Efficient Solution of Acoustic and Electromagnetic Scattering Problems in Three-Dimensional Periodic Media

Oscar Bruno[1,*], **Stephen Shipman**[2], **Catalin Turc**[3], **Stephanos Venakides**[4]
[1] ACM Caltech, Pasadena, USA
[2] Department of Mathematics LSU, Baton Rouge, USA,
[3] Department of Mathematics CWRU, Cleveland, USA,
[4] Department of Mathematics Duke, Durham, USA. *Email: obruno@caltech.edu

Abstract

We present an accurate and efficient numerical method, based on integral Nyström discretizations, for the solution of three dimensional wave propagation problems in piece-wise homogeneous media that have two-dimensional (in-plane) periodicity (e.g. photonic crystal slabs). Our approach uses (**1**) A fast, high-order algorithm for evaluation of singular integral operators on surfaces in three-dimensional space, and (**2**) A new, representation of the three-dimensional quasi-periodic Green's functions, which, based on use of infinitely-smooth windowing functions and equivalent-source representations, converges super-algebraically fast throughout the frequency spectrum—even for high-contrast problems and at and around the resonant frequencies known as Wood anomalies.

1 Introduction

We consider the problem of transmission of time-harmonic acoustic waves by periodic structures, including (a) Structures $\Omega_{per} = \cup_{(n,m)\in\mathbb{Z}\times\mathbb{Z}}\Omega_{m,n}$, where $\Omega_{0,0} = \Omega$ is a bounded region in $\mathbb{R}^3$ whose boundary Γ is a (possibly singular) closed surface and where $\Omega_{m,n}$ are defined by $\Omega_{m,n} = \Omega + md_1\mathbf{a}_1 + nd_2\mathbf{a}_2$ in terms of given unit vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ and periods d_1 and d_2; (b) Similarly defined periodic arrays of open surfaces, and (c) Combinations of these two types of periodic configurations. For simplicity we restrict our presentation to the acoustic case. The treatment in the electromagnetic case is analogous, albeit more complicated; our results, however, include both examples of scalar and electromagnetic problems. For acoustic problems concerning structures of type (a), for example, we solve the scattering problem

$$\begin{aligned}
\Delta u_1 + k_1^2 u_1 &= 0 \text{ in } \mathbb{R}^3\setminus\Omega_{per},\ k_1 = \omega\sqrt{\epsilon_1}\\
\Delta u_2 + k_2^2 u_2 &= 0 \text{ in } \Omega_{per},\ k_2 = \omega\sqrt{\epsilon_2}\\
u_1 &= u_2,\ \frac{\partial u_1}{\partial n} = \frac{\partial u_2}{\partial n} \text{ on } \Gamma_{per}\\
\Gamma_{per} &= \cup_{(n,m)\in\mathbb{Z}\times\mathbb{Z}}\Gamma + md_1\mathbf{a}_1 + nd_2\mathbf{a}_2
\end{aligned} \quad (1)$$

Here $u_1 = u^{inc} + u^s$, where the incident field u^{inc} is e.g., a given plane wave of the form $u^{inc}(\mathbf{x}) = \exp(ik_1\mathbf{d}\cdot\mathbf{x}) = \exp[i(\alpha x_1 + \beta x_2 - \gamma x_3)]$ with $\alpha = k_1\sin\psi\cos\phi$, $\beta = k_1\sin\psi\sin\phi$, and $\gamma = k_1\cos\psi$. We require that the scattered fields u^s be (α,β) quasi-periodic with respect to x_1 and x_2 and outgoing in the regions above and below Γ_{per}.

Our problems can be posed in terms of boundary integral equations that involve the quasi-periodic Green's functions. For wavenumbers k different from the Wood anomaly values $k^2 = \left(\alpha + \frac{2\pi n}{d_1}\right)^2 + \left(\beta + \frac{2\pi m}{d_2}\right)^2$ (where $(m,n)\in\mathbb{Z}\times\mathbb{Z}$ are arbitrary integers), the (α,β) quasi-periodic Green's function is given by

$$\begin{aligned}
G_k^{per}(\mathbf{x},\mathbf{x}') &= \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} e^{i\alpha md_1}e^{i\beta nd_2}\\
&\times\ G_k(\mathbf{x}-\mathbf{x}'-md_1\mathbf{a}_1-nd_2\mathbf{a}_2),
\end{aligned} \quad (2)$$

where $G_k(\mathbf{z}) = e^{ik|\mathbf{z}|}/(4\pi|\mathbf{z}|)$.

The problem embodied in equation (1) can be recast in terms of the following integral equation formulations on Γ:

$$\begin{pmatrix} I + K_2 - K_1^{per} & S_2 - S_1^{per} \\ N_2 - N_1^{per} & I + (K_1')^{per} - K_2' \end{pmatrix}\begin{pmatrix} u_1 \\ \frac{\partial u_1}{\partial n}\end{pmatrix} = \begin{pmatrix} u^{inc} \\ \frac{\partial u^{inc}}{\partial n}\end{pmatrix}, \quad (3)$$

where S_2, K_2, K_2' and N_2 denote the single layer, double layer, Neumann trace of the single layer and Neumann trace of the double layer potentials on Γ associated with free-space Green's function G_{k_2}, and where S_1^{per}, K_1^{per}, $(K_1')^{per}$ and N_1^{per} denote the corresponding boundary layer operators associated with quasi-periodic Green's functions (2) with $k = k_1$.

The very slow conditional convergence of the periodic Green's function (2) has been extensively discussed in the vast literature devoted to this subject (see e.g. the comprehensive review articles [6], [7]), and several methods to accelerate its convergence, notably Ewald's method [5] and lattice sums methods [7], have been proposed. Following up on ideas introduced in [8], we propose a new approach for fast evaluations of integral operators involving periodic Green's functions: we use a smooth windowing function χ such that $\chi(t) = 1, t \leq 1$ and $\chi(t) = 0, t \geq 2$ and we approximate G_k^{per} in the following manner

$$\begin{aligned} G_k^{per}(\mathbf{x}, \mathbf{x}') &\approx \sum_{(md_1)^2+(nd_2)^2 \leq 4L^2} \chi\left(\frac{d_{mn}}{L}\right) e^{i\alpha n d_1} e^{i\beta m d_2} \\ &\times \; G_k(\mathbf{x} - \mathbf{x}' - md_1\mathbf{a}_1 - nd_2\mathbf{a}_2) \\ &= \; G_k^{per,L}(\mathbf{x}, \mathbf{x}'), \end{aligned} \tag{4}$$

where $d_{mn} = ((md_1)^2 + (nd_2)^2)^{\frac{1}{2}}$. If k is not a Wood anomaly, then $G_k^{per,L}$ converges to G_k^{per} super-algebraically as $L \to \infty$. In the Wood anomaly case, in turn, use of adequate differences of such windowed expressions restores super-algebraic convergence even at an around Wood anomaly frequencies. We thus have the following Theorem.

Theorem 1.1 *(BSTV) If k is not a Wood anomaly, then for all $\mathbf{x} \neq \mathbf{x}'$ and all integers $p \geq 2$*

$$|G_k^{per}(\mathbf{x}, \mathbf{x}') - G_k^{per,L}(\mathbf{x}, \mathbf{x}')| \leq CL^{\frac{1}{2}-p}.$$

Further, substitution of the free space Green function in (4) by a linear combination of multiple reflections across adequately chosen horizontal planes provides super-algebraic convergence even at and around Wood anomalies.

2 Numerical Method

The rapidly convergent quasi-periodic Green's function $G_k^{per,L}$ can be incorporated seamlessly into the high-order Nyström discretizations introduced in [1], [2]. As shown in what follows, further, the acceleration strategy based on use of equivalent sources and 3D sparse FFTs described in [2] can be extended to the treatment of quasi-periodic problems. The first step of the acceleration procedure consists of partitioning a cube C of size A circumscribing Γ into L^3 identical cubic cells c_i of size adjusted so that they do not admit resonances. The main idea of the acceleration algorithm is to seek to substitute the surface "true" sources which correspond to the discretization points on Γ contained in a certain cube c_i by periodic "equivalent sources" on the faces of c_i in a manner such that the fields generated by the c_i-equivalent sources approximate to high order accuracy the fields produced by the true c_i sources at all points in space non-adjacent to c_i. For a fixed value $l = 1, 2, 3$, we associate to a field u and each cell c_i-equivalent sources, acoustic monopoles $\xi_{i,j}^{(m)l}\ G_k^{L,per}(\mathbf{x} - \mathbf{x}_{i,j}^l)$ and dipoles $\xi_{i,j}^{(d)l}\ \partial G_k^{L,per}(\mathbf{x} - \mathbf{x}_{i,j}^l)/\partial x_l$ placed at points $\mathbf{x}_{i,j}^l, l = 1, \cdots, M^{equiv}$ contained within certain subsets Π_i^l. The fields $\psi^{c_i,true}$ radiated by the c_i-true sources are approximated then in the least square sense by fields $\psi^{c_i,eq}$ radiated by the c_i-equivalent sources $\psi^{c_i,eq}(\mathbf{x}) = \sum_{j=1}^{\frac{1}{2}M^{equiv}} (\xi_{i,j}^{(m)l}\ G_k^{L,per}(\mathbf{x}, \mathbf{x}_{i,j}^l) + \xi_{i,j}^{(d)l} \frac{\partial G_k^{L,per}(\mathbf{x}, \mathbf{x}_{i,j}^{(d)l})}{\partial x_l})$. The parameters n_t, M^{equiv} and the unknown monopole and dipole intensities in the representation of $\psi^{c_i,eq}$ are chosen so that the truncated spherical wave expansions of order n_t for $\psi^{c_i,true}$ and $\psi^{c_i,eq}$ differ in no more than $\mathcal{O}(\epsilon)$ outside $\mathcal{S}_i$. The intensities $\xi_{i,j}^{(m)l}$ and $\xi_{i,j}^{(d)l}$ are obtained in practice as the least-squares solution of three overdetermined linear systems $\mathbf{A}\xi = \mathbf{b}$ where $\mathbf{A}$ are $n^{coll} \times M^{equiv}$ matrices. This strategy leads to a computational cost of $\mathcal{O}(4L^2 N^{4/3} \log N)$ for our solver, where N is the number of discretization points.

The evaluation of quasi-periodic Green's functions can be accelerated beyond the fast convergence implicit in Theorem 1.1 by resorting to Taylor expansions of the terms $G_k(\mathbf{x} - \mathbf{x}' - md_1\mathbf{a}_1 - nd_2\mathbf{a}_2)$ in inverse powers of $d_{m,n} = \sqrt{(md_1)^2 + (nd_2)^2}$ for sufficiently large values of $d_{m,n}$—say, for $d_{m,n} \geq T$, where T is a truncation parameter; cf. Table 2 below.

3 Numerical Results

In Table 1 we present results concerning acoustic and electromagnetic transmission problems for a periodic array Γ_{per} of high-contrast dielectric spheres ($\epsilon_1 = 1,\ \epsilon_2 = 40$) for the frequency value $\omega = k_1 = 0.75$ (reduced angular frequency $\omega d/\pi = 0.4775$) in the resonance regime relevant to photonics research. We present errors in conservation of energy (using the energy-balance indicator $\varepsilon = |1 - \mathit{reflected} - \mathit{transmitted}|$) together with computational times and numbers of iterations required by our solvers to reach a GMRES residual of 10^{-4}. Convergence studies we have conducted show that the quantity ε provides, in our context, an accurate measure of maximum errors

Unknowns	L	ε	It/Time
$12 \times 16 \times 16$	20	2.1×10^{-3}	19/5m38sec
$12 \times 16 \times 16$	30	8.4×10^{-4}	19/9m29sec
$12 \times 32 \times 32$	50	4.9×10^{-5}	19/26m10sec
$24 \times 16 \times 16$	20	7.2×10^{-4}	103/28m23sec
$24 \times 16 \times 16$	30	6.3×10^{-4}	103/31m50sec
$24 \times 32 \times 32$	50	3.4×10^{-5}	103/44m8sec

Table 1: Convergence of the periodic transmission solvers using $G_k^{L,per}$ for various L. No additional Taylor-expansion truncations (cf. Section 2) were used to obtain the results in this table. Here and throughout this paper, the notation $P \times n \times n$ indicates that a total of P patches are used to represent Γ, and $n \times n$ discretization points are used in each patch.

Body Γ	L	T	ε	It/Time
Sphere	80	80	1.9×10^{-3}	18/51m4sec
Sphere	80	20	1.4×10^{-2}	18/3m41sec
Cube	80	80	1.3×10^{-5}	70/58m42sec
Cube	80	20	1.9×10^{-3}	70/14m21sec
Disc	80	80	1.4×10^{-5}	17/50m56sec
Disc	80	20	2.0×10^{-2}	17/5m54sec

Table 2: Computational times of periodic solvers using $G_k^{L,per}$ and Taylor-expansion truncations at level T; cf. Section 2. Discretizations containing $6\times16\times16$ points were used for the sphere and cube, while a $5 \times 16 \times 16$ discretization was used for the open disc; in all cases a frequency five times larger than that in Table 1 was assumed.

in the far field.

Remark. *We note that the implementation of one of the most advanced approaches previously put forth for evaluation of periodic Green's functions [3]—which is based use of a combination of techniques, including spatial and spectral representations as well as Kummer transforms and Shanks transforms—has been reported to require several milliseconds per evaluation point in present-day single processors [4]. Thus, even for a small discretization consisting of* $N = 6\times16\times16$ *points (here we are assuming a total of* 6 *patches are used to represent* Γ*, and* 6×6 *discretization points are used in each patch) the number* $2\times N^2 = 4.7\times10^6$ *of values of the quasi-periodic Green's functions that are needed for computation of the four boundary integral operators* (3) *would require, if produced by the method [3], at least* 4.7×10^3 *seconds for a single matrix vector product (assuming a conservative one millisecond per Green function evaluation). In contrast, as it can be seen in Table 1, our method requires about* 83 *seconds to evaluate a matrix vector product in the case under consideration, leading, upon use of a Krylov-subspace iterative solver, to results with 5 digits of accuracy.*

In Table 2 we present results based on the Taylor-expansion truncation strategy described in Section 2 with truncation parameter $T = 20$ and keeping the two leading terms in the Taylor series expansions. This table includes results for sound-soft (Dirichlet) quasi-periodic problems of scattering by various types of periodic arrays, with $\omega = k = 3.75$ (reduced frequency = 2.5, five times larger than that in Ta-

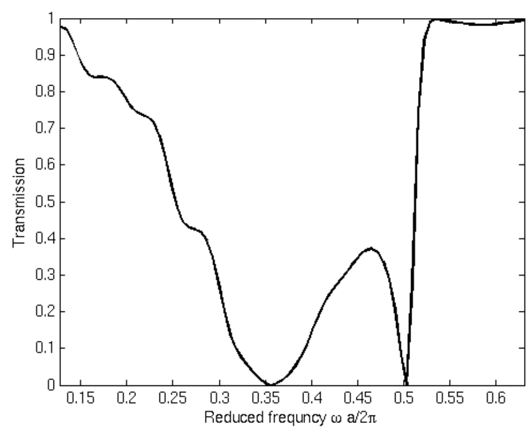

Figure 1: Transmission curve for a 2D array of high-contrast cubes ($\epsilon_1 = 1,\ \epsilon_2 = 40$) at normal incidence.

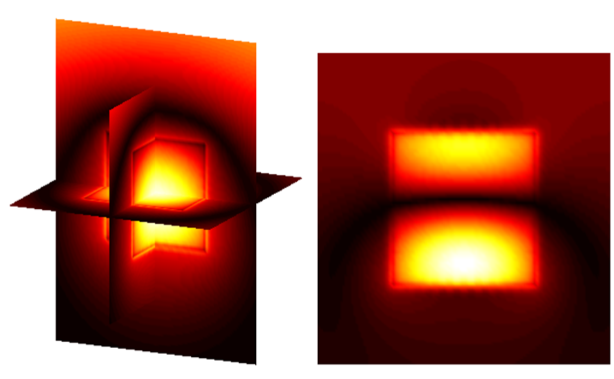

Figure 2: Fields inside and near the scatterer for reduced frequencies equal to 0.36 (left) and 0.51 (right), corresponding to the near-zero transmission cases clearly visible in Figure 1.

ble 1). We see that use of the truncation strategy leads to very fast computations.

In Figures 1 and 2 we display the transmission curve and near fields for the problem of scattering and transmission of plane waves by two-dimensional periodic arrays of high-contrast acoustic cubes at normal incidence (again here $\epsilon_1 = 1,\ \epsilon_2 = 40$). The near-field images correspond to two almost-zero transmission frequencies that can easily be seen in the transmission curve. For the reduced frequency equal to 0.36 (Figure 1 middle) the transmission coefficient is very small (about 10^{-5}). For reduced frequency is 0.51 (Figure 1 bottom) we observe a significant resonant behavior: the amplitude of the fields in the interior of the scatterer is approximately 8 times larger than the amplitude of the fields outside the scatterer.

In Figure 3 we present transmission curves in the electromagnetic case for a 2D array of high-contrast spheres ($\epsilon_1 = 1,\ \epsilon_2 = 40$) with oblique incidence. In Figure 4, finally, we demonstrate the capability of

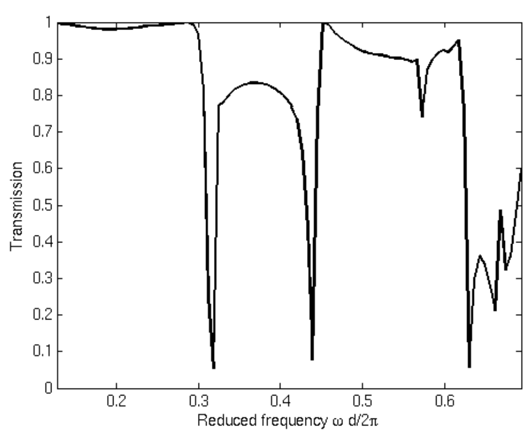

Figure 3: Transmission curves in the electromagnetic case for a 2D array of high-contrast spheres ($\epsilon_1 = 1,\ \epsilon_2 = 40$) at oblique incidence ($\psi = \pi/6, \phi = 0$) and y polarization.

our algorithm to handle problems at and around the classically challenging Wood anomaly values.

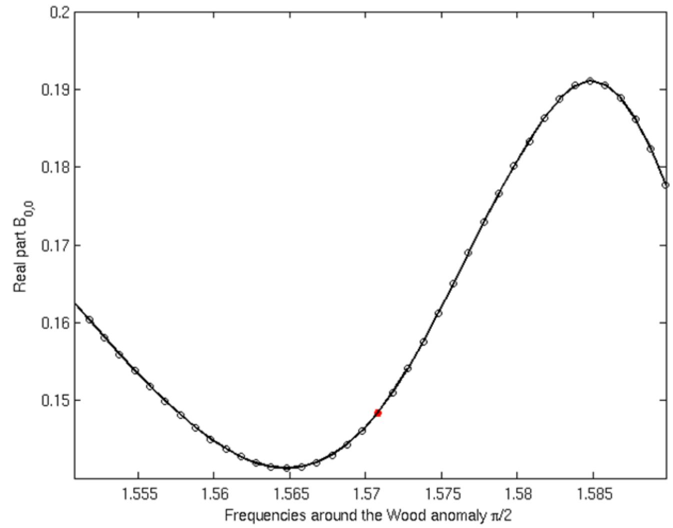

Figure 4: Real part of the backscattered amplitude as a function k at and around the first Wood anomaly $\pi/2$ (marked by a red point), for a sound soft bi-sinusoidal grating at normal incidence.

References

[1] O. Bruno, T. Elling, R. Paffenroth, and C. Turc, “Electromagnetic integral eqns. requiring small numbers of Krylov-subspace iterations”, J. Comput. Phys, 228 (17), 6169-6183, 2009.

[2] O. Bruno and L. Kunyansky, “A fast, high-order algorithm for the solution of surface scatt. problems: basic implementation, tests, and applications”, J. Comput. Physics, 169, 80-110, 2001.

[3] Guerin, S., Enoch, S., and G. Tayeb, “ Combined method for the computation of the doubly periodic Green’s functions”, J. of Electr. Waves and Appls, vol 15, 205-221, 2001.

[4] Bleszynski, E. H., Bleszynski, M. K., and T. Jaroszewicz, “Rigorous modeling of electromagnetic wave interactions with large dense discrete scatterers”, 2010

[5] Ewald, P., “Die Berechnung optischer und elektrostatischen Gitterpotentiale”, Ann. Phys. 64 (1921), 253-268

[6] C. M. Linton, “The Green’s function for the two-dimensional Helmholtz equation in periodic domains”, J. Eng. Math., vol 33, 377-402, 1998.

[7] C. M. Linton, I. Thompson, “One- and two-dimensional lattice sums for the three-dimensional Helmholtz equation”, J. Eng. Mathematics, vol 33, 377-402, 1998.

[8] J. A. Monro, “A Super-Algebraically Convergent, Windowing-Based Approach to the Evaluation of Scattering from Periodic Rough Surfaces”, Thesis, Caltech.