Fast Multipole Method for Periodic Scattering Problems

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1. Abstract

This presentation discusses an FMM for isotropic and anisotropic periodic boundary value problems for Maxwell's equations in 3D. The periodic Green function and its derivatives, which are essential to the present method, are derived with Fourier analysis. We then apply the proposed method to scattering problems for two dimensional array of spheres and silicon woodpile structures, which are standard models in the field of photonic crystals. For the silicon woodpile structures, we compare the obtained energy transmittances with those in the previous studies. We observe good agreements.

2. Introduction

New optical structures in which periodicity plays a significant role are being developed these days. One of most remarkable examples of such structures is the photonic crystal. Photonic crystals are composed of periodic dielectric or metallic structures. By designing the periodic structure properly, we can make band gaps in photonic crystals: we can prohibit propagation of light within certain ranges of frequencies called band gaps. In addition, defects in the periodicity can cause localised modes in the vicinity of defects, which may lead to a pass band in a band gap. Photonic crystals thus enable us to control light freely since we can guide or store light using these phenomena. Nowadays many researchers make great efforts to fabricate new optical devices using photonic crystals: such devices include zero-threshold lasers, large scale optical integrated circuits etc.

Considering such applications, it is concluded very important to develop designing tools for periodic structures, especially in dynamics. Indeed, large scale analyses are required in the design of optical devices such as photonic crystals, since shapes of actual optic devices are very complicated. FM-BIEMs (Fast Multipole Boundary Integral Equation Methods) [1] are good candidates as fast solvers of large scale wave problems since FM-BIEMs require only $O(N(\log N)^{\alpha})$ operations in problems with N boundary elements. The FM-BIEM was first introduced in Laplace's equation [2] and then was applied to many equations which are important in various fields of engineering. In the field of electromagnetics, Chew's group developed the fast multipole solver called MLFMA (Multilevel Fast Multipole Algorithm) [3], which is nowadays one of most standard tools for EM simulations.

However, we can find few researches on large scale periodic scattering problems other than the works of the present author's group [4]. In view of these backgrounds, we develop an FMM for periodic problems for scattering problems in electromagnetics in the present study. The target problems are doubly periodic problems in Maxwell's equations in 3D in frequency domain.

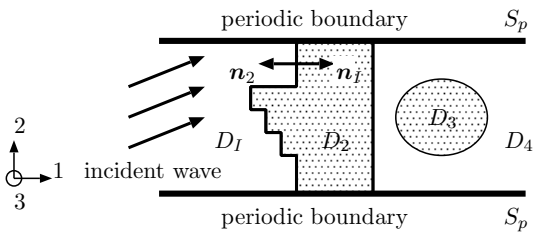

Fig. 1: Periodic boundary value problems

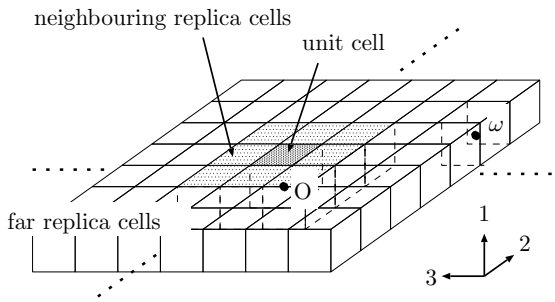

Fig. 2: Replica cells

3. Formulations

In this section we express the formulation of periodic scattering problems for three-dimensional Maxwell's equations. Let D be the domain defined by $D = (-\infty, \infty) \otimes (-L_2/2, L_2/2) \otimes (-L_3/2, L_3/2)$, where L_i is the periodic length in the direction of x_i $(i = 2, 3)$ and we assume $L_2 \geq L_3$. D is further subdivided into N subdomains $D = \overline{D_1 \cup D_2 \cup \cdots \cup D_N}$ (Fig. 1). In each of the subdomains D_i we assume that the following Maxwell's equations are satisfied:

$$\nabla \times \boldsymbol{E} = i\omega\mu^i \boldsymbol{H}, \quad \nabla \times \boldsymbol{H} = -i\omega\epsilon^i \boldsymbol{E} \quad \text{in } D_i,$$

where ω is the frequency (with the $e^{-i\omega t}$ time dependence), ϵ^i and μ^i are the dielectric constant and the magnetic permeability for the material occupying D_i. In the subdomain which extends to $x_1 \to -\infty$, we consider the incident plane wave. On interfaces between different subdomains we impose the continuity conditions on the tangential components of $\boldsymbol{E}$ and $\boldsymbol{H}$. On the periodic boundaries given by $S_p = \{\boldsymbol{x} |\ \boldsymbol{x} \in \partial D,\ |x_2| = L_2/2 \text{ or } |x_3| = L_3/2\}$ we require the following periodic boundary conditions:

$$\boldsymbol{E}(x_1, L_2/2, x_3) = e^{i\beta_2}\boldsymbol{E}(x_1, -L_2/2, x_3), \quad \boldsymbol{E}(x_1, x_2, L_3/2) = e^{i\beta_3}\boldsymbol{E}(x_1, x_2, -L_3/2),$$
$$\boldsymbol{H}(x_1, L_2/2, x_3) = e^{i\beta_2}\boldsymbol{H}(x_1, -L_2/2, x_3), \quad \boldsymbol{H}(x_1, x_2, L_3/2) = e^{i\beta_3}\boldsymbol{H}(x_1, x_2, -L_3/2),$$

where β_i is the phase difference of the incident wave at $x_i = -L_i/2$ and $x_i = L_i/2$, expressed by $\beta_i = L_i k_i^{\text{inc}}$ $(i = 2, 3)$, and k_i^{inc} is the wave number vector of the incident wave.

4. Periodic Green Function

The periodic Green function is one of essential ingredients in our formulation. Because of space limitations, we present just formulae related to the periodic Green function in this paper. Other details will be covered in the presentation.

The periodic Green function for Maxwell's equations is denoted by Γ^{P}_{ip}. The function Γ^{P}_{ip} satisfies the governing equation:

$$e_{ijk}e_{klm}\Gamma^{\text{P}}_{mp,lj}(x - y) - k^2\Gamma^{\text{P}}_{ip}(x - y) = \delta_{ip}\delta(x - y),$$

with periodic boundary conditions. The function Γ^{P}_{ip} is easily seen to be expressed in terms of the following lattice sums:

$$\Gamma^{\text{P}}_{ip}(\boldsymbol{x} - \boldsymbol{y}) = \sum_{\boldsymbol{\omega} \in \mathcal{L}} \Gamma_{ip}(\boldsymbol{x} - \boldsymbol{y} - \boldsymbol{\omega})e^{i\boldsymbol{\beta}\cdot\boldsymbol{\omega}}, \tag{1}$$

where $\mathcal{L}$ stands for the lattice points defined by $\mathcal{L} = \{(0, \omega_2, \omega_3) |\ \omega_2 = pL_2,\ \omega_3 = qL_3,\ p, q \in \mathbb{Z}\}$.

From the lattice sum expression for Γ^{P}_{ip} in (1) we see that the periodic boundary value problems can be interpreted as an ordinary problem in an infinite domain with an infinite repetition of the replicas of the unit cell (Fig. 2).

We now take the unit cell as the level 0 cell in FMM, and divide the set of replica cells into those in the neighbourhood of the unit cell (denoted by C_N) and others (denoted by C_F). Correspondingly, the sum in Γ^{P} is divided into the contribution from C_N, denoted by Γ^{PN} which includes the contributions from the unit cell itself, and those from C_F, denoted by Γ^{PF}. Namely, we have

$$\Gamma_{ij}^{\mathrm{P}} = \Gamma_{ij}^{\mathrm{PF}} + \Gamma_{ij}^{\mathrm{PN}},$$

where

$$\Gamma_{ij}^{\mathrm{PF}}(\boldsymbol{x}-\boldsymbol{y}) = \sum_{\boldsymbol{\omega}\in\mathcal{L}'} \Gamma_{ij}(\boldsymbol{x}-\boldsymbol{y}-\boldsymbol{\omega})e^{i\boldsymbol{\beta}\cdot\boldsymbol{\omega}},$$
$$\Gamma_{ij}^{\mathrm{PN}}(\boldsymbol{x}-\boldsymbol{y}) = \sum_{\boldsymbol{\omega}\in\mathcal{L}''} \Gamma_{ij}(\boldsymbol{x}-\boldsymbol{y}-\boldsymbol{\omega})e^{i\boldsymbol{\beta}\cdot\boldsymbol{\omega}},$$

$\mathcal{L}' = \{(0,\omega_2,\omega_3)|\ \omega_2 = pL_2,\ \omega_3 = qL_3,\ p,q\in\mathbb{Z},\ \sqrt{(pL_2)^2+(qL_3)^2} \geq C\sqrt{2L_2^2+L_3^2}$ and $\mathcal{L}'' = \mathcal{L}\backslash\mathcal{L}'$, where C is a given number and we set $C = \frac{\sqrt{3}}{2}$ in this study.

The evaluation of $\Gamma_{ij}^{\mathrm{PN}}(\boldsymbol{x}-\boldsymbol{y})$ can be carried out using the standard FMM, and needs no further consideration. For the computation of $\Gamma_{ij}^{\mathrm{PF}}(\boldsymbol{x}-\boldsymbol{y})$, we expand $\Gamma_{ij}^{\mathrm{PF}}$ in the following plane wave expansion:

$$\Gamma_{ij}^{\mathrm{PF}}(\boldsymbol{x}-\boldsymbol{y}) = -\frac{ik}{(4\pi)^2}\int_{|\hat{\boldsymbol{k}}|=1}\left(e_{jpk}\frac{\partial}{\partial x_p}e^{i\boldsymbol{x}\cdot\boldsymbol{k}}\right)$$
$$\times\underbrace{\left(\sum_n\sum_m i^n(2n+1)\overline{Y_n^m}(\hat{\boldsymbol{k}})\left(\sum_{\boldsymbol{\omega}\in\mathcal{L}'}O_n^m(-\boldsymbol{\omega})e^{i\boldsymbol{\beta}\cdot\boldsymbol{\omega}}\right)\right)}_{\text{periodised translation operator}}\left(e_{kqi}\frac{\partial}{\partial y_q}e^{-i\boldsymbol{y}\cdot\boldsymbol{k}}\right)dS_{\hat{\boldsymbol{k}}}.$$

In the above equation, the function O_n^m is definded as follows:

$$O_n^m(\overrightarrow{Ox}) = h_n^{(1)}(k|\overrightarrow{Ox}|)Y_n^m\left(\frac{\overrightarrow{Ox}}{|\overrightarrow{Ox}|}\right),$$

where $h_n^{(1)}$ stands for the spherical Hankel function of the 1st kind and nth order. Also, Y_n^m denotes the spherical harmonics. The factor within the second parentheses on the RHS corresponds to the translation operator in the periodised M2L formula. The contribution from the non-adjacent replica cells is evaluated with the periodised M2L formula in level 0.

5. Numerical Results

In this study we deal with standard and important models in the field of photonic crystals. We show examples of the models considered in the present study in Fig. 3, where the left figure shows a model of slab photonic crystals and the right figure gives a model of woodpile photonic crystals. In the case of the woodpile crystal, we computed the energy reflectance and compared the results obtained with the present method with those reported by Gralak et al[5]. We plot the energy reflectance for various wave numbers in Fig. 4. As seen in Fig. 4, our results agreed well with the most accurate results, denoted by '$N = 9\times 9$' (solid line) obtained by Gralak et al.

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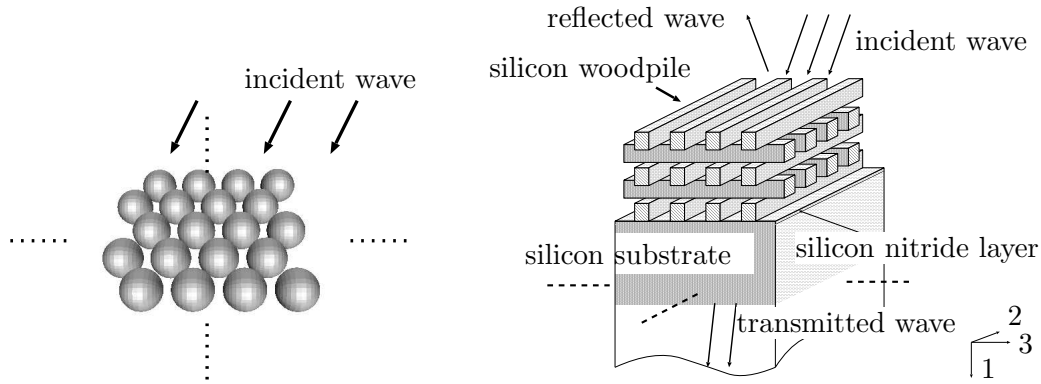

Fig. 3: Examples of models. Left: 2 dimensional array of dielectric spheres, Right: Woodpile crystal

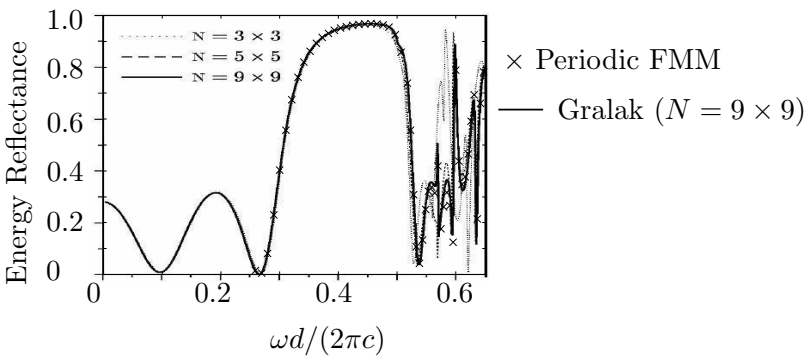

Fig. 4: Reflectance of the woodpile crystal (d: distance between the centres of woodpiles in the x_2 or x_3 direction, ω: frequency, c: light velocity)

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