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The aperiodic Fourier modal method in contrast-field formulation for simulation of scattering from finite structures.

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Abstract

This paper extends the area of application of the Fourier modal method (FMM) from periodic structures to aperiodic ones, in particular for plane-wave illumination at arbitrary angles. This is achieved by placing perfectly matched layers at the lateral sides of the computational domain and reformulating the governing equations in terms of a contrast field which does not contain the incoming field. Due to the reformulation, the homogeneous system of second-order ordinary differential equations from the original FMM becomes non-homogeneous. Its solution is derived analytically and used in the established FMM framework. The technique is demonstrated on a simple problem of planar scattering of TE-polarized light by a single rectangular line.

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1. Introduction

The Fourier modal method (FMM), also referred to as Rigorous Coupled-Wave Analysis (RCWA), has a well established position in the field of rigorous diffraction modeling. It was first formulated by Moharam and Gaylord in 1981 [1]. Being based on Fourier-mode expansions, the method is inherently built for periodic structures such as diffraction gratings. Harmonic functions constitute in fact a natural basis for representing wave-like solutions. This, in turn, means that few such functions are required to approximate the exact solution with a certain accuracy.

The stability and efficiency of the FMM was improved especially due to the *enhanced transmittance matrix approach* for solving the recursive matrix equations [2, 3]. The convergence problems observed for incident waves with TM-polarization, have been overcome by

reconsidering the Laurent’s rule for the product of truncated Fourier series [4, 5]. Shortly after, these rules have been given a sound mathematical background by Li [6], and usually are referred to as the *Li rules*. The Li rules could be easily applied to 2D-periodic structures with rectangular shapes. For non-rectangular shapes a zigzag approximation of the profile had to be used. This inconvenience has been removed by considering separately the tangential and normal components of the field at the interface [7–10]. Another important improvement was the introduction of the technique of *adaptive spatial resolution* [11]. Due to this technique a faster convergence is achieved by increasing the resolution in space around the material interfaces.

As a consequence of the improvements over the last two decades, nowadays the FMM is a well established method. It is robust and efficient, especially for two-dimensional problems. A recent paper [12] benchmarks the performance of state-of-the-art methods in rigorous diffraction modeling, including the FMM, the finite element method (FEM), the finite difference time-domain method (FDTD) and the volume integral method (VIM).

One important limitation of the FMM is given by the fact that it can only be used for computational problems defined for periodic structures (such as diffraction gratings). This is because the modes used to represent the field are themselves periodic. A straightforward workaround for this limitation is the *supercell approach*; the aperiodic structure is still assumed to be periodic but with a large enough period so that the interaction of neighboring structures is negligible.

Lalanne and his co-workers [13–15] have applied the FMM to waveguide problems. The aperiodicity of the waveguide was dealt with by placing *perfectly matched layers* (PMLs) [16] on the lateral sides of the computational domain. PMLs are introduced in the domain by performing the mathematical operations of analytic continuation and coordinate transformation. Physically, PMLs can be seen as some fictitious absorbing and non-reflecting materials. In this way, artificial periodization is achieved, i.e. the structure of interest is repeated in space, but there is no electromagnetic coupling between neighboring cells. The concepts of perfectly matched layers and artificial periodization are carefully explained in the paper.

The above approach, combining standard FMM with PMLs, is applicable only for the case of normal incidence of the incoming field, which is sufficient for waveguide problems. In this paper we show that for oblique incidence we need to reformulate the standard FMM such that the incident field is not part of the computed solution. We propose a decomposition of the total field into a *background field* (containing the incident field) and a *contrast field*. The problem is reformulated with the contrast field as the new unknown. The background field solves a corresponding *background problem* which has a simple analytical solution. The main effect of the reformulation is that the homogeneous system of second-order ordinary differential equations becomes non-homogeneous. The solution of this equation is derived in

closed form, as required for the FMM algorithm.

The ideas conveyed in this paper are demonstrated on two model problems: diffraction of TE-polarized light from a binary one-dimensional grating (periodic model problem) and from a single line (aperiodic model problem). The remainder of the paper is structured as follows. Section 2 briefly describes the standard FMM applied to the periodic model problem. Next, in Section 3, the idea of artificial periodization with PMLs is described as a means of solving the aperiodic model problem for normal incidence of the incoming field. Section 4 constitutes the core of this paper and demonstrates the derivation of the contrast-field formulation for the FMM. The new formulation allows for arbitrary angles of incidence in combination with the PMLs. Finally, numerical results and conclusions are presented in the last two sections.

2. The standard Fourier modal method

The structure considered in the periodic model problem is an infinitely periodic binary grating with a period Λ illuminated by TE-polarized light. The permittivity profile $\epsilon(x, z)$ is invariant in the y direction and is shown in Figure 1. The field is assumed to be time-harmonic, $\check{E}(x, z, t) = E(x, z) \exp(i\omega t)$. The solution of the periodic model problem satisfies

$$\frac{\partial^2}{\partial x^2} E_y(x, z) + \frac{\partial^2}{\partial z^2} E_y(x, z) + k_0^2 \epsilon(x, z) E_y(x, z) = 0, \quad (1)$$

where E_y is the y component of the electric field and the wavenumber k_0 is defined by $k_0 = \omega \sqrt{\epsilon_0 \mu_0}$, with ϵ_0 and μ_0 respectively the electric permittivity and magnetic permeability of vacuum. The incoming field is given by a plane wave

$$E_y^{inc}(x, z) = \exp(-i(k_{x0}x + k_{z0}z)), \quad (2)$$

with $k_{x0} = k_0 n_1 \sin \theta$ and $k_{z0} = k_0 n_1 \cos \theta$. Here, n_1 is the refractive index of the superstrate and θ is the angle the wavevector $[k_{x0}, k_{z0}]^T$ makes with the z axis. The wavelength of the incoming wave is given by $\lambda = 2\pi/(n_1 k_0)$. Note that the incident field satisfies the following condition

$$E_y^{inc}(0, z) = E_y^{inc}(\Lambda, z) \exp(ik_{x0}\Lambda). \quad (3)$$

This condition is referred to as the *pseudo-periodicity condition* or the *Floquet condition*. It may be proven [17, p. 8] that for periodic structures also the resulting total field must be pseudo-periodic.

The first step in the FMM is to divide the computational domain into layers such that the permittivity $\epsilon(x, z)$ is z -independent in each particular layer. For our periodic model problem this division generates three layers as shown in Figure 1.

Then the field in layer l ($l = 1, 2, 3$) satisfies

$$\frac{\partial^2}{\partial x^2} E_{y,l}(x, z) + \frac{\partial^2}{\partial z^2} E_{y,l}(x, z) + \epsilon_l(x) E_{y,l}(x, z) = 0. \quad (4)$$

Fig. 1. Geometry of the periodic model problem and division into layers.

Note that ϵ_l , ($l = 1, 3$) is constant in layers 1 and 3. In this case the solution of (4) may be written in terms of a Rayleigh expansion. However, when the PML is added later, the Rayleigh expansion is not applicable. Therefore, for generality, we treat these layers in the same way as the middle layer(s).

The second step in the FMM is to expand the x -dependent quantities into Fourier modes

$$E_{y,l}(x, z) = \sum_{n=-\infty}^{\infty} s_{n,l}(z) \exp(-ik_{xn}x), \quad (5a)$$

$$\epsilon_l(x) = \sum_{n=-\infty}^{\infty} \hat{\epsilon}_{n,l} \exp\left(i\frac{2\pi n}{\Lambda}x\right), \quad (5b)$$

where

$$k_{xn} = k_0 n_1 \sin \theta - n \frac{2\pi}{\Lambda}, \quad n \in \mathbb{Z}.$$

Note that the modes $\exp(-ik_{xn}x)$ satisfy the condition of pseudo-periodicity. Thus, the solution obtained by superposition will necessarily be pseudo-periodic. By substituting the expansions (5) in (4) and retaining only $2N + 1$ harmonics in the expansion of the field, we get

$$-k_{xn}^2 s_{n,l}(z) + \frac{d^2}{dz^2} s_{n,l}(z) + \sum_{m=-N}^N \hat{\epsilon}_{n-m,l} s_{m,l}(z) = 0, \quad n = -N, \dots, N, \quad (6)$$

or in matrix form

$$\frac{d^2}{dz^2} \mathbf{s}_l(z) = k_0^2 \mathbf{A}_l \mathbf{s}_l(z), \quad \text{with } \mathbf{A}_l = \mathbf{K}_x^2 - \mathbf{E}_l, \quad (7)$$

where $\mathbf{K}_x$ is a diagonal matrix with the values k_{xn}/k_0 on its diagonal and $\mathbf{E}_l$ is a Toeplitz matrix with the (n, m) -entry equal to $\epsilon_{n-m,l}$ for $-N \leq n, m \leq N$.

Equation (7) is a homogeneous second-order ordinary differential equation whose general solution is given by

$$\mathbf{s}_l(z) = \mathbf{s}_l^+(z) + \mathbf{s}_l^-(z) = \mathbf{W}_l(\exp(-\mathbf{Q}_l(z - h_{l-1}))) \mathbf{c}_l^+ + \exp(\mathbf{Q}_l(z - h_l)) \mathbf{c}_l^-, \quad (8)$$

where h_l is the z -coordinate of the top interface of layer l (we take $h_0 = h_1$), $\mathbf{W}_l$ is the matrix of eigenvectors of $\mathbf{A}_l$ and $\mathbf{Q}_l$ is a diagonal matrix with square roots of the corresponding eigenvalues on its diagonal.

The general solution (8) consists of waves traveling upward, $\mathbf{s}_l^-(z)$, and downward, $\mathbf{s}_l^+(z)$. In the top and bottom layer the radiation condition is imposed by requiring that there is no incoming field except for the prescribed incident plane wave

$$\mathbf{s}_1^+(h_1) = \mathbf{d}_0 \exp(-ik_{z0}h_1), \quad (9a)$$

$$\mathbf{s}_3^-(h_2) = \mathbf{0}. \quad (9b)$$

The vector $\mathbf{d}_0 \in \mathbb{R}^{(2N+1)}$ in (9a) is an all-zero vector except for entry $N+1$ which is equal to 1. Conditions (9) fix the vectors $\mathbf{c}_1^+$ and $\mathbf{c}_3^-$. The remaining vectors $\mathbf{c}_l^+$ and $\mathbf{c}_l^-$ are unknown, and can be determined from the interface conditions between the layers [2]. In the case of the standard FMM the top and bottom layers are homogeneous and Rayleigh expansions of the field can be used. It means that the eigenvalues and eigenvectors for these layers are known in advance.

3. Artificial periodization with perfectly matched layers

The goal of this section is to integrate the aperiodic model problem (planar diffraction from one line) into the framework of the FMM. To this end we will use the technique of perfectly matched layers which act as absorbing layers and annihilate the effect of the pseudo-periodic boundary conditions. The section starts with a description of the concepts and ideas behind PMLs and ends by explaining the necessity of reformulating the problem in order to allow for arbitrary angles of incidence.

PMLs were first suggested by Berenger [16] as a method of imposing the radiation condition [18] on the boundary of the computational domain in FDTD. PMLs can be obtained by an analytic continuation of the solution of (1) (defined in real coordinates) to a complex contour

$$\tilde{x} = x + i\beta(x), \quad x \in \mathbb{R}. \quad (10)$$

The function $\beta(x)$ is continuous and has a non-zero value only inside the PMLs. For faster convergence also the continuity of higher order derivatives is desirable. Figure 2 shows an example of such a function when the PMLs are placed in the domains $[0; x_l]$ and $[x_r; \Lambda]$. The analytic continuation (10) transforms propagating waves into evanescent waves. We may observe the damping effect by evaluating a plane wave on the contour $\tilde{x}$

$$\exp(-i(k_{x0}\tilde{x} + k_{z0}z)) = \exp(-i(k_{x0}x + k_{z0}z)) \exp(k_{x0}\beta(x)). \quad (11)$$

It is seen that this right-propagating wave (assume $k_{x0} > 0$) is attenuated exponentially in the right PML, where $\beta(x) < 0$. The left PML would have the same effect on a left-propagating wave. Note that the attenuation is angle dependent.

Fig. 2. The imaginary part $\beta(x)$ of the transformation (10).

The procedure of obtaining a PML requires an analytic continuation from $\mathbb{R}$ to $\mathbb{C}$ followed by a coordinate transformation back to $\mathbb{R}$. The operations can be represented formally as

$$E(x) \xrightarrow{\{1\}} \tilde{E}(\tilde{x}) \xrightarrow{\{2\}} \tilde{E}(x), \text{ with } x \in \mathbb{R}, \tilde{x} \in \mathbb{C}. \quad (12)$$

Operation $\{1\}$ does not formally change the equation but changes its solution by modifying the domain of the space variable x . Operation $\{2\}$ is required in order to avoid working in complex coordinates. It is defined as a coordinate transformation

$$\tilde{x} = f(x) = x + i\beta(x), \quad (13)$$

applied to the equation in $\tilde{x}$. This coordinate transformation eliminates the derivatives with respect to complex variables

$$\frac{\partial}{\partial \tilde{x}} = \frac{dx}{d\tilde{x}} \frac{\partial}{\partial x} = \frac{1}{f'(x)} \frac{\partial}{\partial x}. \quad (14)$$

From the above discussion, we conclude that PMLs modify the underlying equations at the continuous level, therefore they can be used in combination with virtually any discretization technique. For the FMM, PMLs are used to make the solution of an aperiodic problem coincide with the solution of a periodic problem on a subdomain, as explained next.

Suppose we want to solve the aperiodic model problem with normal incidence, that is we want to compute the field scattered by a simple aperiodic structure shown on top of Figure 3 (a single rectangular groove infinitely long in the y direction) when illuminated by a perpendicular plane wave. For this problem, let us refer to it as P_1 , the FMM cannot be used since both the permittivity and field are required to be (pseudo-)periodic functions in order to be represented in terms of Fourier series as in (5). However, we can define an equivalent problem P_2 which is artificially periodized with the help of PMLs as shown in Figure 3. The problems P_1 and P_2 are equivalent in the sense that (for an ideal PML) their

Fig. 3. Problems P_1 (top) and P_2 (bottom) have equal solutions on Ω_0 (for an ideal non-reflecting PML).

solutions on the domain Ω_0 coincide. Problem P_2 fits well in the framework of FMM, due to its periodicity.

To solve P_2 , PMLs have to be added. As explained above, PMLs are implemented by $\{1\}$ an analytic continuation of the solution to a complex contour and $\{2\}$ a back transformation to the real coordinates. The first step is a formal one as it consists of writing the same partial differential equation in the new variable $\tilde{x}$ instead of x . The second step involves the coordinate transformation from $\tilde{x}$ back to x . Under this transformation, described by (13) and (14), Equation (4) becomes

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_{y,l}(x, z) \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_{y,l}(x, z) + k_0^2 \epsilon_l(x) \tilde{E}_{y,l}(x, z) = 0. \quad (15)$$

Note that the permittivity is constant in the PML and is not affected by the transformation. By replacing the field and the permittivity with their corresponding truncated Fourier series (as in Section 2) the equation can be written in matrix form

$$\frac{d^2}{dz^2} \mathbf{s}_l(z) = k_0^2 \mathbf{A}_l \mathbf{s}_l(z), \quad \mathbf{A}_l = (\mathbf{F} \mathbf{K}_x)^2 - \mathbf{E}_l, \quad (16)$$

where $\mathbf{F}$ is the Toeplitz matrix associated with the Fourier coefficients of $1/f'(x)$. Compared to (7), the modification introduced by the PML is minor: a "stretching matrix" $\mathbf{F}$ appears in the computations.

Since the FMM uses an expansion in pseudo-periodic modes the resulting solution has to be pseudo-periodic. We show that the pseudo-periodicity requirement is only satisfied for normal incidence. We write the total field as a sum of the incident and the scattered field

$$\tilde{E}_y = \tilde{E}_y^{inc} + \tilde{E}_y^s.$$

The scattered field (it is an outgoing field) is damped exponentially to “almost zero“ at $x = 0$ and $x = \Lambda$. The original incoming field is given by

$$E_y^{inc}(x, z) = \exp(-i(k_{x0}x + k_{z0}z)). \quad (17)$$

For normal incidence $k_{x0} = 0$, so it is independent of the stretched coordinate x and is not affected by the PML. Thus, the total field is pseudo-periodic. However, for oblique incidence $k_{x0} \neq 0$ and the incoming field will be affected by the analytic continuation. We evaluate the incident field on the complex contour $\tilde{x}$,

$$\tilde{E}_y^{inc}(\tilde{x}, z) = \exp(-i(k_{x0}\tilde{x} + k_{z0}z)) = \exp(-i(k_{x0}x + k_{z0}z)) \exp(k_{x0}\beta(x)). \quad (18)$$

The incident field on the complex contour for $z = 0$ is plotted in Figure 4. Thus, although

Fig. 4. The incident field on the complex contour $\tilde{x}$ for $z = 0$.

the scattered field is still damped exponentially to zero at $x = 0$ and $x = \Lambda$ and satisfies the pseudo-periodic boundary condition, the incoming field on the complex contour violates the pseudo-periodicity

$$\tilde{E}_y^{inc}(f(0), z) \neq \tilde{E}_y^{inc}(f(\Lambda), z) \exp(ik_{x0}\Lambda). \quad (19)$$

Consequently, also the total field violates this condition and cannot be represented by a superposition of the modes in (5a). Therefore, in the next section we remove the part which does not exhibit pseudo-periodicity from the total field and reformulate the problem such that its solution is pseudo-periodic.

4. The contrast-field formulation of the FMM

4.A. Contrast/background decomposition

As shown in the previous section, the presence of PMLs determines the following form of the governing equation

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y + k_0^2 \epsilon(x, z) \tilde{E}_y = 0. \quad (20)$$

The total field is decomposed into a *contrast field* and a *background field* (this can also be viewed as a decomposition into a periodic part and a non-periodic part)

$$\tilde{E} = \tilde{E}^c + \tilde{E}^b, \quad (21)$$

where $\tilde{E}^b$ is chosen to be the field formed in materials defined by $\epsilon^b(x, z)$

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^b \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^b + k_0^2 \epsilon^b(x, z) \tilde{E}_y^b = 0. \quad (22)$$

Subtracting (22) from (20) yields

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^c + k_0^2 \epsilon(x, z) \tilde{E}_y^c = -k_0^2 (\epsilon(x, z) - \epsilon^b(x, z)) \tilde{E}_y^b. \quad (23)$$

Fig. 5. Permittivities involved in the source term of (23).

We can still choose ϵ^b . However, it should be chosen in such a way that the solution of (22) can be computed analytically. Moreover, we want to choose ϵ^b such that the right-hand side of (23) vanishes in the PML. This is required in order to avoid having a non-periodic source in the PML. If ϵ^b is chosen such that it represents the background of ϵ , i.e. ϵ without the scatterer (rectangular line), then the above mentioned requirements are satisfied; the right-hand side vanishes in the PML, and the background field $\tilde{E}^b$ can be expressed analytically inside the scatterer. Figure 5 shows the permittivities ϵ , ϵ^b , $\epsilon - \epsilon^b$, corresponding to the equations for total field (20), background field (22) and contrast field (23).

4.B. The background field

The background field appears on the right-hand side of (23). Therefore, before solving (23), the solution of (22) needs to be found. Since the background field is not pseudo-periodic, we attempt to obtain it analytically and not with the help of FMM. Let us consider the background problem without PMLs

$$\frac{\partial^2}{\partial x^2} E_y^b + \frac{\partial^2}{\partial z^2} E_y^b + k_0^2 \epsilon^b(x, z) E_y^b = 0. \quad (24)$$

The solutions of (22) and (24) coincide in the physical domain (physical domain = domain - PML region). Since on the right-hand side of (23), $\epsilon - \epsilon^b = 0$ in the PMLs, we need not know the background field in the PML region in order to solve (23).

To solve (24), we use knowledge about angles of reflection and refraction. Figure 6 shows the representation of the solution in terms of plane waves. We assume $h_1 = 0$ and $h_2 = h$. In layer 2 ($0 < z < h$, see Figure 6) the field is written as

$$E_{y,2}^b = E_y^{inc} + E_y^r = \exp(-q_2 z) \exp(-ik_{x0} x) + r \exp(q_2 z) \exp(-ik_{x0} x). \quad (25)$$

In layer 3 ($z > h$)

$$E_{y,3}^b = E_y^t = t \exp(-q_3(z - h)) \exp(-ik_{x0} x), \quad (26)$$

where $q_l = \sqrt{k_{x0}^2 - \epsilon_l^b}$, $l = 2, 3$. The amplitudes r and t are unknown. They can be computed by matching the fields and their normal derivatives at the interface $h_2 = h$.

Fig. 6. The background problem.

$$E_y^{inc}(x, h) + E_y^r(x, h) = E_y^t(x, h), \quad (27)$$

$$\frac{\partial}{\partial z} E_y^{inc}(x, h) + \frac{\partial}{\partial z} E_y^r(x, h) = \frac{\partial}{\partial z} E_y^t(x, h). \quad (28)$$

Using the relations (25), (26) and setting $b = e^{-q_2 h}$, we get a linear system of equations for r and t

$$rb^{-1} + b = t, \quad (29)$$

$$rq_2 b^{-1} - q_2 b = -tq_3. \quad (30)$$

This system has the solution

$$r = \frac{q_2 - q_3}{q_2 + q_3} b^2, \quad t = \frac{2q_2}{q_2 + q_3} b. \quad (31)$$

4.C. Solving for the contrast field

The contrast field satisfies Equation (23). In layers 1 and 3 the right-hand side vanishes (see Figure 7) and the equations are similar to the ones in standard FMM

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_{y,l}^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_{y,l}^c + k_0^2 \epsilon_l(x) \tilde{E}_{y,l}^c = 0, \quad l = 1, 3. \quad (32)$$

Fourier expansion and truncation yields the system of ordinary differential equations

$$\frac{d^2}{dz^2} \tilde{s}_l(z) = k_0^2 \mathbf{A}_l \tilde{s}_l(z), \quad l = 1, 3, \quad (33)$$

The general solution of this system is given by (8). In layer 2 the following equation is solved

$$\frac{1}{f'(x)} \frac{\partial}{\partial x} \left(\frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_{y,2}^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_{y,2}^c + k_0^2 \epsilon_2(x) \tilde{E}_{y,2}^c = -k_0^2 (\epsilon_2(x) - \epsilon_2^b) E_{y,2}^b. \quad (34)$$

This equation is non-homogeneous. The following steps are presented in detail since FMM

Fig. 7. The source term in the contrast-field equation.

has not been applied to such equations before. We proceed in the usual way by expanding the x -dependent quantities in Fourier modes

$$\tilde{E}_{y,2}^c(x, z) = \sum_{n=-\infty}^{\infty} \tilde{s}_{2,n}(z) \exp(-ik_{xn}x), \quad (35a)$$

$$E_{y,2}^b(x, z) = \exp(-q_2 z) \exp(-ik_{x0}x) + r \exp(q_2 z) \exp(-ik_{x0}x), \quad (35b)$$

$$\epsilon_2(x) = \sum_{n=-\infty}^{\infty} \hat{\epsilon}_{2,n} \exp\left(i \frac{2\pi n}{\Lambda} x\right), \quad (35c)$$

$$\frac{1}{f'(x)} = \sum_{n=-\infty}^{\infty} \hat{f}_n \exp\left(i \frac{2\pi n}{\Lambda} x\right). \quad (35d)$$

Substituting (35) in (34) and truncating the infinite series by keeping the harmonics $n = -N, \dots, N$ yields

$$\begin{aligned}
& - \sum_{n=-N}^N \sum_{m=-N}^N \left(\hat{f}_{n-m} k_{xm} \sum_{r=-N}^N \hat{f}_{m-r} k_{xr} \tilde{s}_{2,r}(z) \exp(-ik_{xn}x) \right) \\
& + \sum_{n=-N}^N \frac{d^2}{dz^2} \tilde{s}_{2,n}(z) \exp(-ik_{xn}x) + k_0^2 \sum_{n=-N}^N \sum_{m=-N}^N \hat{\epsilon}_{2,n-m} \tilde{s}_{2,m}(z) \exp(-ik_{xn}x) \\
& = -k_0^2 \sum_{n=-N}^N \sum_{m=-N}^N (\hat{\epsilon}_{2,n-m} - \epsilon_2^b \delta_{n-m}) (\exp(-q_2 z) + r \exp(q_2 z)) \delta_n \exp(-ik_{xn}x),
\end{aligned}$$

where δ_n is the Kronecker delta ($\delta_0 = 1, \delta_n = 0, n \in \mathbb{Z} \setminus \{0\}$).

Since the functions $\exp(-ik_{xn}x)$ form a basis, their coefficients must satisfy

$$\begin{aligned}
& - \sum_{m=-N}^N \left(\hat{f}_{n-m} k_{xm} \sum_{r=-N}^N \hat{f}_{m-r} k_{xr} \tilde{s}_{2,r}(z) \right) + \frac{d^2}{dz^2} \tilde{s}_{2,n}(z) + k_0^2 \sum_{m=-M}^M \hat{\epsilon}_{2,n-m} \tilde{s}_{2,m}(z) \\
& = -k_0^2 \sum_{m=-N}^N (\hat{\epsilon}_{2,n-m} - \epsilon_2^b \delta_{n-m}) \delta_n (\exp(-q_2 z) + r \exp(q_2 z)), \quad n = -N, \dots, N.
\end{aligned} \tag{36}$$

In matrix form this system of equations can be written as

$$\frac{d^2}{dz^2} \tilde{\mathbf{s}}_2(z) = k_0^2 \mathbf{A}_2 \tilde{\mathbf{s}}_2(z) + k_0^2 (\epsilon_2^b \mathbf{I} - \mathbf{E}_2) \mathbf{d}_0 (\exp(-q_2 z) + r \exp(q_2 z)), \tag{37}$$

with

$$\mathbf{A}_2 = (\mathbf{F} \mathbf{K}_x)^2 - \mathbf{E}_2.$$

We recall that the vector $\mathbf{d}_0 \in \mathbb{R}^{(2N+1)}$ in (37) is an all-zero vector except for entry $N+1$ which is equal to 1. Equation (37) is a system of non-homogeneous second order ordinary differential equations. The solution vector is of the form

$$\tilde{\mathbf{s}}_2 = \tilde{\mathbf{s}}_{2,hom} + \tilde{\mathbf{s}}_{2,part}. \tag{38}$$

To find the particular solution we use the method of undetermined coefficients applied to systems of equations [19, p. 241]. If the non-homogeneous term contains functions with a finite family of derivatives (e.g. polynomial and trigonometric functions), the solution may be assumed to be a linear combination of those functions. In our case the particular solution is of the form

$$\tilde{\mathbf{s}}_{2,part}(z) = \mathbf{p} (\exp(-q_2 z) + r \exp(q_2 z)), \tag{39}$$

where $\mathbf{p} \in \mathbb{R}^{(2N+1)}$ is a vector of coefficients to be determined. We substitute the ansatz (39) in Equation (37) and get in the end the following linear system which can be solved for $\mathbf{p}$

$$(k_0^2 \mathbf{A}_2 - q_2^2 \mathbf{I}) \mathbf{p} = -k_0^2 (\epsilon_2^b \mathbf{I} - \mathbf{E}_2) \mathbf{d}_0. \tag{40}$$

Note that in case there is no PML, we have $\mathbf{F} = \mathbf{I}$ and $\mathbf{p} = -\mathbf{d}_0$. The general solution of (37) can now be written using (38) and (39)

$$\tilde{\mathbf{s}}_2(z) = \mathbf{W}_2(\exp(-k_0 \mathbf{Q}_2 z) \mathbf{c}_2^+ + \exp(k_0 \mathbf{Q}_2(z - h)) \mathbf{c}_2^-) + \mathbf{p}(\exp(-q_2 z) + r \exp(q_2 z)). \quad (41)$$

The conditions at the layer interface are

$$\tilde{\mathbf{s}}_1(0) = \tilde{\mathbf{s}}_2(0), \quad (42a)$$

$$-\frac{1}{k_0} \frac{d}{dz} \tilde{\mathbf{s}}_1(0) = -\frac{1}{k_0} \frac{d}{dz} \tilde{\mathbf{s}}_2(0), \quad (42b)$$

$$\tilde{\mathbf{s}}_2(h) = \tilde{\mathbf{s}}_3(h), \quad (42c)$$

$$-\frac{1}{k_0} \frac{d}{dz} \tilde{\mathbf{s}}_2(h) = -\frac{1}{k_0} \frac{d}{dz} \tilde{\mathbf{s}}_3(h). \quad (42d)$$

Since there is no incident field in the contrast problem, the radiation condition implies

$$\tilde{\mathbf{s}}_1^+(0) = \mathbf{0}, \quad (43a)$$

$$\tilde{\mathbf{s}}_3^-(h) = \mathbf{0}. \quad (43b)$$

where $\mathbf{s}_1^+$ and $\mathbf{s}_3^-$ represent the fields consisting of respectively downwards and upwards traveling waves (see Equation (8)). By substituting the general solution (41) into (42) and setting $\mathbf{X}_2 = \exp(-\mathbf{Q}_2 h)$, the relations for the three layers considered are obtained

$$\begin{bmatrix} \mathbf{W}_1 \\ -\mathbf{W}_1 \mathbf{Q}_1 \end{bmatrix} \mathbf{c}_1^- = \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2 \mathbf{X}_2 \\ \mathbf{W}_2 \mathbf{Q}_2 & -\mathbf{W}_2 \mathbf{Q}_2 \mathbf{X}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix} + \begin{bmatrix} \tilde{\mathbf{s}}_{2,part}(0) \\ -k_0^{-1} \tilde{\mathbf{s}}'_{2,part}(0) \end{bmatrix}, \quad (44)$$

$$\begin{bmatrix} \mathbf{W}_2 \mathbf{X}_2 & \mathbf{W}_2 \\ \mathbf{W}_2 \mathbf{Q}_2 \mathbf{X}_2 & -\mathbf{W}_2 \mathbf{Q}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix} + \begin{bmatrix} \tilde{\mathbf{s}}_{2,part}(h) \\ -k_0^{-1} \tilde{\mathbf{s}}'_{2,part}(h) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_3 \\ \mathbf{W}_3 \mathbf{Q}_3 \end{bmatrix} \mathbf{c}_3^+, \quad (45)$$

where

$$\tilde{\mathbf{s}}_{2,part}(z) = \mathbf{p}(\exp(-q_2 z) + r \exp(q_2 z)), \quad (46)$$

$$\tilde{\mathbf{s}}'_{2,part}(z) = \mathbf{p}(-q_2 \exp(-q_2 z) + r q_2 \exp(q_2 z)). \quad (47)$$

The equations (44), (45) can be solved for $\mathbf{c}_1^-$, $\mathbf{c}_2^-$, $\mathbf{c}_2^+$, $\mathbf{c}_3^+$. Note that the inversion of matrix $\mathbf{X}_2$ implies growing exponentials and a loss of accuracy due to round-off. This is a general problem encountered by modal methods. Many solutions have been proposed such as the enhanced transmittance matrix approach [3], the S -matrix and R -matrix algorithms [20]. However, due to the non-homogeneous part, our system has a different structure than in standard FMM and the above algorithms cannot be applied without modifications. We use a full-matrix approach [21, 22] in order to guarantee stability.

5. Numerical results

We consider the aperiodic model problem of scattering from an isolated resist line in air with a width of $100nm$ and a height of $20nm$ illuminated by a plane wave with a wavelength $\lambda = 628nm$ incident at an angle $\theta = \pi/6$. The computational domain has a width $\Lambda = 500nm$ and the lateral PMLs have a width of $100nm$. The geometry of the problem can be seen in Figure 8. The refractive index of air and resist are given by $n_1 = 1$, $n_3 = 1.5$.

Fig. 8. The contrast field computed with aFMM-CFF.

The contrast-field formulation of the FMM with PMLs is used to solve the problem. We refer to this method as the aperiodic Fourier modal method in contrast-field formulation (aFMM-CFF). For the implementation of the PMLs we need to define the coordinate transformation function which is chosen to be a polynomial of degree p ,

$$\tilde{x} = f(x) = \begin{cases} x + i\sigma_0|x - x_l|^{(p+1)}/(p+1), & 0 \leq x \leq x_l, \\ x, & x_l < x < x_r, \\ x - i\sigma_0|x - x_r|^{(p+1)}/(p+1), & x_r \leq x \leq \Lambda, \end{cases} \quad (48)$$

where x_l is the endpoint of the left PML, x_r is the start-point of right PML, σ_0 is the damping strength. We chose a quadratic PML ($p = 2$) with a damping strength $\sigma_0 = 10$. In the computations also the derivative of the coordinate transformation function is required,

$$\frac{d}{dx}f(x) = \begin{cases} 1 - i\sigma_0|x - x_l|^p, & 0 \leq x \leq x_l, \\ 1, & x_l < x < x_r, \\ 1 - i\sigma_0|x - x_r|^p, & x_r \leq x \leq \Lambda. \end{cases} \quad (49)$$

We will first confirm that the PML acts as an absorbing layer. Figure 8 shows the contrast field computed with aFMM-CFF. We observe a decay of the field in the PML to 'almost zero' at the lateral boundaries, which implies that the effect of the pseudo-periodic boundary condition is negligible. It is clear that the amplitude of the field near the lateral boundary could be used as an indication on the performance of the PML and consequently the accuracy

of the numerical solution. This is a matter of further investigation. Note that the solution in the PML is not physically relevant. In order to obtain the solution outside the physical domain, a Green's functions approach may be taken [23].

Fig. 9. Logarithmic plots $\log_{10} e_1$ (left) and $\log_{10} e_2$ (right) of the errors defined in (50).

Next, the convergence behavior of aFMM-CFF and supercell FMM (standard FMM with a large period Λ) is investigated. For this purpose we define

$$e_1(N, \Lambda) = \|E_y^c(N, \Lambda) - E_{ref}\|_2, \quad (50a)$$

$$e_2(N, \sigma_0) = \|\tilde{E}_y^c(N, \sigma_0) - E_{ref}\|_2, \quad (50b)$$

where $\tilde{E}_y^c(N, \sigma_0)$ is the numerical solution obtained with aFMM-CFF for $2N + 1$ harmonics and a damping strength σ_0 , while $E_y^c(N, \Lambda)$ is the numerical solution obtained with supercell FMM for $2N + 1$ harmonics and a period Λ . The reference solution is taken $E_{ref} = E_y^c(800, 15000)$. Figure 9 displays the logarithmic plots of the absolute error for the two methods. Note that since the amplitude of the total field is close to unity, the relative and absolute errors have the same order.

The convergence plots demonstrate that the aFMM-CFF solution converges to the supercell solution. The error of aFMM-CFF has a globally monotonic behavior with respect to N and σ_0 . In other words, increasing either N or σ_0 will not worsen the accuracy of the solution. The supercell FMM has a non-monotonic behavior with respect to Λ . In order to obtain a better solution, increasing Λ would require also taking more harmonics. This behavior is undesirable since it requires following certain 'rules of thumb' when choosing Λ and N .

Also quantitative statements may be made based on Figure 9. It indicates that aFMM-CFF exhibits faster convergence. For instance, an absolute error in the range $10^{-2.7} \dots 10^{-3}$, is attained by the Supercell FMM for N around 80, and by the aFMM-CFF for $N \approx 10$. Note that the plots have different color scales.

6. Conclusions

We have presented an extension of the FMM which enables simulation of scattering from two-dimensional finite structures (invariant in the third dimension) illuminated by plane waves at arbitrary planar angles. A detailed derivation has been provided for the case of planar incidence and TE-polarization. The approach can be generalized to planar TM and conical incidence by following similar steps to the ones presented in the paper. This is technically more involved since in these cases the interface conditions for the contrast field are modified. A detailed presentation of the TM and conical cases is beyond the scope of the paper.

The formulation in terms of a contrast field presented in this paper resembles the scattered field formulations used in FEM and FDTD [24]. However, the reformulation for the FMM is less straightforward, since it requires solutions which can be written in analytical form.

It has been shown how the FMM can be adapted in order to solve non-homogeneous equations. Besides the application demonstrated in the paper, this has far-going implications on the modeling capabilities of the method, such as internal sources inside the domain.

The convergence study has shown that for the aperiodic model problem aFMM-CFF needs less harmonics than the supercell FMM. In view of the fact that the number of operations performed by the eigenvalue solver (which is computationally the most demanding step in the method) scales cubically with the number of harmonics, this results in a considerable reduction of computational time. In our example, for an accuracy of 10^{-3} , a speed-up by a factor of 8^3 is reached.

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