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Split-step finite-difference time-domain method with perfectly matched layers for efficient analysis of two-dimensional photonic crystals with anisotropic media

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This Letter presents a split-step (SS) finite-difference time-domain (FDTD) method for the efficient analysis of two-dimensional (2-D) photonic crystals (PhCs) with anisotropic media. The proposed SS FDTD method is formulated with perfectly matched layer boundary conditions and caters for inhomogeneous anisotropic media. Furthermore, the proposed method is derived using the efficient SS1 splitting formulas with simpler right-hand sides that are more efficient and easier to implement. A 2-D PhC cavity with anisotropic media is used as an example to validate the efficiency of the proposed method. © 2012 Optical Society of America

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Photonic crystals (PhCs) involving anisotropic media have attracted a considerable amount of interest over recent years. For example, one-dimensional (1-D) PhCs with unit cells composed of anisotropic media can yield dispersion relations with stationary inflection points (SIPs) [1], degenerate, and split band edges [2]. Electromagnetic waves operating at frequencies near these points or band edges can propagate with unique effects such as large field enhancement and unidirectionality (for the SIP case). Anisotropic media can also be used in the form of localized defects to tune the frequency of defect modes. Such anisotropic media include liquid crystals [3] and ferrites [4] that have permittivity and permeability tensors tunable by external fields, respectively. This feature can be used to develop tunable PhC devices such as cavities and filters [5].

PhCs with anisotropic media can be analyzed with the finite-difference time-domain (FDTD) method [3,6]. In modeling certain PhCs, the FDTD method can however suffer from a Courant-limit time-step bound that can be computationally demanding. This is especially so when highly refined grids are required to model sharp field variations or long simulation times are needed to model resonant modes with high quality factors [7]. To overcome this computational limitation, implicit FDTD methods based on the alternating-direction-implicit scheme have recently been proposed in [8,9] specifically for 1-D anisotropic PhCs. In this Letter, we propose an alternate implicit FDTD method based on the split-step (SS) scheme for the efficient analysis of two-dimensional (2-D) anisotropic PhCs. The proposed method is an extension of [10] in that it includes perfectly matched layer (PML) boundary conditions [11–13] and caters for inhomogeneous anisotropic media. In addition, the proposed method is formulated using the fundamental SS1 splitting formulas [14], which is in the simplest basic (fundamental) form without matrix operators on its right-hand sides.

Consider the following frequency-domain Maxwell's equations in anisotropic media:

$$j\omega\epsilon_0\tilde{\mathbf{E}} = \kappa\tilde{\nabla} \times \tilde{\mathbf{H}}, \quad (1)$$

$$j\omega\mu_0\tilde{\mathbf{H}} = -\nu\tilde{\nabla} \times \tilde{\mathbf{E}}. \quad (2)$$

κ and ν represent the relative inverse permittivity ($\kappa = \epsilon^{-1}$) and permeability ($\nu = \mu^{-1}$) tensors, respectively. $\tilde{\nabla}$ is the modified nabla operator that incorporates the complex-space version of the PML. $\tilde{\nabla}$ is given as

$$\tilde{\nabla} = \frac{1}{s_x} \frac{\partial}{\partial x} \hat{x} + \frac{1}{s_y} \frac{\partial}{\partial y} \hat{y} + \frac{1}{s_z} \frac{\partial}{\partial z} \hat{z}, \quad (3)$$

with coordinate-stretching variables $s_\xi = 1 + \frac{\sigma_\xi}{j\omega\epsilon_0}$ and PML conductivity σ_ξ along the direction $\xi = x, y, z$ [8]. In a split-field formulation, Eq. (1) can be decomposed as

$$j\omega\tilde{\mathbf{E}}_{s_\xi} s_\xi = \frac{\kappa}{\epsilon_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \tilde{\mathbf{H}}, \quad (4)$$

for $\{\zeta, \xi\} = \{1, x\}, \{2, y\}$, and $\{3, z\}$. The original electric field vector $\tilde{\mathbf{E}}$ is related to its split-field vectors $\tilde{\mathbf{E}}_{s_\xi}$ as $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}_{s1} + \tilde{\mathbf{E}}_{s2} + \tilde{\mathbf{E}}_{s3}$. A similar split-field formulation can be obtained for Eq. (2). Using the inverse Fourier transform, the corresponding time-domain split-field equations can be attained as

$$\frac{\partial \mathbf{E}_{s_\xi}^\zeta}{\partial t} + \frac{\sigma_\xi}{\epsilon_0} \mathbf{E}_{s_\xi}^\zeta = \frac{\kappa}{\epsilon_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \mathbf{H}, \quad (5)$$

$$\frac{\partial \mathbf{H}_{s_\xi}^\zeta}{\partial t} + \frac{\sigma_\xi}{\epsilon_0} \mathbf{H}_{s_\xi}^\zeta = -\frac{\nu}{\mu_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \mathbf{E}, \quad (6)$$

with $\mathbf{E} = \mathbf{E}_{s1} + \mathbf{E}_{s2} + \mathbf{E}_{s3}$ and $\mathbf{H} = \mathbf{H}_{s1} + \mathbf{H}_{s2} + \mathbf{H}_{s3}$.

Assuming a 2-D TM_z problem with scalar permittivity and tensor permeability (with elements $\mu_{xz} = \mu_{zx} = \mu_{yz} = \mu_{zy} = 0$), Eqs. (5) and (6) reduce to six equations that can be expressed as a first-order differential system,

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{M}\mathbf{U}, \quad (7)$$

in which split-field vector U is

$$U = [E_{s1,z} \ E_{s2,z} \ H_{s1,x} \ H_{s1,y} \ H_{s2,x} \ H_{s2,y}]^T \quad (8)$$

and matrix $\mathbf{M}$ comprises the differential operator. The original fields can be obtained from components of U as

$$\begin{aligned} E_z &= E_{s1,z} + E_{s2,z}, H_x = H_{s1,x} + H_{s2,x}, H_y \\ &= H_{s1,y} + H_{s2,y}. \end{aligned} \quad (9)$$

By splitting matrix $\mathbf{M}$ into two matrices and using them in the fundamental SS1 splitting formulas [14], the following SS formulation with PML boundary conditions in anisotropic media can be attained, in compact form:

$$\text{Input initialization : } \hat{U}^n = \mathbf{D}^{-1}U^n. \quad (10)$$

$$\text{Substep 1 : } \left(\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}\right)V^{n+\frac{1}{2}} = \hat{U}^n, \quad (11)$$

$$\hat{U}^{n+\frac{1}{2}} = \mathbf{D}^{-1}V^{n+\frac{1}{2}} - \hat{U}^n. \quad (12)$$

$$\text{Substep 2 : } \left(\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}\right)V^{n+1} = \hat{U}^{n+\frac{1}{2}}, \quad (13)$$

$$\hat{U}^{n+1} = \mathbf{D}^{-1}V^{n+1} - \hat{U}^{n+\frac{1}{2}}. \quad (14)$$

$$\text{Output : } U^{n+1} = \mathbf{D}\hat{U}^{n+1}. \quad (15)$$

V is an auxiliary vector denoted as

$$V = [e_{s1,z} \ e_{s2,z} \ h_{s1,x} \ h_{s1,y} \ h_{s2,x} \ h_{s2,y}]^T, \quad (16)$$

and $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{D}$ are 6×6 matrices selected as

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\nu_{xy} \partial}{\mu_0 \partial x} & \frac{\nu_{xy} \partial}{\mu_0 \partial x} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ \frac{\nu_{yy} \partial}{\mu_0 \partial x} & \frac{\nu_{yy} \partial}{\mu_0 \partial x} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (17)$$

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\epsilon_0 \partial y} & 0 & -\frac{1}{\epsilon_0 \partial y} & 0 \\ 0 & 0 & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\nu_{xy} \partial}{\mu_0 \partial y} & \frac{\nu_{xy} \partial}{\mu_0 \partial y} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ \frac{\nu_{yx} \partial}{\mu_0 \partial y} & \frac{\nu_{yx} \partial}{\mu_0 \partial y} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (18)$$

$$\mathbf{D} = \text{diag}\left(\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}\right). \quad (19)$$

Note that, for zero initial fields, input initialization Eq. (10) need not be performed. In addition, the final fields can be output using Eq. (15), only when required.

Next, we discuss the actual numerical update of $\hat{U}$. For spatial discretization, we consider Yee's grid with inhomogeneous media and split-field components $\{E_{s1,z}, E_{s2,z}\}$, $\{H_{s1,x}, H_{s2,x}\}$, and $\{H_{s1,y}, H_{s2,y}\}$ located at positions (i, j) , $(i, j + \frac{1}{2})$, and $(i + \frac{1}{2}, j)$, respectively. Consider the update of $\hat{U}^{n+\frac{1}{2}}$ in Substep 1 as an example.

(1) Implicit updating $e_{s1,z}|_{i,j}^{n+\frac{1}{2}}$ in Eq. (11):

$$\begin{aligned} & -\beta_{ij}\gamma_{i-\frac{1}{2},j}^{yy}e_{s1,z}|_{i-1,j}^{n+\frac{1}{2}} + (1 + \beta_{ij}\gamma_{i-\frac{1}{2},j}^{yy} + \beta_{ij}\gamma_{i+\frac{1}{2},j}^{yy})e_{s1,z}|_{i,j}^{n+\frac{1}{2}} \\ & - \beta_{ij}\gamma_{i+\frac{1}{2},j}^{yy}e_{s1,z}|_{i+1,j}^{n+\frac{1}{2}} \\ & = \hat{E}_{s1,z}|_{i,j}^n + \beta_{ij}\gamma_{i-\frac{1}{2},j}^{yy}\hat{E}_{s2,z}|_{i-1,j}^n \\ & - (\beta_{ij}\gamma_{i-\frac{1}{2},j}^{yy} + \beta_{ij}\gamma_{i+\frac{1}{2},j}^{yy})\hat{E}_{s2,z}|_{i,j}^n + \beta_{ij}\gamma_{i+\frac{1}{2},j}^{yy}\hat{E}_{s2,z}|_{i+1,j}^n \\ & + \beta_{ij}(\hat{H}_{s1,y}|_{i+\frac{1}{2},j}^n + \hat{H}_{s2,y}|_{i+\frac{1}{2},j}^n - \hat{H}_{s1,y}|_{i-\frac{1}{2},j}^n - \hat{H}_{s2,y}|_{i-\frac{1}{2},j}^n), \end{aligned} \quad (20)$$

in which

$$\beta_{ij} = \frac{\frac{\Delta t}{4\epsilon_{ij}\epsilon_0\Delta x}}{\frac{1}{2} + \frac{\sigma_x|_{i,j}\Delta t}{8\epsilon_0}},$$

$$\gamma_{i+\frac{1}{2},j}^{yy} = \frac{\frac{\nu_{yy}|_{i+\frac{1}{2},j}\Delta t}{4\mu_0\Delta x}}{\frac{1}{2} + \frac{\sigma_x|_{i+\frac{1}{2},j}\Delta t}{8\epsilon_0}}.$$

(2) Explicit updating of remaining fields in Eq. (11):

$$\begin{aligned} h_{s1,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} &= \hat{H}_{s1,y}|_{i+\frac{1}{2},j}^n \\ &+ \gamma_{i+\frac{1}{2},j}^{yy}(e_{s1,z}|_{i+1,j}^{n+\frac{1}{2}} - e_{s1,z}|_{i,j}^{n+\frac{1}{2}} + \hat{E}_{s2,z}|_{i+1,j}^n \\ &- \hat{E}_{s2,z}|_{i,j}^n), \end{aligned} \quad (21)$$

$$h_{s1,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{H}_{s1,x}|_{i,j+\frac{1}{2}}^n + \left\{ \frac{\nu_{xy}}{\nu_{yy}}(h_{s1,y}^{n+\frac{1}{2}} - \hat{H}_{s1,y}) \right\}_{i,j+\frac{1}{2}}, \quad (22)$$

$$e_{s2,z}|_{i,j}^{n+\frac{1}{2}} = \hat{E}_{s2,z}|_{i,j}^n, \quad (23)$$

$$h_{s2,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{H}_{s2,x}|_{i,j+\frac{1}{2}}^n, \quad (24)$$

$$h_{s2,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{H}_{s2,y}|_{i+\frac{1}{2},j}^n. \quad (25)$$

Fig. 1. Normalized resonant frequency of PhC cavity versus anisotropy angle ϕ using explicit and SS FDTD method.

First, the update of $V^{n+\frac{1}{2}}$ components is performed using Eq. (11). $e_{s1,z}|_{i,j}^{n+\frac{1}{2}}$ is first updated implicitly by solving a system of linear equations, formed using Eq. (20) with a tridiagonal matrix coefficient. $h_{s1,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$ is then updated explicitly using Eq. (21). $h_{s1,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$ is subsequently updated using Eq. (22), which includes a nondiagonal term from the anisotropic permeability tensor. In Eq. (22), the fields $h_{s1,y}^{n+\frac{1}{2}}$ and $\hat{H}_{s1,y}^n$ need to be interpolated at $(i, j + \frac{1}{2})$ from neighboring points, as they are computed at $(i + \frac{1}{2}, j)$ [15]. The remaining components of $V^{n+\frac{1}{2}}$ are then updated explicitly with Eqs. (23–25). Finally, the update of $\hat{U}^{n+\frac{1}{2}}$ is attained by using auxiliary Eq. (12). A similar set of update procedures can be deduced for Substep 2 to complete the update of $\hat{U}^{n+1}$.

Next, we demonstrate the proposed SS FDTD method for efficient modeling of a 2-D tunable anisotropic PhC cavity. Consider a 5×5 square PhC cavity consisting of dielectric rods with scalar permittivity $\epsilon = 11.56$ in air, as shown in the inset of Fig. 1. The gray and black shaded rods have free space and anisotropic permeability (tensor elements $\mu_{xx} = 1.3 \cos^2 \phi + 1.1 \sin^2 \phi$, $\mu_{yy} = 1.3 \sin^2 \phi + 1.1 \cos^2 \phi$, $\mu_{xy} = \mu_{yx} = 0.2 \sin \phi \cos \phi$), respectively. The rod radius is $r = 0.2a$ with $a = 1.55 \mu\text{m}$. The cavity center is excited by a Gaussian pulse: $\cos(\omega_c t) e^{-\frac{t-t_0}{\tau}}$ with $\omega_c = 0.3762 \frac{2\pi c_0}{a}$ (c_0 is speed of light in free space), $t_0 = 300$ fs, and $\tau = 90$ fs. The simulation runs for $\frac{300000}{\text{CFLN}}$ time steps of size $\Delta t = \text{CFLN} \frac{\Delta}{c_0 \sqrt{2}}$. The uniform cell size is $\Delta = 19.38$ nm, corresponding to cell per minimum wavelength of 44. CFLN is the Courant number. The simulation is terminated with 20 PML layers. Figure 1 plots the cavity resonant frequency over various tuning angles ϕ using the explicit Eq. [13] and proposed SS FDTD methods. The figure first shows that the PhC cavity has a tunable frequency range of 0.503 THz over $\phi = 0^\circ$ to 90° with maximum tunability within $\phi = 20^\circ$ and 70° . Second, the proposed SS FDTD methods require lower computational times compared to the explicit FDTD method, while main-

Fig. 2. (Color online) E_z field over PhC for $\phi = 30^\circ$ using SS FDTD method at CFLN = 5.

taining good agreement. Specifically, the SS FDTD method at CFLN = 6 requires about 44% of the central processing unit (CPU) time with a low frequency error of 0.17%, with respect to the explicit FDTD method. Figure 2 further plots the well-localized E_z field within the defect (cavity) region of the PhC using the proposed SS FDTD method at CFLN = 5 and $\phi = 30^\circ$.

In conclusion, this Letter has presented an SS FDTD method for the efficient analysis of 2-D PhCs with anisotropic media. The proposed method has been formulated with PML boundary conditions for the case of TM_z wave propagation with anisotropic permeability. A similar formulation can be attained for a TE_z case with anisotropic permittivity. Numerical demonstration of a tunable PhC cavity has verified the proposed method's efficiency and good agreement with the explicit FDTD.

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