A Mode-Preserving Perfectly Matched Layer for Optical Waveguides

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***Abstract*—For numerical simulation of wave propagation in optical waveguides, we develop a mode-preserving boundary condition for the popular perfectly matched layer (PML) which truncates the unbounded transverse plane. The method is particularly useful for single mode longitudinally varying wave-guiding structures and it is easy to use for step-index planar waveguides. With this boundary condition, accurate numerical solutions can be obtained in a much smaller computational window. Numerical results based on the beam propagation method for a tapered waveguide are used to demonstrate the capacity of this boundary condition.**

***Index Terms*— Perfectly matched layer, optical waveguides, optical propagation, approximation methods, beam propagation method.**

I. INTRODUCTION

An optical waveguide is typically an open waveguide with an unbounded transverse plane. Numerical simulation of wave fields propagating in an optical waveguide can only be carried out in a finite computational domain. Therefore, it is important to use accurate transverse boundary conditions or absorbing layers to simulate the radiation condition which allows only outgoing waves to propagate away from the waveguide axis [1]. The perfectly matched layer (PML) [2]-[4] is a popular method for truncating an unbounded domain for wave propagation problems. It corresponds to a complex coordinate stretching that changes a transverse variable x to $\hat{x} = x + i\int_0^x \sigma(\tau)d\tau$, where σ is a prescribed function. The effect of this transformation is to force the outgoing waves to decay exponentially in the x direction (away from the axis of the waveguide). At the boundary of the computational domain, simple boundary conditions such as $u = 0$ are typically used.

For waveguide problems, it is important to minimize the side-effect of the PML on propagating modes. Using a PML of finite thickness, the propagation constant becomes complex. Although the imaginary part is typically very small, it leads to unphysical power gain or loss. The error can be significant if the mode is propagated for a large distance in the waveguide.

In this letter, we propose a boundary condition for the PML that can preserve the fundamental propagating mode. It is useful for simulations of wave propagation in slowly varying waveguides, especially step-index planar waveguides. We demonstrate the effect of this boundary condition for transverse magnetic (TM) waves propagating in a tapered waveguide [5] using the beam propagation method (BPM) [6]-[13]. Notice that the method applies equally well to the transverse electric case.

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II. MODE-PRESERVING PML

For TM polarized waves in a planar wave-guiding structure, the governing equation is the Helmholtz equation:

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

where k_0 is the wavenumber in vacuum, $n = n(x, z)$ is the refractive index, z is a variable along the axis of the waveguide, x is the transverse variable and u is the y-component of the magnetic field. The time dependence is $e^{-i\omega t}$ for a angular frequency ω. If the refractive index is a constant, say $n = n_+$, for $x \ge H_+ > 0$, we can define a continuous function σ, such that $\sigma(x) = 0$ for $x \le H_+$ and $\sigma(x) \ne 0$ for $x > H_+$. Similarly, if $n = n_-$ for $x \le H_- < 0$, the function σ is changed to non-zero for $x < H_-$. For the PML, we introduce the complex variable

$$\hat{x} = x + i\int_0^x \sigma(\tau)d\tau, \qquad (2)$$

and replace ∂_x in (1) by $\partial_{\hat{x}}$. This leads to

$$n^2\partial_z\left(\frac{1}{n^2}\partial_z u\right) + \frac{n^2}{1+i\sigma}\partial_x\left(\frac{n^{-2}}{1+i\sigma}\partial_x u\right) + k_0^2 n^2 u = 0. \qquad (3)$$

For practical numerical computation, the variable x is truncated to $D_- < x < D_+$, where $D_+ > H_+$ and $D_- < H_-$. The actual PML corresponds to the intervals (H_+, D_+) and (D_-, H_-) in which the equations (1) and (3) are different. Boundary conditions at $x = D_+$ and $x = D_-$ are needed for (3). Usually, simple boundary conditions such as $u = 0$ are used.

The effect of the PML can be understood through a reflection coefficient calculation. Assume that the refractive index n is also the constant n_+ for x slightly less than H_+, that is, $n = n_+$ for $x > H_+ - \delta$, where δ is a small positive constant. The Helmholtz equation (1) supports the plane wave solution $u^+ = e^{i(\alpha x+\beta z)}$ (for $x > H_+ - \delta$) that propagates toward $x = +\infty$. Here $\alpha^2 + \beta^2 = k_0^2 n_+^2$ and $\alpha > 0$. For the modified equation (3), the boundary condition $u = 0$ at $x = D_+$ gives rise to a reflected wave $u^- = Re^{i(-\alpha x+\beta z)}$ for $H_+ - \delta < x \le H_+$. The reflection coefficient R satisfies

$$|R| = e^{-2\alpha\int_{H_+}^{D_+}\sigma(\tau)d\tau}.$$

If σ is real and positive for $x > H_+$, the above coefficient can be small. For a propagating mode with the propagation constant β, say $u = e^{-\gamma(x-H_+)+i\beta z}$ for $x \ge H_+$, where $\gamma = \sqrt{\beta^2 - k_0^2 n_+^2} > 0$, the PML with the boundary condition $u = 0$ at $x = D_+$ again induces a reflected wave $Re^{\gamma(x-H_+)+i\beta z}$ for $H_+ - \delta < x \le H_+$. The reflection coefficient satisfies

$$|R| = e^{-2\gamma(D_+ - H_+)},$$

if σ is real. Clearly, the magnitude of R is related to the natural decay rate γ of the mode and it is not related to σ in the PML [3]. For a weakly guided mode, γ is small, the mode decays slowly in the cladding region and a large D_+ is necessary to reduce the undesired reflection from the boundary.

With the PML and simple boundary conditions at $x = D_+$ and $x = D_-$, a mode corresponding to an eigenfunction of the modified transverse operator $(1+i\sigma)^{-1}\partial_x[(1+i\sigma)^{-1}\partial_x \cdot] + k_0^2 n^2$ usually has a complex propagation constant. Although the imaginary part of the propagation constant is small, it gives rise to exponential increase or decrease in the propagation direction. For waveguide problems, the length scale in the z direction is much larger than the wavelength, thus the small imaginary part of the propagation constant can lead to significant error in the computed solution. One way to reduce this side-effect is to enlarge the computational domain, but the computation cost is also increased. Our approach is to use the following mode-preserving boundary conditions at $x = D_+$ and $x = D_-$:

$$\partial_x u = -[1 + i\sigma(D_+)]\sqrt{\beta^2 - k_0^2 n_+^2}\, u \quad \text{at} \ \ x = D_+, \qquad (4)$$

$$\partial_x u = [1 + i\sigma(D_-)]\sqrt{\beta^2 - k_0^2 n_-^2}\, u \quad \text{at} \quad x = D_-, \qquad (5)$$

where β is the propagation constant of the fundamental propagating mode of the waveguide. Our interest is to use the above boundary conditions for wave propagation simulations in slowly varying waveguides. Therefore, the propagating mode is defined locally for each z and β varies with z. In the original open waveguide, the propagating mode decays in the increasing x direction exponentially as $\exp\{-\sqrt{\beta^2 - k_0^2 n_+^2} x\}$ for $x > H_+$. When the complex coordinate change (2) is applied, it turns to $\exp\{-\sqrt{\beta^2 - k_0^2 n_+^2}\hat{x}\}$. Therefore, we have

$$\partial_{\hat{x}} u = (1+i\sigma)^{-1}\partial_x u = -\sqrt{\beta^2 - k_0^2 n_+^2}\, u$$

for $x > H_+$. Equation (4) is simply the above condition at $x = D_+$.

Notice that the boundary conditions (4) and (5) only preserve one propagating mode. For a multi-mode waveguide, the propagation constants of other modes will still have undesired imaginary parts. Our approach is thus useful for those waveguides when the local leading propagating mode dominates the wave field. Also, the propagation constant β is in general unknown and it has to be calculated or estimated. Fortunately, for planar step-index waveguides, β can be easily calculated.

III. Numerical Results

For a numerical example, we consider a tapered waveguide studied earlier in [5]. This is a step index waveguide with n=3.3 in the core and n=3.17 in the cladding. The core is given by $0 < x < d(z)$, where $d(z) = 0.2\,\mu m$ for $z \le 0$, $d(z) = 0.1\,\mu m$ for $z \ge a$ and d is continuous and linear for $0 < z < a$. The length a is determined from an opening angle of $0.1°$. That is, $a = 0.1\cot(0.1\pi/180) = 57.296\,\mu m$. The waveguide is excited by the local fundamental mode at the input side ($z = 0$). The free space wavelength is $\lambda = 1.55\,\mu m$.

For such a slowly varying waveguide where the wave field is dominated by its component propagating in one direction along the waveguide, the beam propagation method (BPM) [6]-[8] can be used. In this letter, we use the energy-conserving one-way equation [11]-[13]:

$$\partial_z \phi = ik_0 n_* \frac{1}{n}\sqrt{1+X}(n\phi) \ \text{for} \ \phi = \frac{1}{n}(1+X)^{1/4}u, \qquad (6)$$

where n_* is a reference refractive index and

$$X = \frac{1}{k_0^2 n_*^2}\left[\frac{n^2}{1+i\sigma}\frac{\partial}{\partial x}\left(\frac{n^{-2}}{1+i\sigma}\frac{\partial}{\partial x}\right) + k_0^2 n^2 - k_0^2 n_*^2\right].$$

The use of ϕ implies that the power flux is continuous even at a longitudinal discontinuity of the waveguide. Padé approximants of $(1+X)^{\pm 1/4}$ can be used to efficiently transform u to ϕ or ϕ to u. Equation (6) can be discretized based on a Padé approximant of the operator $P = \exp\{is\sqrt{1+X}\}$, where s is proportional to the step size in z.

In our calculations, the function σ that defines the PML is given by

$$\sigma(x) = \alpha_\pm \tau^3/(1+\tau^2) \quad \text{for} \quad \tau = (x - H_\pm)/(D_\pm - H_\pm),$$

where $x \in (H_+, D_+)$ or $x \in (D_-, H_-)$. The coefficients α_+ and α_- are positive parameters. The mode-preserving boundary conditions (4) and (5) keep the propagation constant (of the fundamental propagating mode) unchanged when the PML is used. This is the ideal result where the exact eigenmode of the transverse operator is concerned. In practical BPM calculations, the transverse operator will be discretized. Here, we compare the numerical values of the propagation constant for the fundamental mode at $z = 0$ using the simple zero boundary condition ($u = 0$ at $x = D_+$ and $x = D_-$) and our boundary conditions (4,5). We choose $D_+ = -D_- = 1\,\mu m$, $H_+ = -H_- = 0.8\,\mu m$ and $\alpha_+ = \alpha_-$. The exact value of the propagation constant is $12.9054\,(\mu m)^{-1}$. The transverse operator is approximated by a tridiagonal matrix based on a second order finite difference method using the grid size $\delta x = 0.005\,\mu m$. The numerical values of the propagation constant are calculated as a matrix eigenvalue problem and are listed in Table 1. A set of different values of $\alpha_\pm$ is used for comparison. Clearly, when x is discretized, the mode-preserving boundary conditions are still more accurate than the simple zero boundary condition.

To simulate the propagation and interaction of various modes in a slowly varying waveguide, the BPM can be used. For this purpose, we first calculate a reference solution. This is obtained with a large computational window where the effect of PML is negligible. We choose $D_+ = -D_- = 10\,\mu m$, $H_+ = -H_- = 9.8\,\mu m$, $\alpha_+ = \alpha_- = 40$ and use the simple zero boundary condition $u = 0$ at $x = D_\pm$. The energy-conserving equation (6) is used in our calculations and it is

TABLE I

NUMERICAL VALUES OF THE PROPAGATION CONSTANT FOR THE FUNDAMENTAL MODE AT $z = 0$. THE EXACT VALUE IS $\beta = 12.9054\,(\mu m)^{-1}$.

$\alpha_\pm$	zero boundary condition	mode-preserving PML
10	$12.888 + 2.62 \times 10^{-2} i$	$12.9049 + 3.01 \times 10^{-4} i$
20	$12.913 + 2.47 \times 10^{-2} i$	$12.9053 + 5.54 \times 10^{-4} i$
30	$12.924 + 9.76 \times 10^{-3} i$	$12.9057 + 4.89 \times 10^{-4} i$
40	$12.921 - 2.73 \times 10^{-3} i$	$12.9059 + 2.47 \times 10^{-4} i$
50	$12.916 - 9.60 \times 10^{-3} i$	$12.9060 - 6.52 \times 10^{-5} i$
60	$12.909 - 1.22 \times 10^{-2} i$	$12.9058 - 3.67 \times 10^{-4} i$
70	$12.903 - 1.21 \times 10^{-2} i$	$12.9055 - 5.67 \times 10^{-4} i$
80	$12.898 - 1.04 \times 10^{-2} i$	$12.9051 - 5.52 \times 10^{-4} i$
90	$12.893 - 7.76 \times 10^{-3} i$	$12.9048 - 2.35 \times 10^{-4} i$

solved with a $[(p-1)/p]$ Padé approximant for $p = 4$ with the reference refractive index $n_* = 3.18$. The transverse variable x is discretized with $\delta x = 0.005\,\mu m$. Under the second order finite difference approximation, the operator X is approximated by a tridiagonal matrix. In the z direction, we use a large step size $h = \delta x\,\cot(0.1\pi/180) = 2.8648\,\mu m$. This is possible because the Padé approximants of the one-way propagator $P = e^{is\sqrt{1+X}}$ are accurate even for a relatively large s. Here, $s = k_0 n_* h = 36.929$. The power loss of the fundamental mode is calculated. The value we obtained is 3.389% and it is consistent with other results published in [5].

Next, we calculate the solution in a much smaller computational window. In the first case, we set $D_+ = -D_- = 1\,\mu m$, $H_+ = -H_- = 0.8\,\mu m$ and $\alpha_\pm = 40$. The same energy-conserving equation (6) is used with the same reference refractive index and the same $[3/4]$ Padé approximant for the propagator. The grid size δx and step size h also remain unchanged. The solutions at $z = a$ calculated with our mode-preserving boundary conditions (4,5) and the simple zero boundary condition are compared with the reference solution in Fig. 1(a). The solution obtained with the zero boundary condition is much too small compared with the reference solution. In another calculation, we set $D_+ = -D_- = 2\,\mu m$, $H_+ = -H_- = 1.8\,\mu m$. All other computational parameters remain the same. The solutions at $z = a$ are compared with the reference solution in Fig. 1(b). In both cases, it is clear that the solutions calculated with the mode-preserving boundary conditions are much more accurate than the solutions calculated with the zero boundary condition.

IV. CONCLUSIONS

We have developed a mode-preserving boundary condition that can be used with a PML. It is simply the exact boundary condition of the local fundamental propagating mode consistent with the complex coordinate change of the PML. The method is mainly useful for single mode waveguides and it requires to calculate the propagation constant of the local fundamental propagating mode. For step-index planar waveguides, the propagation constant can be easily computed. The mode-preserving boundary condition reduces the error in the propagation constant when a PML with finite thickness is used and it allows

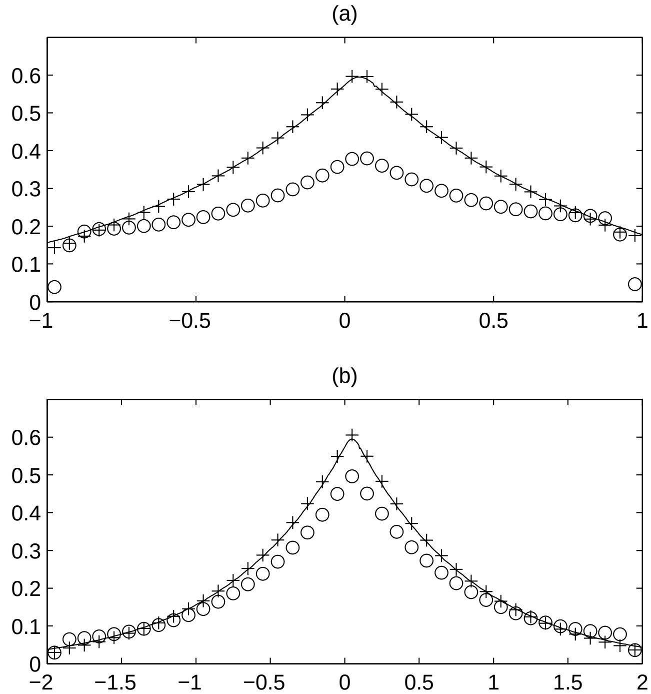

Fig. 1. Magnitudes of solutions of the energy-conserving equation (6) at $z = a$. The reference solution (solid lines) is compared with the solutions calculated with the zero boundary condition ("$\circ$") and the mode-preserving boundary conditions ("$+$"). The computational windows are: (a) $-1\,\mu m < x < 1\,\mu m$ and (b) $-2\,\mu m < x < 2\,\mu m$.

us to accurately calculate the wave fields propagating in slowly varying waveguides using a much smaller computational domain.

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