib width is  $W = 3.0 \mu\text{m}$ , and  $n = 1.0$  (air), 3.44, and 3.4 for the upper cladding, the core, and the substrate, respectively. The operating wavelength is  $\lambda = 1.15 \mu\text{m}$ . The fundamental

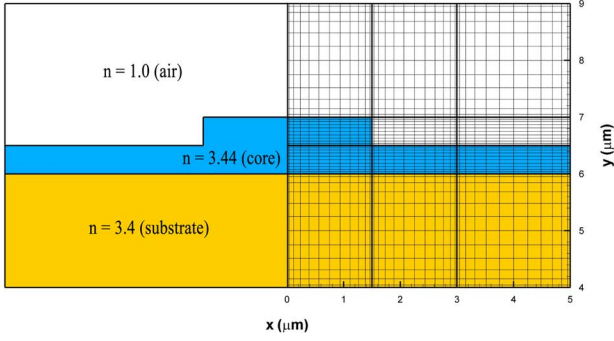


Fig. 14. Sub-domain arrangement and grid mesh for the rib waveguide.

TABLE VII  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL TE MODE OF THE RIB WAVEGUIDE

$N$	$n_{eff}$
4	3.414329827640850
6	3.413414917379402
8	3.413183007067949
10	3.413138730115563
12	3.413132756729537
14	3.413132183989132
16	3.413132136900558
20	3.413132130779760
24	3.413132132794152
28	3.413132135245575
32	3.413132137218818

TE guided mode of this rib waveguide is not a leaky one, but it is a good case for examining the effect of the sharp corners in a more complicated waveguide structure than the simple channel waveguide, since it has long been an example for benchmarking waveguide mode solvers including in [32]. And such examination would be useful before studying the photonic wire waveguide in the next subsection. Fig. 14 shows the rib waveguide structure and the designed sub-domain arrangement for half structure due to symmetry. PML regions (not shown) are put outside the right, bottom, and top sides with thicknesses  $6 \mu\text{m}$  (three sub-domain layers),  $4 \mu\text{m}$  (two sub-domain layers), and  $2 \mu\text{m}$  (one sub-domain layer), respectively. The PSFD computed effective indexes for different  $N$ s are listed in Table VII, and the finite-difference method obtained value of  $n_{eff} = 3.413132 \pm 3 \times 10^{-6}$  provided in [32] is used for comparison. Apparently, the PSFD calculation reaches 3.413132 when  $N = 12$ , and then the convergent rate slows down. However, with larger  $N$  used, as seen in Table VII for  $N$  from 16 to 32, better accuracy can be obtained, and we can achieve two more accuracy digits than that in [32], i.e.,  $n_{eff} = 3.41313214$  (after rounding) with self-convergent accuracy on the order  $10^{-8}$ .

The calculated  $|E_x|$ ,  $|E_y|$ ,  $|E_z|$ ,  $|H_x|$ ,  $|H_y|$ , and  $|H_z|$  profiles for the fundamental TE mode are shown in Fig. 15(a)–(f), respectively. The mode fields are well guided in the thicker portion of the rib region, and field singular points can be seen in Fig. 15(b).

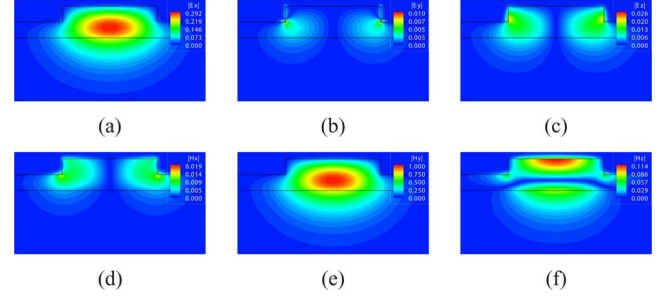
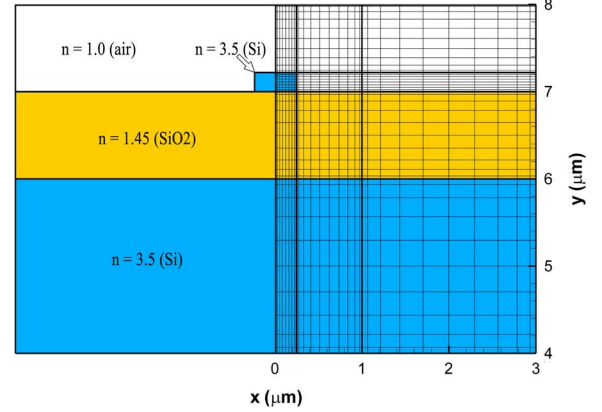
Fig. 15. Field profiles of the fundamental TE mode of the rib waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

Fig. 16. Sub-domain arrangement and grid mesh for the photonic wire waveguide.

#### H. Photonic Wire Waveguide

The photonic wire waveguide or photonic wire has been an essential structure in recently developed high-density photonic integrated circuits, and the computed effective indexes of its fundamental mode have been compared among ten different numerical methods or solvers in [30]. As shown in Fig. 16, the guiding core and the substrate are both made of silicon with  $n = 3.5$  and there is a  $\text{SiO}_2$  buffer layer between them with  $n = 1.45$ . The upper cover medium is air, resulting in a high-index-contrast structure. The rectangular core has of course sharp corners. One important characteristic is that the limited thickness of the  $\text{SiO}_2$  buffer causes the fundamental mode to leak power into the substrate, and the accurate determination of  $\text{Im}[n_{eff}]$  becomes a main concern. To compare with the results in [30], we adopt the same parameters: the width and the height of the core being  $0.5 \mu\text{m}$  and  $0.22 \mu\text{m}$ , respectively, the thickness of the buffer layer being  $1.0 \mu\text{m}$ , and  $\lambda = 1.55 \mu\text{m}$ . The designed sub-domain arrangement for half structure is also shown in Fig. 16. Again, PML regions (not shown) are put outside the right, bottom, and top sides with thicknesses  $4 \mu\text{m}$  (three sub-domain layers),  $4 \mu\text{m}$  (two sub-domain layers), and  $2 \mu\text{m}$  (one sub-domain layer), respectively. The PSFD computed complex effective indexes for different  $N$ s are listed in Table VIII, and with  $N$  up to 32. From the convergence trend, we would have confidence that  $\text{Re}[n_{eff}] = 2.41237$  (order of  $10^{-5}$  accuracy) and  $\text{Im}[n_{eff}]$  falls between  $2.91 \times 10^{-8}$  and  $2.92 \times 10^{-8}$ , showing slow convergent rate for this high-index-contrast structure with corners compared with all cases discussed above.

The calculated effective indexes by ten different methods or solvers, as given in Table VI of [30], are similarly listed in



TABLE VIII  
PSFD COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL MODE OF THE PHOTONIC WIRE WAVEGUIDE

$N$	$\text{Re}[n_{eff}]$	$\text{Im}[n_{eff}]$
4	2.390482909644422	$2.2502459 \times 10^{-8}$
6	2.412928964014647	$3.0647138 \times 10^{-8}$
8	2.412454190888035	$4.9832197 \times 10^{-8}$
10	2.412413768252360	$3.5744559 \times 10^{-8}$
12	2.412398013885063	$2.3180120 \times 10^{-8}$
14	2.412389601631874	$4.5563542 \times 10^{-8}$
16	2.412384521810727	$3.1565139 \times 10^{-8}$
20	2.412379043823438	$3.0185470 \times 10^{-8}$
24	2.412376369646066	$2.9509228 \times 10^{-8}$
28	2.412374903200264	$2.9279178 \times 10^{-8}$
32	2.412374029676081	$2.9198372 \times 10^{-8}$

TABLE IX  
COMPUTED EFFECTIVE INDEXES FOR THE FUNDAMENTAL MODE OF THE PHOTONIC WIRE WAVEGUIDE FROM TEN METHODS AS LISTED IN TABLE VI OF [30] AND FROM THE PSFD METHOD

Method	$\text{Re}[n_{eff}]$	$\text{Im}[n_{eff}]$
Effective index	2.45	$2.4 \times 10^{-3}$
Perturbation	2.35	$3.0 \times 10^{-7}$
BPM Obayya	2.413340	$2.7 \times 10^{-8}$
FEM Uranus	2.4131	$2.97 \times 10^{-8}$
FEM Parma	2.41233	$2.45 \times 10^{-8}$
Olympios	2.413	$2.9 \times 10^{-8}$
FimmWave	2.41235	$2.688 \times 10^{-8}$
CAMFR	2.412372	$2.9135 \times 10^{-8}$
Aperiodic Fourier modal	2.412372	$2.91348 \times 10^{-8}$
Plane wave admittance	2.4126	$2.910 \times 10^{-8}$
PSFD (this work)	2.412374	$2.9198 \times 10^{-8}$

Table IX together with our PSFD result using  $N = 32$  for comparison. It was concluded in [30] that for  $\text{Re}[n_{eff}]$ , four solvers agree on five significant digits 2.4123 with CAMFR and aperiodic fourier modal method even agreeing up to seven significant digits, and for  $\text{Im}[n_{eff}]$ , three solvers agree on three significant digits  $2.91 \times 10^{-8}$  with CAMFR and aperiodic fourier modal method again agreeing on five significant digits after rounding. It is seen that our PSFD result agrees with CAMFR and aperiodic fourier modal method on six significant digits for  $\text{Re}[n_{eff}]$  (2.41237) and with a deviation less than  $0.01 \times 10^{-8}$  for  $\text{Im}[n_{eff}]$  ( $2.92 \times 10^{-8}$  after rounding). As mentioned in the first paragraph of the previous subsection for rib waveguide, the sharp dielectric corners are with electric-field singular points and ruin the spectral convergence [24]. Therefore, although Table III shows the possible decreasing trend for the values of both  $\text{Re}[n_{eff}]$  and  $\text{Im}[n_{eff}]$ , such decrease would be slow with  $N$ . We did not pursue further computation since the  $N = 32$  one has already been expensive.

Fig. 17 shows the  $\text{Re}[E_x]$  profile along the  $y$ -axis at  $x = 0$  together with the waveguide refractive-index profile. The mode field is seen mostly guided in the core, decaying in the  $\text{SiO}_2$  buffer layer, leaking into the Si substrate, and absorbed by the PML layer. The PML is placed at  $y < 4 \mu\text{m}$  (substrate) and the enlarged field profile depicted in the inset of Fig. 17 clearly shows the leaky behavior and the well-absorption by the PML.

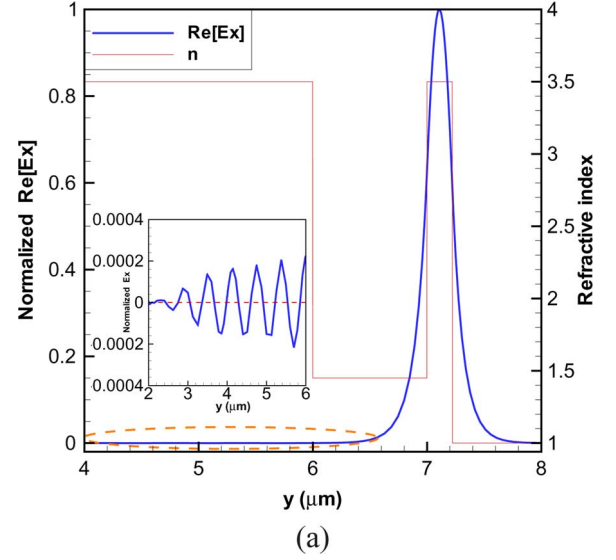


Fig. 17. Structural refractive-index profile along the  $y$ -axis at  $x = 0$  and  $\text{Re}[E_x]$  of the fundamental mode versus  $y$  distribution at  $x = 0$  for the photonic wire waveguide with the enlarged  $\text{Re}[E_x]$  profile for  $2 \mu\text{m} < x < 6 \mu\text{m}$  in the inset showing the leaky-wave characteristic.

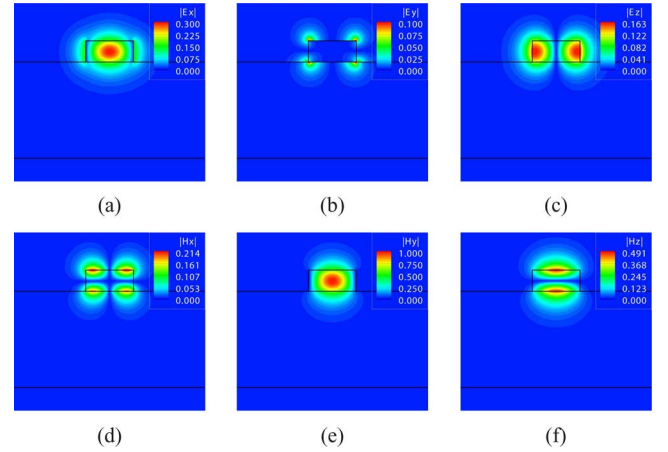


Fig. 18. Field profiles of the fundamental mode of the photonic wire waveguide. (a)  $|E_x|$ . (b)  $|E_y|$ . (c)  $|E_z|$ . (d)  $|H_x|$ . (e)  $|H_y|$ . (f)  $|H_z|$ .

The PSFD calculated  $|E_x|$ ,  $|E_y|$ ,  $|E_z|$ ,  $|H_x|$ ,  $|H_y|$ , and  $|H_z|$  profiles for the fundamental mode are shown in Fig. 18(a)–(f), respectively. The field singular points can be seen in Fig. 18(b).

## V. CONCLUDING REMARKS

We have incorporated the stretched coordinate PMLs into the recently developed pseudospectral frequency-domain (PSFD) method waveguide mode solver which employs a penalty scheme [24] so that leaky modes can be determined with high-accuracy complex effective indexes. Applications of the new PSFD solver to several standard leaky-mode slab and circular waveguides, including the W-type and M-type ones, demonstrate that computational accuracy for the effective indexes of their fundamental modes can be on the order of  $10^{-15}$ . For the popularly studied more complicated microstructured six-air-hole fiber, our PSFD solver can achieve self convergence of accuracy in the effective index on the order of  $10^{-14}$ , and the comparison with a new high-order boundary-integral-equation (BIE) method reported recently [19] shows that



the agreement between the two solvers is up to the order of  $10^{-13}$  for both the real and imaginary parts of the computed effective index for the  $p = 3$  mode. As for rectilinear waveguides with sharp corners, PSFD analyses of the rib waveguide and the photonic wire have been conducted. As investigated in [24], sharp dielectric corners are associated with electric-field singular points and ruin the exponential-convergence characteristic of the PSFD computation. Nevertheless, compared with the prior high-accuracy finite-difference analysis of the rib waveguide in [32], we can achieve two more accuracy digits, with self-convergent accuracy on the order  $10^{-8}$ , for the computed effective index of the fundamental TE mode. For the high-index-contrast photonic wire with substrate leakage, the PSFD solver provides an effective index for the fundamental mode close to the possible best results offered by CAMFR and aperiodic fourier modal method among ten methods compared in [30] with the agreement on six significant digits for the real part and on three digits for the imaginary part.

Some remarks regarding the advantages of this proposed PSFD method waveguide mode solver are addressed below. Solving second-order Helmholtz equations in terms of the two transverse-magnetic field components has been a popular approach in full-vectorial waveguide analysis. The PSFD formulation of [21] was based on such approach with PMLs implemented. The present PSFD formulation is constructed using first-order differential equations written from Maxwell's equations and the six field components are included. Obviously, under the same sub-domain arrangement, the number of unknowns becomes larger, which could be the major disadvantage. In [24], on which the present formulation is based, the possibility of reducing the total number of discrete equations as well as the field components included to reduce the computational work has been discussed in its concluding remarks, where it was also pointed out that one advantage of the first-order-equation formulation is its easiness to include tensor permittivity in the waveguide structure. One useful aspect of directly obtaining six field components from the waveguide analysis lies in the combined application of the PSFD and PSTD methods in analyzing or simulating some device structures involving waveguide input. The complete profiles of the six field components of the input waveguide eigenmode can be readily used as the input functions to the PSTD computation with the same sub-domain mesh arrangement considered in the waveguide-mode calculation and the time-domain simulation.

One key technique utilized in the present formulation is the same penalty scheme formulated in [24] for treating interface boundary conditions between adjacent sub-domains although we make the generalization here by implementing the stretched coordinate PML. Note that in the PSFD method of [21], directly matching interface conditions was employed. As discussed also in Subsection V.B in [33] which reported a PSFD method for solving scattering problems, the penalty scheme provides an edge-by-edge approach to impose interface conditions between sub-domains and it avoids the problematic issue of specifying a unique normal vector at a vertex point of a sub-domain by specifying two normal vectors at the vertex point using the normal vectors on the edges that intersect at the vertex. Every vertex point is thus enforced with two penalty interface conditions. We

have found that the numerical convergence behavior through this penalty treatment appears to be better than that of [21] using the direct matching of interface conditions. One example is the analysis of the  $p = 3$  mode shown in Table VI of the six-air-hole waveguide. Some comparison between the analysis results of [19] and [21] for this mode was discussed in Section V of [19], which showed an agreement not as superior as that between those of [19] and this work.

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