Robust high-order numerical scattering from multi-layer dielectric gratings using a new integral representation for quasi-periodic fields

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Abstract

Many numerical problems arising in modern photonic and electromagnetic applications involve the scattering of a plane wave from a piecewise-homogeneous medium, periodic in one direction. Boundary integral equations are an efficient approach to solving such boundary-value problems with high-order convergence. The standard way to periodize is then to replace the free-space Green's function kernel with its quasi-periodic cousin. However, a major drawback is that the quasi-periodic Green's function fails to exist for parameter families known as Wood's anomalies, even though the underlying scattering problem remains well-posed. We propose a new integral representation that relies on the *free-space* Green's function alone, adding auxiliary layer potentials on the walls of the unit cell, while enforcing quasi-periodicity with an expanded linear system. The result is a 2nd kind scheme which is immune to Wood's anomalies, avoids lattice sums, is fast-multipole friendly, and allows arbitrary aspect ratios.

Introduction

The design and optimization of modern photonic, electromagnetic and acoustic devices relies heavily on numerical modeling. There has been an explosion of recent interest in devices which are periodic in one or more directions, such as thin film solar cells [4], photonic crystals (including slab guides), meta-materials, and specialized dielectric gratings [6]. Computational efficiency and robustness are paramount because predicting real-world device performance often requires thousands of solutions at different incident wavenumbers and angles. In recent work we presented a robust integral equation scheme for the scattering problem of an infinite periodic array of isolated obscacles [5]. However, in most realistic situations, obstacles or inclusions exist near or on a substrate, possibly with multiple homogeneous layers; see Fig. 1a. Here we extend our previous work to cover these more complicated cases.

To showcase our approach, we focus on the problem of a periodic single dielectric interface (Fig. 1b). Given an incident wavevector $\mathbf{k} = (\kappa^{\rm i}, k^{\rm i}) := (\omega\cos\theta, \omega\sin\theta)$, hence an incoming plane wave $u^{\rm i} = e^{i\mathbf{k}\cdot\mathbf{x}}$ in $\Omega \subset \mathbb{R}^2$,

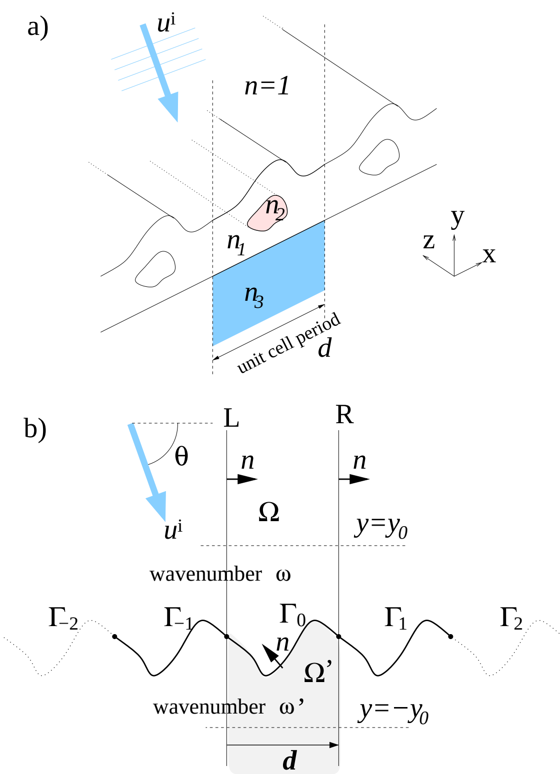

Figure 1: a) General geometry for multi-layer periodic scattering, invariant in the z-direction. b) 2D setup for single dielectric interface (diffraction grating) $\Gamma = \cup_{j\in\mathbb{Z}}\Gamma_j$, with translation vector **d**. Directly-summed images Γ_{-P} to Γ_P are shown as solid lines.

and $u^{\rm i} = 0$ in $\Omega' := \mathbb{R}^2\backslash\overline{\Omega}$, we seek the scattered field u such that the total field $u^{\rm t} = u^{\rm i} + u$ has continuous value and normal derivative across the material interface Γ. The wavenumber below Γ is $\omega' \neq \omega$. Thus one seeks the scattered wave u satisfying the Helmholtz equations

$$(\Delta + \omega^2)u = 0 \quad \text{in } \Omega \quad (1)$$

$$(\Delta + \omega'^2)u = 0 \quad \text{in } \Omega', \quad (2)$$

the inhomogeneous jumps at the interface

$$u^+ - u^- = -u^{\rm i}, \quad u_n^+ - u_n^- = -u_n^{\rm i} \qquad \text{on } \Gamma, \quad (3)$$

where $\pm$ indicates limiting values either side of Γ and

$u_n = \boldsymbol{n} \cdot \nabla u$ the normal derivative, and the quasi-periodicity condition

$$u(x+d, y) = \alpha u(x,y) \qquad \forall (x,y) \in \mathbb{R}^2$$

determined by the indicent wave via $\alpha = e^{i\kappa^{\text{i}} d}$. This situation describes z-invariant acoustics or Maxwell equations (in TM polarization).

A radiation condition is also needed: u has uniformly-convergent upwards and downwards Rayleigh–Bloch expansions,

$$\begin{aligned} u(x,y) &= \sum_{n\in\mathbb{Z}} c_n e^{i\kappa_n x} e^{ik_n(y-y_0)}, \quad y > y_0,\ x \in \mathbb{R} \\ u(x,y) &= \sum_{n\in\mathbb{Z}} d_n e^{i\kappa_n x} e^{ik'_n(-y-y_0)}, \quad y < -y_0,\ x \in \mathbb{R} \end{aligned}$$

where Γ lies within the strip $-y_0 < y < y_0$. Here the horizontal wavenumbers are $\kappa_n = \kappa^{\text{i}} + 2\pi n/d$, and corresponding vertical wavenumbers $k_n = +\sqrt{\omega^2 - \kappa_n^2}$ in Ω, and $k'_n = +\sqrt{\omega'^2 - \kappa_n^2}$ in Ω'. The complex coefficients c_n, d_n, for the propagating modes—that is, $|\kappa_n| \le \omega$ upwards, and $|\kappa_n| \le \omega'$ downwards—are the desired Bragg diffraction amplitudes. All other modes are evanescent. This boundary-value problem (BVP) is known [7] to have a unique solution at all wavenumbers $\omega, \omega' > 0$, and incident angles θ (i.e., there are no guided modes). Whenever $k_n = 0$ or $k'_n = 0$ for some n, i.e. a Bragg scattered wave points along the grating, this is known as a *Wood's anomaly*. Note that the BVP remains well-posed at Wood's anomalies, yet they cause numerical difficulties discussed below.

Boundary integral equations

The standard Müller-Rokhlin [11], [8] integral equation scheme for a closed dielectric interface Γ is to represent the scattered field by

$$u = \begin{cases} \mathcal{S}_\Gamma^{(\omega)}\sigma + \mathcal{D}_\Gamma^{(\omega)}\tau & \text{in } \Omega, \\ \mathcal{S}_\Gamma^{(\omega')}\sigma + \mathcal{D}_\Gamma^{(\omega')}\tau & \text{in } \Omega', \end{cases} \tag{4}$$

where $\mathcal{S}_\Gamma^{(\omega)}$ and $\mathcal{D}_\Gamma^{(\omega)}$ are the standard single and double layer representations [8] on Γ at wavenumber ω, and σ, τ are density functions on Γ. Imposing (3) and using the standard jump relations [8] gives the Fredholm integral equation system

$$A\eta = b, \qquad \eta := \begin{bmatrix} \tau \\ -\sigma \end{bmatrix}, \qquad b := \begin{bmatrix} -u^{\text{i}} \\ -u^{\text{i}}_n \end{bmatrix} \tag{5}$$

where A is of the form identity plus compact. Hence the system is 2nd kind, a numerically desirable feature since it implies a well-conditioned linear system even upon fine Nyström discretization.

One may solve the case of Γ unbounded and periodic by restricting (4) to one period Γ_0, while replacing the free space Green's function kernels $G(\mathbf{x},\mathbf{y}) = \frac{i}{4}H_0^{(1)}(\omega|\mathbf{x}-\mathbf{y}|)$, $\mathbf{x},\mathbf{y} \in \mathbb{R}^2$, in the operators by the *quasi-periodic Green's function* $G_{\text{QP}}(\mathbf{x},\mathbf{y}) := \sum_{j=-\infty}^{\infty} \alpha^j G(\mathbf{x}, \mathbf{y} + j\mathbf{d})$. Computation of G_{QP} is difficult and slow [3], and requires evaluation of *lattice sums* [9] if the integral equation is to be compatible with fast-multipole acceleration. Lattice sums converge in a disc, placing an inconvenient limit on the aspect ratio of Γ.

More severely, G_{QP} does not exist at Wood's anomalies, so this numerical method fails. In the multi-layer setting, each layer has its own set of Wood's anomalies, exacerbating this problem. Chandler-Wilde and co-workers [10], [2] prevent this failure in the single-interface case by using the quasi-periodic Green's function for a Dirichlet or impedance half-space; however, their idea does not help in the case of isolated obstacles [5], and becomes cumbersome for multiple layers. We now present a periodizing scheme with significant advantages over all of the above: it is flexible, robust at all scattering parameters, and requires only evaluation of the free-space Green's function and simple exponentials.

Proposed periodizing scheme

We return to representation (4) with unknown densities σ and τ lying on Γ_0, and duplicate these densities (with the appropriate phases) on its nearest neighboring images. The remaining field (due to the remaining infinite image sums) we represent by auxiliary densities lying on the L and R unit cell walls, thus, in Ω,

$$\begin{aligned} u = &\sum_{j=-P}^{P} \alpha^j \left(\mathcal{S}_{\Gamma_j}^{(\omega)}\sigma + \mathcal{D}_{\Gamma_j}^{(\omega)}\tau \right) + \\ &\left(\mathcal{S}_L^{(\omega)} + \alpha\mathcal{S}_R^{(\omega)} \right)\mu + \left(\mathcal{D}_L^{(\omega)} + \alpha\mathcal{D}_R^{(\omega)} \right)\nu \end{aligned} \tag{6}$$

We use a similar representation in Ω' with wavenumber ω', the same σ and τ, but independent wall densities μ',ν'. Typically $P = 2$. We stack the wall unknown densities as $\xi := [\nu; -\mu; \nu'; -\mu']$. We define the wall *discrepancies* $f = u|_L - \alpha^{-1}u|_R$ and $f_n = u_n|_L - \alpha^{-1}u_n|_R$, and impose the new condition that $[f; f_n]$ vanish. The latter becomes the second block row of an expanded version of (5) (the first block row imposing the matching condition on Γ_0), giving the larger system,

$$\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \eta \\ \xi \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}. \tag{7}$$

Operator B describes the effect of wall densities on Γ_0, C describes the effect of interface densities on the discrepancy, and Q the effect of wall densities on the discrepancy. By our careful choice of neighboring copies of interface densities we get beneficial cancellations of close interactions in C. Likewise, by the placement of wall densities on L and R, Q is the identity plus only distant interactions.

To handle densities on unbounded walls L and R, we choose to work in Fourier variables in the vertical (y) direction. This relies on the representation for the Green's function

$$G^{(\omega)}(\mathbf{x}) = \frac{i}{4\pi}\int_{-\infty}^{\infty} e^{iky}\,\frac{e^{i\sqrt{\omega^2-k^2}\,|x|}}{\sqrt{\omega^2-k^2}}\,dk\,, \quad \mathbf{x}=(x,y) \tag{8}$$

where the Sommerfeld integral passes through the origin, from the 2nd to 4th quadrants in the complex k plane. Since explicit direct summation of nearby images of Γ_0 has been done, the remaining field that ξ needs to represent in the solution is smooth: since $|x| > d$ the above integrand has exponential tails. We approximate the Fourier transforms to spectral accuracy using M quadrature points along a suitable k contour. Near a Wood's anomaly, the integrand has poles (at the wavenumbers $\pm k_n$ or $\pm k'_n$) which merge at the origin, rendering this contour quadrature inaccurate. We fix this by translating the contour in the complex plane so that it passes an $O(1)$ distance from all poles, and correct the change in radiation boundary conditions thus introduced by the addition of a single plane wave into the representation of u. Finally the coefficient of this plane wave is determined by the linear condition that the fields in Ω and Ω' each obey the correct radiation condition (as in [5]). This adds an extra row and column to the discretized system matrix, and renders the scheme oblivious to Wood's anomalies [5].

Quadrature on the interface Γ

The A operator involves the self-interaction of Γ_0, which requires the approximation of the action of integral operators with (at most) logarithmic singularity on the diagonal. Alpert [1] has designed quadrature corrections for such integrands based upon replacing the periodic trapezoid rule nodes in a neighborhood of the singularity by a new set of unequally spaced nodes. We use the 16th order rule, which replaces 10 grid nodes on either side. Lagrange barycentric polynomial interpolation from the local regular grid is used to get the density function at these new nodes. In terms of the matrix approximation of A, these corrections live along a (periodic) diagonal band which includes northeast and southwest corners of the matrix. In order to 'unwrap' this periodic rule for the quasi-periodic case of an *open* segment Γ_0, these corners need to be modified to account for interactions with Γ_{-1} and Γ_1. Finally, the uncorrected periodic trapezoid quadrature can be used for the B and C blocks since they involve only *distant* interactions.

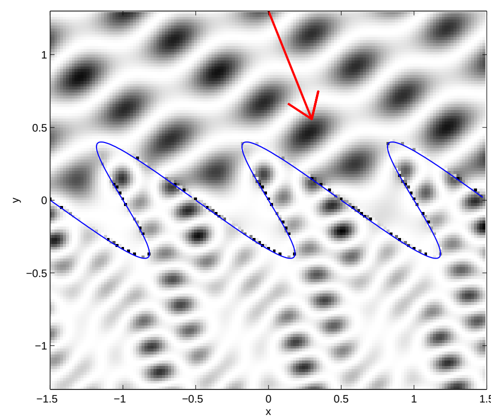

Figure 2: Square of real part of full field for sheared sinusoidal dielectric interface, wavenumbers $\omega = 10, \omega' = 20$, at a Wood's anomaly for the upper half-place, $\theta = -\cos^{-1}(1 - \frac{2\pi}{\omega})$, shown by arrow. Accuracy is 12 digits.

Results

Fig. 2 shows a dielectric grating scattering problem at a Wood's anomaly solved with an error of 10^{-12} (verified by flux conservation), solved in 2 sec, with a further 10 sec to plot u on a grid of 6500 points. (All timings are reported for a 2006-era laptop, 2GHz Intel Core Duo CPU, 2GB RAM, running MATLAB and `MPSpack` [5].) This needs $N = 120$ nodes on Γ_0, and $M = 100$ Fourier quadrature points on the Sommerfeld contour, giving a dense square linear system of size $2N + 4M + 1 = 661$. Condition number (after row and column rescaling) is 900, and if GMRES is used, 129 iterations are needed.

Fig. 3 shows an interface of height 10 periods, needing more quasi-periodizing degrees of freedom ($M = 260$). Errors are 10^{-7}, $N = 550$, giving matrix size 2140, and taking 21 secs to fill and solve, then 70 sec to plot. Finally, the ability to combine inclusions and interfaces at a Wood's anomaly is shown by Fig. 4, which has error 2×10^{-12}, solution time 1.3 sec, and matrix size 521.

Our robust 2nd kind scheme generalizes simply to multi-layer media with inclusions; we will present results on this case at the conference.

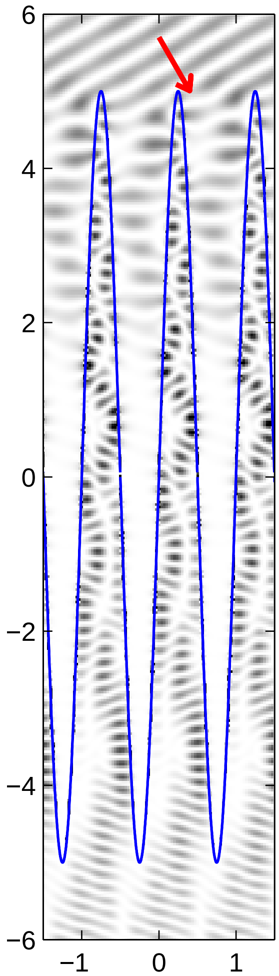

Figure 3: High-aspect ratio dielectric interface, $\omega = 10$, $\omega' = 20$. The structure is 32λ tall at the higher wavenumber.

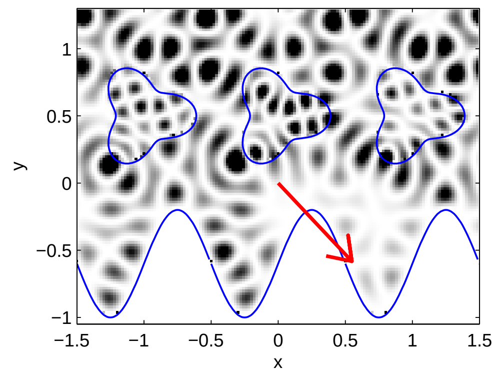

Figure 4: Dirichlet (PEC or sound-soft) grating with nearby inclusions (of wavenumber $\omega' = 30$), incident wavenumber $\omega = 20$, at a Wood's anomaly. Accuracy is 12 digits.

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