Application of modified Padé approximant operators to time-domain beam propagation methods

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We demonstrate the usefulness of the recently introduced modified Padé approximant operators for the solution of time-domain beam propagation problems. We show this both for a wideband method, which can take reflections into account, and for a split-step method for the modeling of ultrashort unidirectional pulses. The resulting approaches achieve high-order accuracy not only in space but also in time.

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1. INTRODUCTION

The beam propagation method (BPM) has become one of the most widely used techniques for the study of light propagation in longitudinally varying optical waveguide devices. A large number of BPM versions exist [1,2], including a wide-angle (WA) BPM based on Padé approximant operators using a new complex Jacobi iterative (CJI) method [3]. This new technique can significantly reduce computational efforts even if the WA beam propagation is treated in three-dimensional (3D) optical waveguides. However, this approach assumes only forward propagating waves, and thus, it is difficult to take into account backward propagating waves, which are indispensable for the analysis of many optical components and devices [4].

One method usually employed to study reflected waves is the finite-difference time-domain (FDTD) technique [5]. This technique is very powerful and versatile and has been adapted to optical waveguide devices [6,7]. However, the FDTD method requires a very small time step size to fulfill the stability criterion that leads to a substantial increase in the computation resources required for the analysis of large optical waveguides [8,9].

Recently, simple and efficient BPMs in the time domain have been developed for dealing with reflected waves, and these have been successfully employed for the analysis of both TE and TM modes propagating in photonic crystal structures [9–11]. Most of these existing TD-BPMs are based on the slow-wave approximation where the second-order derivative with respect to time was ignored [12]; if it is included (thus resulting in wideband time-domain propagation), the approximate solution of this term is commonly obtained by the rational real Padé approximant operators [10,11]. However, as we mentioned in our earlier efforts [3,13] these rational Padé propagators incorrectly propagate evanescent modes in the frequency domain as their denominators gradually approach zero. This not only leads to additional errors in the final solution, but it also causes serious instability problems. To overcome this problem we proposed the so-called modified Padé approximant operators, which not only give evanescent waves a desired damping, but also allow a more accurate approximation to the wave equation than those based on the conventional ones [13]. In this work, the modified Padé approximant operators are extended to approximate the wideband solution of time-domain propagation in reflective waveguides.

Besides using time-domain BPMs for dealing with reflected waves, these BPMs have also become widely used techniques for the analysis of ultrashort pulses propagating (unidirectionally) in optical waveguide structures [14,15]. In this paper, we also derive a description of modified Padé approximant operators suitable for that application.

2. FORMULATIONS

A. Basic Equation

We start with the formation of the modified Padé approximant operators for the solution of time-domain beam propagation methods by considering a two-dimensional (2D) scalar wave equation where the computational domain is on the xz-plane [9]:

$$\frac{\partial^2\Psi}{\partial z^2}+\frac{\partial^2\Psi}{\partial x^2}=\frac{n^2}{c^2}\frac{\partial^2\Psi}{\partial t^2}, \tag{1}$$

where n is a refractive index profile and c is the speed of light in free space. From this equation, two common approaches for dealing with reflected waves and for the modeling of ultrashort pulse propagation in wide-angle

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structures can be obtained as follows in Subsection 2.B.

B. Method 1: Time-Domain BPMs for Treating Reflected Waves

The formal solution of Eq. (1) with a slowly varying complex amplitude is given by

$$\Psi(x,z,t) = \psi(x,z,t)\exp(i\omega_0 t). \tag{2}$$

(We obviously only consider waves propagating forward in time; the method is fully reflective since no approximation is made in the propagation direction). By substituting Eq. (2) into Eq. (1), we obtained

$$\frac{\partial^2 \psi}{\partial t^2} + 2i\omega_0 \frac{\partial \psi}{\partial t} = P\psi, \tag{3}$$

where $P=c^2/n^2(\partial^2/\partial x^2+\partial^2/\partial z^2)+\omega_0^2$ and ω_0 is the center angular frequency. A formal solution of Eq. (3) can be written in the following well-known form [16]:

$$\frac{\partial \psi}{\partial t} = -i\omega_0(1-\sqrt{1-X})\psi, \tag{4}$$

with $X=P/\omega_0^2$. In addition, to allow numerical methods to solve Eq. (3) effectively its approximate solution is usually obtained by the conventional Padé approximant method. The conventional Padé propagators are well known and result from the recurrence relation with the initial value of $\partial/\partial t|_0=0$ in the following form:

$$\left.\frac{\partial}{\partial t}\right|_{n+1} = -i\omega_0 \frac{\frac{X}{2}}{1-\frac{j}{\omega_0}\left.\frac{\partial}{\partial t}\right|_n}. \tag{5}$$

For $\partial/\partial t|_2$, this gives us the well-known Padé (1,1) approximant-based wideband beam propagation formula:

$$\frac{\partial \psi}{\partial t} \approx -i\omega_0 \frac{\frac{X}{2}}{1-\frac{X}{4}}\psi. \tag{6}$$

If Eq. (6) is compared to the formal solution of wave equation given in Eq. (4), we obtain the approximation formula

$$1-\sqrt{1-X} \approx \frac{\frac{X}{2}}{1-\frac{X}{4}}. \tag{7}$$

Since the operator X has a real spectrum, it is useful to consider the approximation of $1-\sqrt{1-X}$ by the conventional Padé approximant propagation operator. Figure 1 shows the absolute value of $1-\sqrt{1-X}$ and its first-order Padé (1,1) approximant as a function of X.

However, as the denominator of the Padé (1,1) approximant gradually approaches zero its absolute value approaches ∞, as can clearly be seen in Fig. 2. Physically this means that the conventional Padé approximant in-

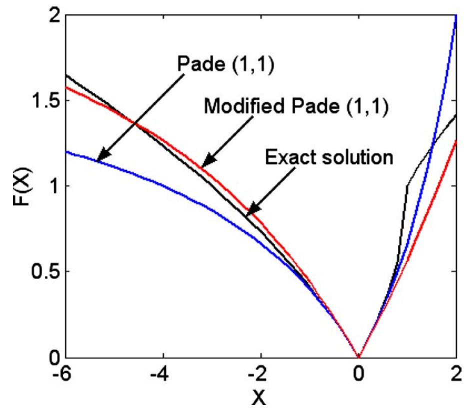

Fig. 1. (Color online) The absolute values of $1-(1-X)^{1/2}$, its first-order standard Padé approximant (X/2)/(1−X/4) and modified Padé approximant (X/2)/(1−X/{4(1+ibeta/2)}) with respect to X.

correctly propagates the evanescent modes. To circumvent this problem we proposed the so-called modified Padé approximant operators [3] by using a different initial value. To apply the modified operators for the time-domain wave equation in this work, the initial value is set at $\partial/\partial t|_0=-\omega_0\beta$ where β is a damping parameter. For $\partial/\partial t|_2$ the first-order modified Padé (1,1) approximant operator is given as follows:

$$\frac{\partial \psi}{\partial t} \approx -i\omega_0 \frac{\frac{X}{2}}{1-\frac{X}{4\left(1+i\frac{\beta}{2}\right)}}\psi. \tag{8}$$

The absolute value of the modified Padé (1,1) approximant of $1-\sqrt{1-X}$ is also depicted in Fig. 1. It is seen that our modified Padé approximant operator (with $\beta=2$) allows more accurate approximations to the true equation than the conventional Padé approximant operator. Furthermore, the conventional rational Padé approximant incorrectly propagates the evanescent modes as their denominator gradually approaches zero while the modified

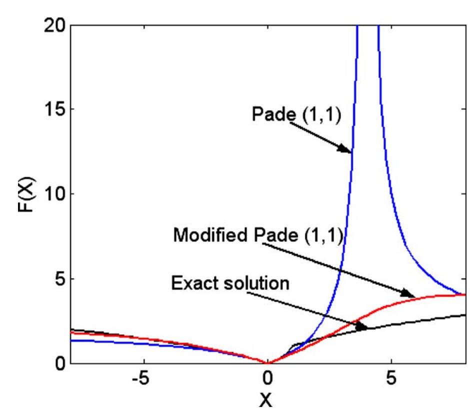

Fig. 2. (Color online) The absolute values of 1−(1−X)1/2 (black line), its first-order standard Padé approximant (X/2)/(1−X/4) and modified Padé approximant (X/2)/(1−X/{4(1+ibeta/2)}) with respect to X.

Padé approximant gives the waves propagating in the evanescent region the desired damping as clearly seen in Fig. 2.

C. Method 2: Time-Domain BPMs for Modeling Ultrashort Pulses in Wide-Angle Structures

Apart from being successful in treating reflected waves, these time-domain BPMs have also found a wide-range application in the analysis of ultrashort pulses propagating in wide-angle waveguides. To do so, the formal solution of the time-domain wave equation is rewritten under the slowly varying envelope approximation as follows [14]:

$$\Psi(x,z,t) = \psi(x,z,t)\exp(ikz)\exp(i\omega_0 t), \qquad (9)$$

with $k=k_0 n_{ref}$, n_{ref} the reference refractive index, k_0 the vacuum wavevector. Here, only waves that are propagating forward in space are retained.

By substituting Eq. (9) into Eq. (1), we obtain

$$\frac{\partial^2\psi}{\partial z^2} + 2ik\frac{\partial\psi}{\partial z} + \frac{\partial^2\psi}{\partial x^2} - \frac{n^2}{c^2}\left(\frac{\partial^2\psi}{\partial t^2} + 2i\omega_0\frac{\partial\psi}{\partial t}\right) + k_0^2(n^2-n_{ref}^2)\psi = 0. \qquad (10)$$

In order to calculate this efficiently, a moving time window is needed. Since a pulse will eventually disappear from the window after a certain number of propagation steps, the computational window should move along with the pulse at the group velocity of the pulse envelope. Therefore, a moving time coordinate $\tau=t-v_g^{-1}z$ with arbitrary v_g should be used and Eq. (10) can be expressed in the following form [15]:

$$\frac{\partial^2\psi}{\partial z^2} + 2ik\frac{\partial\psi}{\partial z} = Q\psi, \qquad (11)$$

with $Q=n^2/c^2\partial^2/\partial\tau^2+2ik_0n^2(1/c-1/v_g)\partial\psi/\partial\tau-\partial^2/\partial x^2 -k_0^2(n^2-n_{ref}^2)$ and $k_0=\omega_0/c$. It is easy to see that Eq. (11) is in the same form as Eq. (3). Therefore, by following the same steps as described in the above section one can easily obtain the modified Padé approximation to the time-domain wave equation.

3. EXAMPLES

In this section, we employ the modified Padé (1,1) approximant operator for the two methods developed in the previous section, and numerically compare the results to those obtained by the conventional Padé (1,1) operator. For verification, we employ two different solvers to solve the time-domain Padé (1,1) approximant-based propagation equation effectively including the biconjugate gradients stabilized method (Bi-CGSTAB) [17], and the CJI method [3].

A. Optical Grating

We consider an optical grating as shown in Fig. 3, where the number of grating periods is eight and the guiding core thickness is 0.3 μm. Obviously, reflections are important in such a structure, so we use the method described in Subsection 2.B. The input pulse has a transverse profile $\psi_0(x)$ corresponding to the fundamental mode of the planar waveguide and a Gaussian profile in the longitudinal direction. At time $t=0$, it is given as

$$\psi(x,z,t=0) = \psi_0(x)\exp\left[-\left(\frac{z-z_0}{w_0}\right)^2\right]\exp[-ik_{eff}(z-z_0)], \qquad (12)$$

where k_{eff} is the effective propagation constant, z_0 is the center position of the input pulse, and w_0 is the spot size. Here, we choose $z_0=1$ μm, $w_0=0.5$ μm, and carrier center wavelength $\lambda=1.5$ μm, respectively. The spatial distribution of the pulse at time $t=0$ is superimposed on Fig. 3.

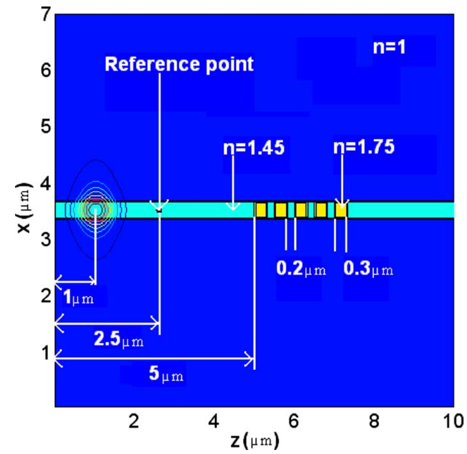

Fig. 3. (Color online) Optical grating with modulated refractive index with input pulse at time $t=0$ superimposed.

The reflected pulse is monitored inside the waveguide at a certain reference point, which is indicated in Fig. 3. Figure 4 shows the evolution of the field profile at that reference point. In order to show the benefits of the modified Padé (1,1) approximant operator, we calculate as a function of time the relative error (RE) of the field profile at the reference point defined as

$$RE = \left[\frac{|\psi_p^{\Delta t} - \psi_p^{0.1\text{ fs}}|^2}{|\psi_p^{0.1\text{ fs}}|^2}\right]^{1/2}, \qquad (13)$$

where $\psi_p^{\Delta t}$ is the field profile at the reference point obtained with various time step resolutions and $\psi_p^{0.1\text{ fs}}$ is the reference solution obtained with the smallest time step resolution used of 0.1 fs. Figure 5 shows this error both for the conventional Padé (cPade) and the modified one

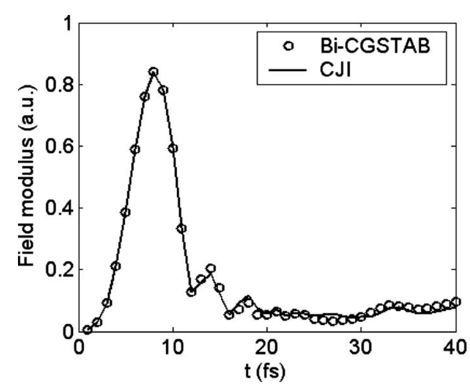

Fig. 4. Time evolution of the field monitored at the reference point.

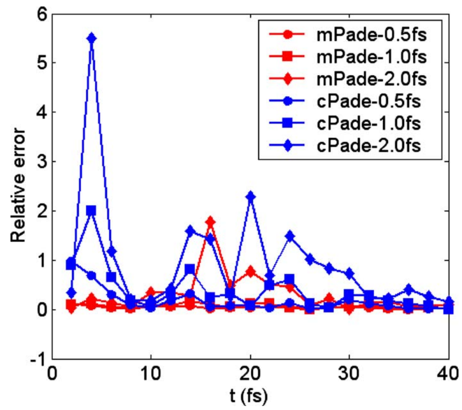

Fig. 5. (Color online) Relative error of the field monitored at the reference point calculated by the modified gray curves (red online) and conventional black curves (blue online) Padé-based TD-BPM with various time steps using the field at 0.1 fs as a reference.

(mPade) with various time step resolutions (0.5 fs, 1 fs, 2 fs). The relative errors obtained by TD-BPM based on the modified Padé (1,1) operator are much smaller than those obtained by the conventional one. This is attributed to more accurate approximations to the wave equation of the modified operator. It leads to the conclusion that using the modified Padé operator allows for propagation with larger time steps for a given accuracy, which is beneficial for runtime.

B. Y-Branch Waveguide

As a second example, we look into the simulation of ultrashort pulse propagation in a Y-branch waveguide structure. Here, reflections are negligible, but the problem is wide-angle, so we use the method described in Subsection 2.C. In this waveguide the initial waveguide is split into two 10-degree tilted waveguides. The guiding core has an index of 3.6 and has a thickness 0.25 μm while the refractive index of the cladding is 3.24, as shown in Fig. 6, and the wavelength is $\lambda = 1.55$ μm.

The input source is given by

$$\psi(x,\tau) = \psi_0(x)\exp\left[-\left(\frac{c\tau - c\tau_0}{cT}\right)^2\right] \tag{14}$$

with $\psi_0(x)$ being the fundamental mode of the planar waveguide and $\tau_0 = 60$ fs, T=20 fs as shown in Fig. 7(a).

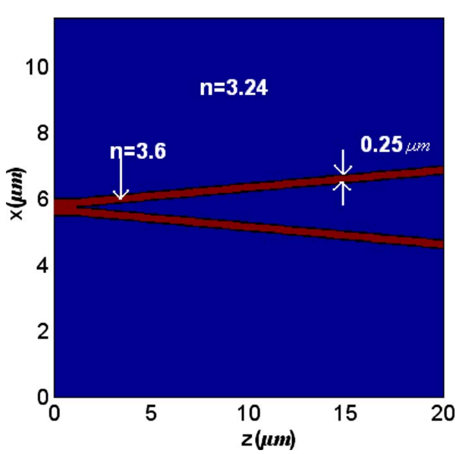

Fig. 6. (Color online) 2D Y-branch waveguide.

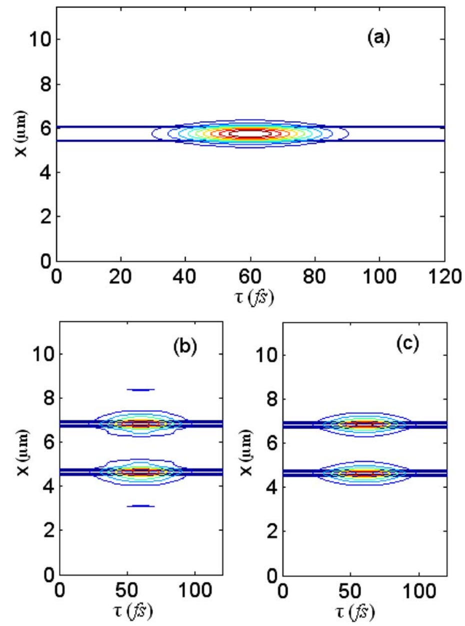

Fig. 7. (Color online) Time evolution of transverse input field (a) and output fields after propagating 20 μm calculated by TD-BPM based on the conventional (b) and the modified (c) Padé(1,1) approximant operator in the Y-branch waveguide. Each part of the figure shows the moving time window of width 120 fs used to monitor the pulse. The local waveguide geometry has been superimposed as a guide to the reader.

The same figure shows the ultrashort pulse after propagating 20 μm calculated by the TD-BPM based on the conventional (b) and the modified (c) Padé (1,1) operator. We can see that the results of the conventional method are much more noisy compared to those of the modified method. To quantify the relative error this time we use the following formula:

$$RE = \left[\frac{\int\int |\psi^{\Delta z} - \psi^{0.02\,\mu\mathrm{m}}|^2 dx d(c\tau)}{\int\int |\psi^{0.02\,\mu\mathrm{m}}|^2 dx d(c\tau)}\right]^{1/2}, \tag{15}$$

where $\psi^{\Delta z}$ are the output pulses obtained for various propagation steps and $\psi^{0.02\,\mu\mathrm{m}}$ is the reference pulse obtained at a propagation step of 0.02 μm. In Table 1 we show these relative errors for pulses calculated by the conventional and the modified Padé-based TD-BPM with various propagation step resolutions (0.2 μm, 0.1 μm, 0.05 μm). It is clearly seen that the relative errors ob-

Table 1. Relative Error (%) of Ultrashort Pulses Calculated by the Modified and Conventional Padé-Based TD-BPM with Various Propagation Steps Using a Pulse Modeled with 0.02 μm Step as a Reference

	Grid Size (μm)		
Operators	0.2	0.1	0.05
Modified Padé	47.9	4.78	3.22
Conventional Padé	69.1	22.81	8.61

tained by the modified Padé-based TD-BPM are much smaller than those obtained by the conventional one for the same propagation step. Thus, TD-BPMs based on the modified Padé operators can offer the advantage of using larger propagation steps than the conventional method for the same accuracy, with an associated reduction in computational effort.

4. CONCLUSIONS

The modified Padé approximant operators have been extended to the solution of wideband time-domain wide-angle beam propagation methods. These modified propagators are promising for more accurate approximation to the time-domain wave equation than conventional approximant operators. Via certain examples chosen here, we showed this both for the propagation of an optical beam in a grating, as well as for the propagation of ultrashort pulses in wide-angle waveguides. In both cases, similar accuracy as compared to the traditional method was obtained, but with much larger step size.

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