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A numerical method for the solution of time-harmonic Maxwell equations for two-dimensional scatterers

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Abstract. The Fourier modal method (FMM) is a method for efficiently solving Maxwell equations with periodic boundary conditions. In a recent paper [1] the extension of the FMM to non-periodic structures has been demonstrated for a simple two-dimensional rectangular scatterer illuminated by TE-polarized light with a wavevector normal to the third (invariant) dimension. In this paper we present a generalized version of the aperiodic Fourier modal method in contrast-field formulation (aFMM-CFF) which allows arbitrary profiles of the scatterer as well as arbitrary angles of incidence of light.

Keywords: Fourier modal method, FMM, aperiodic, aFMM-CFF, perfectly matched layer, PML

PACS: 02.60.Cb, 02.60.Lj, 02.70.Dh, 42.25.Fx

INTRODUCTION

The Fourier modal method (FMM), also known under the name of Rigorous Coupled-Wave Analysis (RCWA), originated in the diffractive optics community and was first introduced in [2]. The method has a history of more than three decades marked by considerable improvements on stability [4] and convergence [5, 6, 7]. The monograph [8] gives an overview of the evolution and the implementation of Fourier modal methods. For a mathematical view on the open problems related to the method the reader is referred to [9].

The FMM is an efficient method for solving periodic scattering problems. Its performance is compared to other state-of-the-art numerical methods in [10]. The desire to keep the efficiency advantage of the FMM and allow modeling of aperiodic structures led to the introduction of the aperiodic Fourier modal method in contrast-field formulation (aFMM-CFF) [1, 11]. This method is based on the classical FMM applied to a set of reformulated equations. The periodic boundary conditions are replaced by radiation conditions with the help of perfectly matched layers (PMLs).

PROBLEM STATEMENT

We are concerned with solving the time-harmonic Maxwell equations for non-magnetic materials on the domain $(x, y, z) \in [0, \Lambda] \times \mathbb{R} \times \mathbb{R}$.

$$\nabla \times \mathbf{E}(\mathbf{x}) = -k_0 \mathbf{H}(\mathbf{x}), \quad (1a)$$

$$\nabla \times \mathbf{H}(\mathbf{x}) = -k_0 \varepsilon(x, z) \mathbf{E}(\mathbf{x}), \quad (1b)$$

where $\mathbf{x} = (x, y, z)$ is the position vector, $\mathbf{E} = (E_x, E_y, E_z)$ is the electric field and $\mathbf{H} = (H_x, H_y, H_z)$ is the magnetic field scaled by $-i\sqrt{\varepsilon_0/\mu_0}$. The temporal frequency ω is incorporated into the constant $k_0 = \omega\sqrt{\varepsilon_0\mu_0}$. The electric permittivity ε is assumed y -invariant. See Figure 1 (left) for a sample geometry. The incident field is given by

$$\mathbf{E}^{inc}(\mathbf{x}) = \mathbf{a}e^{-i\mathbf{k}^{inc} \cdot \mathbf{x}}, \quad (1c)$$

where $\mathbf{k}^{inc} = (k_x^{inc}, k_y^{inc}, k_z^{inc})$ is the wavevector and $\mathbf{a} = (a_x, a_y, a_z)$ is the amplitude vector. Note that the Maxwell equations require that $\mathbf{k}^{inc} \cdot \mathbf{a} = 0$.

We are looking for a solution of (1) on the stripe $(x, y, z) \in [0, \Lambda] \times \mathbb{R} \times \mathbb{R}$. Two possible boundary conditions (BCs) at $x = 0$ and $x = \Lambda$ are considered: periodic BCs and radiation (or transparent) BCs. The periodic case is solved with the classical FMM and the aperiodic case is tackled with the generalized version of the newly proposed aFMM-CFF.

FIGURE 1. Slicing of the scatterer profile

PERIODIC SCATTERER

The classical FMM is used in order to solve the Maxwell equations for a periodic scatterer. The first step is to divide the computational domain into layers such that the permittivity may be considered z -independent in each single layer. Thus, the profile of the scatterer is approximated by a staircase as in Figure 1. Now in each layer $j = 1, \dots, M$ the permittivity $\epsilon_j(x)$ is independent of z and y . This allows elimination of the y and z components of the fields.

$$\frac{\partial^2}{\partial z^2} E_{x,j}(x, y, z) = -\mathfrak{L}_{E,j} E_{x,j}(x, y, z), \quad \text{with } \mathfrak{L}_{E,j} = \frac{\partial^2}{\partial y^2} + \frac{\partial}{\partial x} \frac{1}{\epsilon_j(x)} \frac{\partial}{\partial x} \epsilon_j(x) + \epsilon_j(x), \quad (2a)$$

$$\frac{\partial^2}{\partial z^2} H_{x,j}(x, y, z) = -\mathfrak{L}_{H,j} H_{x,j}(x, y, z), \quad \text{with } \mathfrak{L}_{H,j} = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial x^2} + \epsilon_j(x). \quad (2b)$$

The next step is to discretize the equations in the x -direction by using a Galerkin approach with Fourier harmonics as basis functions and test functions,

$$\phi_n(x, y) = e^{-i(k_{xn}x + k_{yn}y)}, \quad \text{where } k_{xn} = k_x^{inc} + n \frac{2\pi}{\Lambda}, \quad k_y = k_y^{inc}, \quad \text{for } n = -N, \dots, +N. \quad (3)$$

In each layer the electric and magnetic fields are expanded as

$$E_{x,j}(x, y, z) = \sum_{n=-N}^N s_{j,n}(z) \phi_n(x, y), \quad H_{x,j}(x, y, z) = \sum_{n=-N}^N u_{j,n}(z) \phi_n(x, y). \quad (4)$$

The standard inner product on the interval $[0, \Lambda]$ is used. After the application of the Galerkin method, Equations (2) become

$$\mathbf{s}_j''(z) = -\mathbf{L}_{s,j} \mathbf{s}_j(z), \quad \mathbf{u}_j''(z) = -\mathbf{L}_{u,j} \mathbf{u}_j(z), \quad (5)$$

with matrices $\mathbf{L}_{s,j}, \mathbf{L}_{u,j} \in \mathbb{R}^{(2N+1) \times (2N+1)}$ and vectors $\mathbf{s}_j, \mathbf{u}_j \in \mathbb{R}^{(2N+1)}$. These are homogeneous second-order ordinary differential equations whose general solution is given by

$$\mathbf{s}_j(z) = \mathbf{W}_{s,j}(e^{-\mathbf{Q}_{s,j}(z-h_j)} \mathbf{c}_{s,j}^+ + e^{\mathbf{Q}_{s,j}(z-h_{l+1})} \mathbf{c}_{s,j}^-), \quad (6a)$$

$$\mathbf{u}_j(z) = \mathbf{W}_{u,j}(e^{-\mathbf{Q}_{u,j}(z-h_j)} \mathbf{c}_{u,j}^+ + e^{\mathbf{Q}_{u,j}(z-h_{l+1})} \mathbf{c}_{u,j}^-), \quad (6b)$$

where h_j is the z -coordinate of the top interface of layer j , $\mathbf{W}_{\cdot,j}$ is the matrix of eigenvectors of $\mathbf{L}_{\cdot,j}$ and $\mathbf{Q}_{\cdot,j}$ is a diagonal matrix with square roots of the corresponding eigenvalues on its diagonal.

The vectors $\mathbf{c}_{\cdot,1}^+$ and $\mathbf{c}_{\cdot,M}^-$ are fixed by the incident field and radiation conditions. The remaining vectors $\mathbf{c}_{\cdot,j}^+$ and $\mathbf{c}_{\cdot,j}^-$ are unknown, and can be determined from the interface conditions derived from the Maxwell equations [3].

APERIODIC SCATTERER

In order to solve the Maxwell equations for an aperiodic scatterer, a generalized version of the aFMM-CFF is used. The periodic basis functions (3) force the solution to be periodic. For an aperiodic scatterer we need to implement

the radiation BC at the lateral boundaries. One way of achieving this without changing the basis is to place perfectly matched layers (PMLs) [12] of a certain thickness just before the boundary. This approach has been previously used to apply the FMM to waveguide problems [13, 14, 15]. The PML changes the x -derivative in the differential equations (2) as follows

$$\frac{\partial}{\partial x} \rightarrow \frac{1}{f'(x)} \frac{\partial}{\partial x}, \text{ with } f(x) = x + i\beta(x). \quad (7)$$

The function $\beta(x)$ is continuous and non-zero only in the PMLs which are placed in the stripes $[0, x_l]$ and $[x_r, \Lambda]$. An example of such a function is shown in Figure 2. The operators $\mathfrak{L}_{E,j}$ and $\mathfrak{L}_{H,j}$ with the change of x -derivative in (7) will be denoted respectively by $\tilde{\mathfrak{L}}_{E,j}$ and $\tilde{\mathfrak{L}}_{H,j}$.

FIGURE 2. Slicing of the scatterer profile

For each field (magnetic and electric) there is a corresponding incident field which is given in advance and which is part of the unknown total field. In order to avoid modifications of the incident field by the PML, the computed solution should consist of only outgoing waves [11]. Therefore the equations are reformulated such that the incident field, i.e. the known part of the solution, is moved into the source. Since the reformulations are similar for both the electric and magnetic field, we demonstrate the derivation only for the former. In addition to the total field problem

$$\frac{\partial^2}{\partial z^2} \tilde{E}_{x,j}(\mathbf{x}) = -\tilde{\mathfrak{L}}_{E,j} \tilde{E}_{x,j}(\mathbf{x}), \quad E_x^{inc}(\mathbf{x}) = a_x e^{-i\mathbf{k}^{inc} \cdot \mathbf{x}} \quad (8)$$

we define a background problem with PMLs

$$\frac{\partial^2}{\partial z^2} \tilde{E}_{x,j}^b(\mathbf{x}) = -\tilde{\mathfrak{L}}_{E,j}^b \tilde{E}_{x,j}^b(\mathbf{x}), \quad E_x^{b,inc}(\mathbf{x}) = a_x e^{-i\mathbf{k}^{inc} \cdot \mathbf{x}}, \text{ where } \tilde{\mathfrak{L}}_{E,j}^b = \frac{\partial^2}{\partial y^2} + \frac{1}{f'(x)} \frac{\partial}{\partial x} \frac{1}{f'(x)} \frac{1}{\varepsilon_j^b} \frac{\partial}{\partial x} \varepsilon_j^b + \varepsilon_j^b \quad (9)$$

and a background problem without PMLs

$$\frac{\partial^2}{\partial z^2} E_{x,j}^b(\mathbf{x}) = -\mathfrak{L}_{E,j}^b E_{x,j}^b(\mathbf{x}), \quad E_x^{b,inc}(\mathbf{x}) = a_x e^{-i\mathbf{k}^{inc} \cdot \mathbf{x}}, \text{ where } \mathfrak{L}_{E,j}^b = \frac{\partial^2}{\partial y^2} + \frac{\partial}{\partial x} \frac{1}{\varepsilon_j^b} \frac{\partial}{\partial x} \varepsilon_j^b + \varepsilon_j^b \quad (10)$$

Note that ε_j^b is chosen to be x -independent, i.e. it represents a multilayer stack. This implies that the background problem without PMLs has an analytical solution. Since the PML effectively implements the radiation conditions, for an ideal PML the two background problems have equal solutions in the physical domain (the region between the PMLs).

$$\tilde{E}_{x,j}^b(\mathbf{x}) = E_{x,j}^b(\mathbf{x}), \text{ for } \mathbf{x} \in [x_l, x_r] \times \mathbb{R} \times \mathbb{R}. \quad (11)$$

Subtracting (9) from (8) and defining the contrast field $\tilde{E}^c = \tilde{E} - \tilde{E}^b$, we get

$$\frac{\partial^2}{\partial z^2} \tilde{E}_{x,j}^c(\mathbf{x}) = -\tilde{\mathfrak{L}}_{E,j} \tilde{E}_{x,j}^c(\mathbf{x}) - (\tilde{\mathfrak{L}}_{E,j} - \tilde{\mathfrak{L}}_{E,j}^b) \tilde{E}_{x,j}^b(\mathbf{x}), \quad E_x^{c,inc}(\mathbf{x}) = 0. \quad (12)$$

The incident field has been removed, and a non-homogeneous term appears on the right-hand side. The background permittivity is chosen such that $\varepsilon(x, z) - \varepsilon^b(z)$ vanishes in the PML and has compact support. As a consequence, $\tilde{\mathfrak{L}}_{E,j} - \tilde{\mathfrak{L}}_{E,j}^b \neq 0$ only for $x \in [x_l, x_r]$, which according to (11) entitles the substitution of $\tilde{E}_{x,j}^b(\mathbf{x})$ by $E_{x,j}^b(\mathbf{x})$ in (12).

Once the source-term is determined, Equation (12) may be solved. For this purpose, the source term must also be expanded into Fourier modes. After truncation a non-homogeneous system of ordinary differential equations is obtained for each layer. The field is found by matching the general solutions at the layer interfaces.

NUMERICAL EXAMPLE

We solve problem (1) on the domain $[0, 5] \times \mathbb{R} \times \mathbb{R}$ with the incident field defined by $(k_x^{inc}, k_y^{inc}, k_z^{inc}) = (0, 0, 1)$ and $(a_x, a_y, a_z) = (\sqrt{3}/2, 1/2, 0)$. In this example the scatterer is a single triangular groove. The permittivity is discretized in the z -direction with seven layers, $M = 7$. The left plot of Figure 3 shows the sliced geometry which is defined by the refractive index of the material $n(x, z) = \sqrt{\epsilon(x, z)}$. The PMLs are placed in the stripes $x \in [0, 1]$ and $x \in [4, 5]$. The right plot of Figure 3 shows the computed magnitude of the y -component of the magnetic field.

FIGURE 3. Scattering from a single y -invariant triangular groove; Geometry of the sliced problem (left) and the computed field $|\hat{H}_y(x, y, z)|$ at $y = 0$ (right).

CONCLUSIONS

We discussed the application of Fourier modal methods for solving the two-dimensional time-harmonic Maxwell equations numerically. The classical FMM suitable for periodic structures has been formulated based on the Galerkin approach. A generalization of the aFMM-CFF to arbitrary 2D shapes and angles of incidence has been presented.

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