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A fast and robust solver for the scattering from a layered periodic structure containing multi-particle inclusions

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ABSTRACT

We present a solver for plane wave scattering from a periodic dielectric grating with a large number M of inclusions lying in each period of its middle layer. Such composite material geometries have a growing role in modern photonic devices and solar cells. The high-order scheme is based on boundary integral equations, and achieves many digits of accuracy with ease. The usual way to periodize the integral equation—via the quasi-periodic Green's function—fails at Wood's anomalies. We instead use the free-space Green's kernel for the near field, add auxiliary basis functions for the far field, and enforce periodicity in an expanded linear system; this is robust for all parameters. Inverting the periodic and layer unknowns, we are left with a square linear system involving only the inclusion scattering coefficients. Preconditioning by the single-inclusion scattering matrix, this is solved iteratively in $\mathcal{O}(M)$ time using a fast matrix-vector product. Numerical experiments show that a diffraction grating containing $M = 1000$ inclusions per period can be solved to 9-digit accuracy in under 5 minutes on a laptop.

1. Introduction

The modeling and design of periodic dielectric structures plays a central role in modern optics. Tools such as diffraction gratings, photonic crystals, meta-materials, plasmonics, and other micro-scale structures, are becoming key to efficient devices, including lasers, sensors, anti-reflective surfaces and absorbers [21], and solar cells [3]. For instance, in thin-film solar cell design [44,29] the use of periodic structures, and nanoparticle inclusions, in ordered or disordered composites, enhances absorption. One then seeks a grating structure with a specific arrangement of inclusions that maximizes absorption. Other optimization problems include the design of photonic crystal lenses [35]. Related is the inverse problem of inferring a structure from measurements [37,5]. Such tasks demand a large number of solutions of the direct (forward) scattering problem. Similar periodic and multi-particle wave scattering problems arise in acoustics and elastodynamics, and in general whenever a *super-cell* is used to approximate the response of a random composite material (e.g. [36]). Such considerations have spurred the development of efficient methods for solving Helmholtz and Maxwell frequency-domain boundary value problems in periodic geometries [21,7,14,9,10,23,13,18]. High accuracy can be challenging to achieve due to guided modes, resonances, and extreme parameter sensitivity.

Therefore, in this paper we consider the monochromatic scattering from a layered periodic structure containing a large number M of inclusions ("particles") at given locations, as in a (generalized) photonic crystal. As shown in Fig. 1, the

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structure is periodic in the x direction, layered in the y direction and invariant along the z direction. Because of the two-dimensional (2D) geometry, there exist two fundamental polarizations in the electromagnetic scattering: transverse electric (TE) where the magnetic field is transverse to the (x, y) plane, and transverse magnetic (TM) where the electric field is transverse to the (x, y) plane. We will focus on TE polarization, noting that our technique applies to TM polarization without any essential difficulty.

The grating scattering problem has been mathematically very well studied. It has been proved that for an arbitrary periodic dielectric and incident angle the problem has a unique solution for all frequencies with the possible exception of a countable set of resonances (singular frequencies [11]) at which the solution is not unique. Such physical resonances are not to be confused with *Wood's anomalies* (for the definition see the next section), which are frequencies where at least one of the Bragg diffraction orders points along the grating, i.e. in the x direction. A Wood's anomaly does not prevent the solution from being unique, although it does cause arbitrarily large sensitivity with respect to the incident wave angle or frequency [33], and also causes problems with certain integral equation methods [10]. One of the advantages of our scheme is that it is applicable and accurate at or near Wood's anomalies, without any modifications.

There exists a wide range of numerical methods for periodic diffraction, including boundary integral equations [2,14,10,23,13,18], finite element methods [4,8], Fourier expansion based methods [38], and continuation methods [15]. In the time domain, the finite difference scheme has been discussed in [26]. The advantages of the integral approach over finite elements and finite differences are that it reduces the dimension by one (vastly reducing the number of unknowns), and achieves high-order accuracy with appropriate surface quadratures. However, the resulting linear system is often dense, making a naive matrix-vector product expensive when the number of unknowns is large. In this paper, we will reduce this cost via the fast multipole method (FMM) [24].

More specifically, we propose an integral approach based on the free space Green's function; this bypasses the considerable complexities of computing the periodic Green's function [30,13]. We split the representation of the scattered field in the grating structure into near field and far field components. The near field is represented by standard free-space Helmholtz single- and double-layer potentials on the material interfaces, while the far field is taken care by a *local expansion* (Fourier–Bessel or J expansion) whose coefficients are fixed by enforcing the periodic boundary condition explicitly in the linear system. This builds upon recent ideas of the last author and co-workers [9,10,18].

Solving for discretized layer densities on each of the M inclusion boundaries would introduce an unnecessarily large number of unknowns. Hence, following [22,32], we precompute the inclusion *scattering matrices*, then treat the set of outgoing scattering coefficients as a reduced set of unknowns. When particles are sub-wavelength, and not extremely close to each other, this is highly accurate with only 20 or so unknowns per particle [32]. The full rectangular linear system then couples these to the grating interface densities and periodizing J-expansion coefficients. By eliminating the last two (via a Schur complement and pseudoinverse) we are left with a square linear system for the particle scattering coefficients, which we precondition with a block-diagonal matrix and then solve via GMRES with FMM acceleration, with effort scaling linearly in M. The result is a robust, efficient, high-order accurate solver that we expect to be useful for design and optimization problems for periodic photonic devices.

The outline of the paper is as follows. Section 2 gives the mathematical formulation of the periodic problem. Section 3 proposes the integral approach for the scattering from a periodic structure without particle inclusions, based on the free space Green's function. Section 4 reviews classical multi-particle scattering and discusses the evaluation of the scattering matrix. The quasi-periodizing scheme combining all the above techniques is given in Section 5, and numerical experiments are shown in Section 6. We draw conclusions in Section 7.

2. Problem formulation

Consider the plane-wave incident time harmonic scattering (with time dependence $e^{-i\omega t}$) from a 2D periodic (or grating) structure with period d. As shown in Fig. 1, the unit cell $\Omega = [-d/2, d/2] \times \mathbb{R}$ consists of three layers, denoted by Ω_1, Ω_2 and Ω_3. Let Γ_1 and Γ_2 denote the two smooth interfaces separating the layers. The left and right boundaries of Ω_j are denoted by L_j and R_j, $j = 1, 2, 3$. Assume the permittivity ε is given as ε_1, ε_2 and ε_3 in the three layers respectively. A large number M of particles, collectively denoted by Ω_p, with the same permittivity ε_p, are located inside Ω_2. The permeability μ is assumed to be constant everywhere.

For TE polarization, in which case the total electric field is $E(x, y) = (0, 0, u)$, the full time harmonic Maxwell equations

$$\begin{cases} \nabla \times E = i\omega\mu H \\ \nabla \times H = -i\omega\varepsilon E \end{cases}$$

are reduced to the Helmholtz equation:

$$\Delta u + k(\mathbf{x})^2 u = 0, \tag{1}$$

where $\mathbf{x} := (x, y)$, and where the wavenumber k takes one of four values,

$$k(\mathbf{x}) = \begin{cases} k_1 := \omega\sqrt{\mu\varepsilon_1}, & \mathbf{x} \in \Omega_1 \\ k_2 := \omega\sqrt{\mu\varepsilon_2}, & \mathbf{x} \in \Omega_2 \backslash \overline{\Omega_p} \\ k_3 := \omega\sqrt{\mu\varepsilon_3}, & \mathbf{x} \in \Omega_3 \\ k_p := \omega\sqrt{\mu\varepsilon_p}, & \mathbf{x} \in \Omega_p \end{cases} \tag{2}$$