

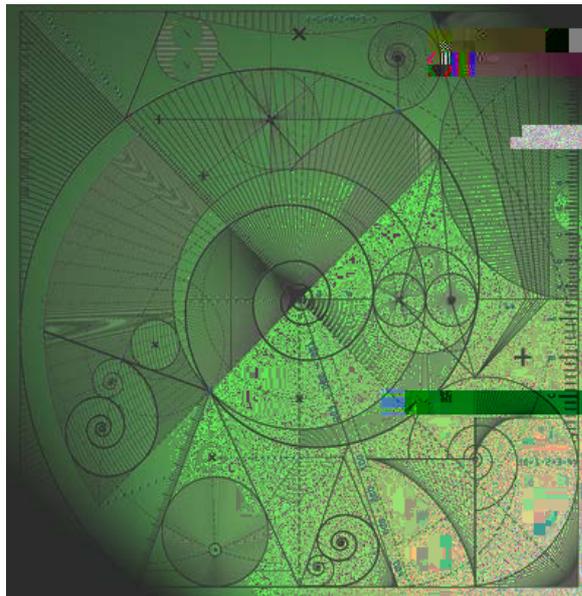
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Acoustic scattering: high frequency boundary element methods and unified transform methods

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Abstract

We describe some recent advances in the numerical solution of acoustic scattering problems. A major focus of the paper is the efficient solution of high frequency scattering problems via hybrid numerical-asymptotic boundary element methods. We also make connections to the unified transform method due to A. S. Fokas and co-authors, analysing particular instances of this method, proposed by J. A. DeSanto and co-authors, for problems of acoustic scattering by diffraction gratings.

1 Introduction

The reliable simulation of processes in which acoustic waves are scattered by obstacles is of great practical interest, with applications including the modelling of sonar and other methods of acoustic detection, and the study of problems of outdoor noise propagation and noise control, for example associated with road, rail or aircraft noise. Unless the geometry of the scattering obstacle is particularly simple, analytical solution of scattering problems is usually impossible, and hence in general numerical schemes are required.

Most problems of acoustic scattering can be formulated, in the frequency domain, as linear elliptic boundary value problems (BVPs) on the exterior of a bounded domain. The boundary conditions are typically of Dirichlet, Neumann or mixed type. The boundary conditions are typically of Dirichlet, Neumann or mixed type. The boundary conditions are typically of Dirichlet, Neumann or mixed type.

solve such problems, and we summarise in particular recent progress in tackling high frequency scattering problems by combining classical BEMs with insights from ray tracing methods and high frequency asymptotics. We

Equation (1) models acoustic propagation in a homogeneous medium at rest. We are often interested in applications in propagation through a medium with variable wave speed. The BEM is well-adapted to compute solutions in the case when the wave speed is piecewise constant. In particular, when a homogeneous region with a different wave speed is embedded in a larger homogeneous medium, acoustic waves are transmitted across the boundary between the two media, (1) holds on either side of with different values of $k = \omega/c$, and, at least in the simplest case when the density of the two media is the same, the boundary conditions on Γ (so-called "transmission conditions") are that u and $\partial u/\partial n$ are continuous across Γ .

The domain D can be a bounded domain (e.g. for applications in room acoustics), but in many practical applications it may be unbounded (e.g. for outdoor noise propagation). In this case, the complete mathematical formulation must also include a condition to represent the idea that the acoustic field (or at least some part of it, e.g. the part reflected by a scattering obstacle) is travelling outwards. The usual condition imposed is the Sommerfeld radiation condition,

$$\frac{\partial u}{\partial r}(x) - iku(x) = o(r^{-(d-1)/2}); \quad (4)$$

as $r \rightarrow \infty$.

and thus work throughout in a Sobolev space setting (see, e.g., [65]; for the simpler case of smooth boundaries we refer to [28]). We then consider the numerical solution of these BIEs in x_3 , focusing in particular, in $x_{3.3}$, on schemes that are well-adapted to the case when the wavenumber k is large. As we report, for many scattering problems these methods provably compute solutions of any desired accuracy with a cost, in terms of numbers of degrees of freedom and size of matrix to be inverted, that is close to frequency independent.

There is a wide literature on boundary integral equation formulations for acoustic scattering problems and boundary element methods for linear elliptic BVPs: see, e.g., [6, 28, 57, 60, 65, 68, 72, 73, 74], and see also, e.g., [59] for a comparison with finite element methods. The question of how to develop schemes efficient for large k

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of $H^s(\mathbb{R}^d)$, while, for $n \in \mathbb{N}$, $W^n(D)$ will denote those $u \in L^2(D)$ whose partial derivatives of order $\leq n$ are also in $L^2(D)$: in particular $W^1(D) = \{u \in L^2(D) : \nabla u \in L^2(D)\}$.

Next we state the exterior BVPs. Suppose that

rather than constant: precisely that, for some constantsk

for $x, y \in \mathbb{R}^d$, $x \neq y$

introduce the single-layer potential operator $S_k : H^{-1/2}(\Gamma) \rightarrow H^1_{loc}(\mathbb{R}^d)$ and the double-layer potential operator $D_k : H^{-1/2}(\Gamma) \rightarrow H^1_{loc}(\mathbb{R}^d)$, defined by

$$S_k(x) := \int_{\Gamma} k(x; y) \phi(y) ds(y); \quad x \in \mathbb{R}^d \setminus \Gamma;$$

and

$$D_k(x) := \int_{\Gamma} \frac{\partial k(x; y)}{\partial \nu(y)} \phi(y) ds(y); \quad x \in \mathbb{R}^d \setminus \Gamma;$$

respectively, where the normal ν is directed into Ω_+ . These layer potentials provide solutions to (1) in $\mathbb{R}^d \setminus \Gamma$; moreover, they also automatically satisfy the radiation condition (4). In general all the standard BVPs for the Helmholtz equation (1) can be formulated as integral equations on Γ using these layer potentials.

Specifically, we can use Green's representation theorems, which lead to so-called direct BIE formulations (as we shall see in §3.3 these lend themselves particularly well to efficient approximation strategies when k is large). Denoting the exterior and interior trace operators, from Ω_+ and Ω_- , respectively, by γ_+ and γ_- , and the exterior and interior normal derivative operators by ∂_+ and ∂_- , respectively, we have the following result for interior problems (see [19, Theorem 2.20]).

Theorem 2.1. If $u \in H^1(\Omega_-) \cap C^2(\Omega_-)$ and, for some $k > 0$, $u + k^2 u = 0$ in Ω_- , then

$$S_k \partial_+ u(x) - D_k \gamma_- u(x) = \begin{cases} u(x); & x \in \Omega_-; \\ 0; & x \in \Omega_+; \end{cases} \quad (18)$$

The following is the corresponding result for exterior problems (see [19, Theorem 2.21]).

Theorem 2.2. If $u \in H^1_{loc}(\Omega_+) \cap C^2(\Omega_+)$ and, for some $k > 0$, $u + k^2 u = 0$ in Ω_+ and u satisfies the Sommerfeld radiation condition (4) in Ω_+ , then

$$S_k \partial_+ u(x) + D_k \gamma_+ u(x) = \begin{cases} u(x); & x \in \Omega_+; \\ 0; & x \in \Omega_-; \end{cases} \quad (19)$$

The formulae (18) and (19) lie at the heart of boundary integral methods. Each expresses the solution throughout the domain in terms of its Dirichlet and Neumann traces on the boundary. Thus for Dirichlet problems, if the Neumann data can be computed then these formulae immediately give a

representation for the solution anywhere in the domain. Likewise, for Neumann or impedance problems, knowledge of the Dirichlet data is sufficient to determine the solution anywhere in the domain.

In order to derive BIEs for (1), for which the "unknown" to be computed will be the complementary boundary data required to complete the representation formula for the solution, we need to take Dirichlet and Neumann

where $c_u = [u; @_u]$

All these equations are BIEs of the form

$$Av = f \tag{29}$$

where A is a linear boundary integral operator, or a linear combination of such operators and the identity, v is the solution to be determined and f is given data. Noting that the same operator A can arise from both interior and exterior problems, it is immediately apparent that, although exterior acoustic problems are generically uniquely solvable, the natural BIE formulations of these problems need not be uniquely solvable for all wavenumbers. As a specific instance, we noted above that the homogeneous interior Dirichlet problem has non-trivial solutions at a sequence k_n of positive wavenumbers. If $k = k_n$ and u is such a solution then u is a non-trivial solution of (28) with $h = 0$ (see, e.g., [19, Theorem 2.4]) and so, for $k = k_n$, the BIE (26) for the exterior Dirichlet problem (7) has infinitely many solutions.

Similar BIE formulations (with the same problems of non-uniqueness) can be derived by utilising the fact that the layer potentials satisfy (1) and (4); to satisfy the BVPs, it just remains to take the Dirichlet or Neumann trace of the layer potentials (using the jump relations as above), and then to match with the boundary data. The resulting formulations are known as indirect BIEs; we do not discuss these further here. As discussed above we will focus on direct formulations in which the unknown to be determined is the normal derivative or trace of the solution in the domain; it is possible as we discuss in §3.3 to bring high frequency asymptotics to bear to understand the behaviour of these solutions and so design efficient

The corresponding direct formulation for the exterior impedance problem is

$$C_{k; \cdot} u = A_{k; \cdot}^0 h; \quad (31)$$

where

$$C_{k; \cdot} := B_{k; \cdot} + i k A_{k; \cdot}^0; \quad u \in H^{1/2}(\cdot); \quad (32)$$

is invertible (considered as an operator between an appropriate pair of Sobolev spaces) for all $k > 0$ provided $\text{Re } \epsilon > 0$; again see [19, Theorem 2.27].

That the exterior Dirichlet, Neumann and impedance BVPs can be solved by combined potential direct integral equation formulations follows from, e.g., [19, Corollary 2.28]. Specifically:

Corollary 2.4. Suppose that $k > 0$ and $\epsilon \in \mathbb{C}$ with $\text{Re } \epsilon > 0$. Then both the following statements hold.

(i) If u is the unique solution of (7) then $\mathcal{D}u \in H^{1/2}(\cdot)$ is the unique solution of (30). Further, if $h = \mathcal{D}u \in H^s(\cdot)$ with $1/2 < s < 1$ then $\mathcal{D}u \in H^{s-1/2}(\cdot)$.

(ii) If u is the unique solution of (8) then $\mathcal{D}u \in H^{1/2}(\cdot)$ is the unique solution of (31). Further, if $h = \mathcal{D}u \in H^s(\cdot)$ with $1/2 < s < 0$ then $\mathcal{D}u \in H^{s+1/2}(\cdot)$.

Although the combined potential integral equations (30) and (31) are the most common integral equation formulations for exterior Dirichlet and impedance scattering problems, other formulations are possible. One that is of particular interest for boundary element methods is the so called "star-combined integral equation", proposed for the exterior Dirichlet problem in the case when Ω is star-shaped with respect to an appropriately chosen origin in [77].

Specifically, if u satisfies the exterior Dirichlet problem (7) with $h \in H^1(\cdot)$, then for $\mathcal{D}u(x) := k|x| + i(d-1)/2, x \in \mathbb{R}^d$, we have

$$A_k \mathcal{D}u = (x \cdot \nabla_k + r \cdot D_k - \frac{1}{2}r \cdot i - \frac{1}{2}l + D_k)h; \quad (33)$$

then A

$H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$, with

$$A = \begin{pmatrix} I + D_k & D_{k+} \\ H_k & H_{k+} \end{pmatrix} \begin{pmatrix} S_{k+} & S_k \\ I + D_{k+}^0 & D_k^0 \end{pmatrix}; \quad f = \begin{pmatrix} \frac{1}{2}h - D_k h + S_k g \\ \frac{1}{2}g + D_k^0 g - H_k h \end{pmatrix}; \quad (38)$$

The operator A is bounded and invertible as an operator on $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$, but also, adapting arguments of [82], as an operator on $H^1(\Omega) \times L^2(\Gamma)$, and as an operator on $L^2(\Omega) \times L^2(\Gamma)$ [50].

We conclude this section by stating precisely direct boundary integral

while (18) holds in .

where $A : V \rightarrow V^0$ is a linear boundary integral operator mapping some Hilbert space V to its dual space V^0 , or a linear combination of such operators and the identity, $v \in V$ is the solution to be determined and $f \in V^0$ is given data. Specifically: for the integral equation (43), we have $A = A_k^0$, $V = V^0 = L^2(\Gamma)$, $v = \frac{\partial u}{\partial n}$, and $f = f_k$; for (44), we have $A = A_k$, $V = V^0 = L^2(\Gamma)$, $v = \frac{\partial u}{\partial n}$, and $f = f_k$; for (45)_n we have $A = C_k$, $V = H^{1/2}(\Gamma)$, $V^0 = H^{-1/2}(\Gamma)$, $v = u$, and $f = \frac{\partial u}{\partial n} - i u^l$; and for (46) we have $A = S_k$.

Although Nyström and collocation methods are both simpler to implement than Galerkin methods, we focus on the Galerkin method here. One part of the rationale for this choice is that a key step (and our major focus below) in designing both Galerkin and collocation methods is designing subspaces V_N that can approximate the solution accurately, with a relatively low number of degrees of freedom N . Everything we say below about designing V_N for the Galerkin method applies equally to the collocation method, and indeed to other numerical schemes where we select the numerical solution from an approximating subspace. The second part of our rationale is that, for collocation and Galerkin and other related methods, choosing a subspace from which we select the numerical solution is only part of the story. We have also to design our numerical scheme so that the numerical solution selected is "reasonably close" to the exact solution.

compact and $B : V \rightarrow V'$ is coercive, by which we mean that, for some $\alpha > 0$ (the coercivity constant),

$$(Bv, v) \geq \alpha \|v\|^2$$

will be highly k -dependent. For example, if v is $p + 1$ times continuously differentiable on each mesh interval then standard estimates for piecewise polynomial approximation of degree p suggest that we might be able to

scattering problem, and also to the standard combined potential formulation (43) for a certain range of geometries (see [79] for details). It is sometimes presumed, since the standard domain-based variational formulations of BVPs for the Helmholtz equation are standard examples of indefinite problems where coercivity does not hold, at least for sufficiently large k , that the same should hold true for weak formulations arising via integral equation formulations. However recent results, discussed in [19, 5] and see also [77, 10, 9, 79, 20]), show that coercivity holds for these BIEs for a range of geometries, with β bounded away from zero for all sufficiently large k , moreover with the k -dependence of β and C in (54) explicitly known in many cases.

The advantage of using this version of Cea's lemma, as opposed to that stated in Theorem 3.1, is that, if the k

when k is very large.

To ease this problem, much effort has been put into developing preconditioners (see, e.g., [52, 13, 55]), efficient iterative solvers (see, e.g., [2, 26, 43]), fast multipole methods (see, e.g., [30, 38, 31, 25, 69]), and matrix compression techniques (see, e.g., [7, 8]) for Helmholtz and related problems.

this oscillatory solution by conventional (piecewise polynomial) boundary elements must also grow with order $k^d - 1$. This lack of robustness with respect to increasing values of k (which puts many problems of practical interest beyond the reach of standard algorithms) is the motivation behind

HNA scheme in the context of a problem of scattering by a single sound-soft screen (equivalently, scattering by an aperture in a single sound-hard screen, see [53] for details), then describing how this idea extends to scattering by sound-soft convex polygons, outlining the added difficulties that arise in the case that the obstacle is nonconvex (presenting sharper results in terms of k -dependence than those outlined in [19]), and finally considering scattering by penetrable polygons (the transmission problem). We demonstrate that HNA methods have the potential to solve scattering problems accurately in a computation time that is (almost) independent of frequency.

3.3.1 Scattering by screens

To get the main ideas across, we first describe an HNA BEM for a simple 2D geometry, scattering by a single planar sound-soft screen. This problem, indeed the more general problem of scattering by an arbitrary collinear array of such screens, has been treated by HNA BEM methods with a complete numerical analysis in [53].

To be precise then, we consider the 2D problem of scattering of the time harmonic incident plane wave (13) by a sound soft screen

$$:= f(x) - 4.504x$$

The HNA method for solving (46) uses an approximation space that is specially adapted to the high frequency asymptotic behaviour of the solution u on D , which we now consider. Representing a point $x \in D$ parametrically by $x(s) := (s; 0)$, where $s \in (0; L)$, the following theorem is proved in [53] (this is derived directly from (16) using an elementary representation for the solution in the half-plane above the screen in terms of a Dirichlet half-plane Green's function - for details see [53] and cf. [22, Theorem 3.2 and Corollary 3.4] and [54, x3]):

Theorem 3.3. Suppose that $k_0 > 0$. Then

$$u(x(s)) = u(x(s)) + v^+(s)e^{iks} + v^-(L-s)e^{-iks}; \quad s \in (0; L); \quad (56)$$

where $v := u|_{\partial D}$, and the functions $v^\pm(s)$ are analytic in the right half-plane $\text{Re}[s] > 0$, where they satisfy the bound

$$|v^\pm(s)| \leq C_1 M |k| |s|^{-\frac{1}{2}};$$

where

$$M := \sup_{x \in D} |u(x)| \leq C(1 + k);$$

and the constants $C, C_1 > 0$ depend only on k_0 and L .

The representation (56) is of the form (55), with $V_0(x(s); k$

conventional piecewise polynomials we instead use the representation (56) with $v^+(s)$ and $v(L-s)$ replaced by piecewise polynomials supported on overlapping geometric meshes, graded towards the singularities $s = 0$ and $s = L$ respectively. We proceed by describing our mesh, which is illustrated in Figure 2.

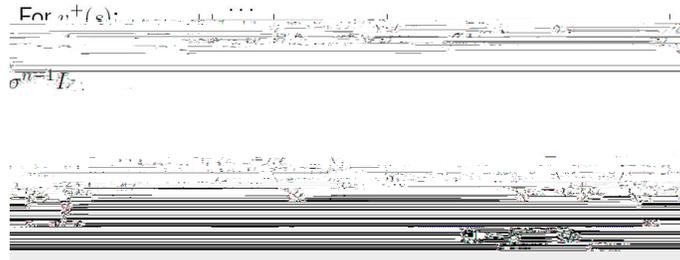


Figure 2: Overlapping geometric meshes for approximation of v^+ and v

Definition 3.4. Given $L > 0$ and an integer $n \geq 1$ we denote by $G_n(0; L)$ the geometric mesh on $[0; L]$ with n layers, whose meshpoints x_i

Theorem 3.5. Let n and p satisfy $n > cp$ for some constant $c > 0$ and suppose that $k_0 > 0$. Then, there exist constants $C; \epsilon > 0$, dependent only on k_0, L , and c , such that

$$\inf_{w_N \in V_{N;k}} \|k' - w_N\|_{H^{\frac{1}{2}}(\cdot)} \leq C k \epsilon^p :$$

Identifying Ω with $(0; L)$, here $H^{\frac{1}{2}}(\cdot) = H^{\frac{1}{2}}(0; L) \times H^{\frac{1}{2}}(R)$, $H^{\frac{1}{2}}(0; L)$ just the subspace of those $u \in H^{\frac{1}{2}}(R)$ that have support in $[0; L]$. And then $\|k\|_{H^{\frac{1}{2}}(\cdot)}$ is just the standard norm on the Sobolev space $H^{\frac{1}{2}}(R)$ (see, e.g., [65]).

Having designed an appropriate approximation space $V_{N;k}$, we use a Galerkin method to select an element w_N so as to efficiently approximate k' . That is, we seek $w_N \in V_{N;k}$ such that

$$(w_N, v_N)_{V_{N;k}} = \frac{1}{k} (u', v_N)_{L^2(\Omega)}$$

\reference" solution to be γ . In Figure 3 we plot $j - \gamma_j - j' - j$, for $k = 20$ and for $k = 10240$. The singularities at the edge of the screen can be clearly seen, as can the increased oscillations for larger k (the apparently shaded area is an artefact of the rapidly oscillating solution).

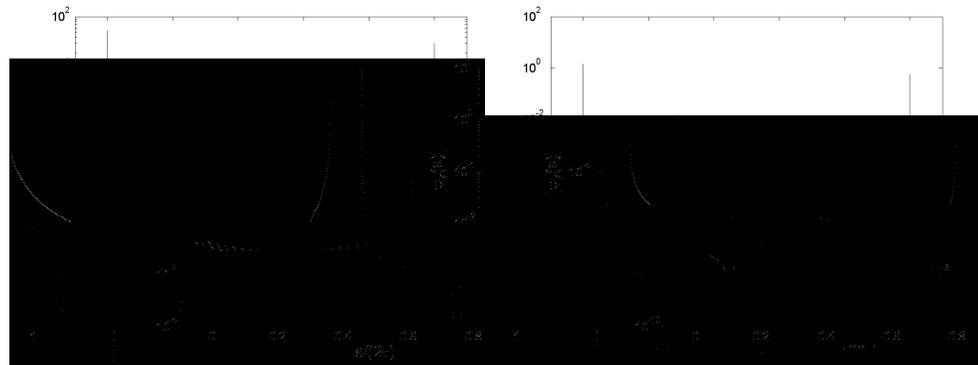


Figure 3: The boundary solution $j - \gamma_j - j' - j$, as given by (57), for $k = 20$ (left) and $k = 10240$ (right), scattering by a screen

In Figure 4 we plot on a logarithmic scale the relative L^1 errors

$$\frac{k - \gamma - p k_{L^1(\cdot)}}{k - \gamma + k k_{L^1(\cdot)}};$$

against p for a range of k (area

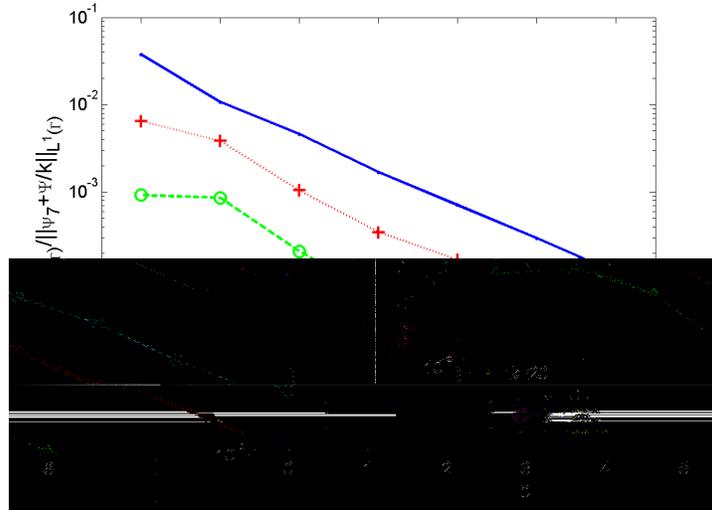


Figure 4: Relative errors in our approximation to $\frac{1}{k}[\mathcal{A}u]$, scattering by a screen

3.3.2 Scattering by convex polygons

The ideas outlined above for the screen problem can also be applied to the case of scattering by polygons. First, we consider the 2D problem of scattering of the time harmonic incident plane wave (13) by a sound-soft polygon with boundary Γ , i.e. problem (14). The solution u then has the representation (39), where $\mathcal{A}u$ satisfies (43) and, if Γ is star-shaped, (44).

We denote the number of sides of the polygon by n_s , and the corners (labelled in order counterclockwise) by P_j , $j = 1; \dots; n_s$. We set $P_{n_s+1} := P_1$, and then for $j = 1; \dots; n_s$

follows from [54, Theorem 3.2, Theorem 4.3].

Theorem 3.7. Let $k = k_0 > 0$. Then on any side j

$$\textcircled{a} u(x(s)) = (x(s) + v_j^+(s)e^{iks} + v_j^-(L_j - s)e^{-iks}; x(s) \in \Omega_j; \quad (60)$$

Having designed an appropriate approximation space $\mathcal{V}_{N;k}$ we use the Galerkin method to select an element to approximate u . Since convex polygons are star-shaped, in this case we can use the integral equation formulation (44), i.e. we seek $u_N \in \mathcal{V}_{N;k}$ such that

$$\langle A_k u_N, w_N \rangle = \frac{1}{k} \langle f, w_N \rangle; \text{ for all } w_N \in \mathcal{V}_{N;k}; \quad (63)$$

Thanks to the coercivity of the integral operator A_k , we have the following error estimate (cf. [54, Corollary 6.2]):

Theorem 3.9. If the assumptions of Theorem 3.8 hold then there exist constants $C; \epsilon > 0$, dependent only on k_0, c and ϵ , such that

$$\|u - u_N\|_{L^2(\Omega)} \leq C k \log^{1+2\epsilon}(2+k) e^{-\epsilon P};$$

To compute the solution in the domain, we rearrange (62) to get

$$\mathcal{G}u(x(s)) = k u(s) + \int_{\partial\Omega} u(y) \mathcal{G}u(y) ds(y); \quad x(s) \in \Omega; \quad (64)$$

and then we insert this approximation to $\mathcal{G}u$ into the representation formula (39) to get an approximation to u , which we denote by u_N . We then have the following error estimate (cf. [54, Theorem 6.3], [21, Corollary 64]):

Theorem 3.10. If the assumptions of Theorem 3.8 hold then there exist constants $C; \epsilon > 0$, dependent only on k_0, c and ϵ , such that

$$\frac{\|u - u_N\|_{L^1(\Omega)}}{\|u\|_{L^1(\Omega)}} \leq C k \log(2+k) e^{-\epsilon P};$$

Similarly, we can derive an approximation to the far field pattern (FFP) of the scattered field, given explicitly for $\mathfrak{x} = |x| > R$ by

$$F(\mathfrak{x}) = \int_{\partial\Omega} e^{ik\mathfrak{x} \cdot y} \mathcal{G}u(y) ds(y); \quad \mathfrak{x} \in S^1; \quad (65)$$

where S^1 denotes the unit circle. Efficient computation of the far field pattern is of interest in many applications, see, e.g., [27]. To compute an approximation F_N to F , we again just insert the approximation (64) into the integral (65). We then have the following estimate (cf. [54, Theorem 6.4], [21, Corollary 64]):

Theorem 3.11. If the assumptions of Theorem 3.8 hold then there exist constants $C; \epsilon > 0$, dependent only on k_0, c and ϵ , such that

$$\|F - F_N\|_{L^1(S^1)} \leq C k^{1+\epsilon} \log^{1+2\epsilon}(2+k) e^{-\epsilon P};$$

Note that the estimates above for the solution in the domain and the FFP follow from results in [21] and are actually a little sharper than those in [54].

The algebraically k -dependent prefactors in the error estimates of Theorems 3.9, 3.10 and 3.11 can be absorbed into the exponentially decaying factors by allowing p to grow modestly ($O(\log^2 k)$) with increasing k . In practice, numerical results [54, 19] suggest that this is pessimistic, and that in many cases a fixed accuracy of approximation can be achieved without any requirement for the number of degrees of freedom to increase with k .

To illustrate the approach described above, we present numerical results for the problem of scattering by a sound soft equilateral triangle, of side length 2 , so that the number of wavelengths per side is equal to k . The total field for $k = 10$ is plotted in Figure 5

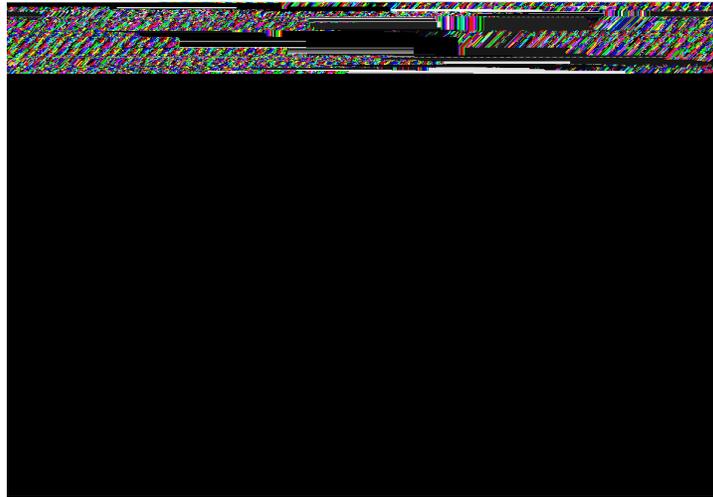


Figure 5: Total field, scattering by a triangle

In our computations we choose $n = 2(p + 1)$, as for the screen results above, so that the total number of degrees of freedom is $N = 6n(p + 1) = 12(p + 1)^2$. Since the total number of degrees of freedom depends only on p , we again adjust our notation by defining $u_p(s) := u_N(s)$. In Figure 6 we plot on a logarithmic scale the relative L^2 errors

$$\frac{k^{-6} \|u_p\|_{L^2(\Omega)}^2}{\|u\|_{L^2(\Omega)}^2};$$

against p for a range of values of k , this quantity an estimate of the relative error in our approximation (64) to u . (Again we take the "reference" solution, our approximation to the true solution u , to be u_6 .) This example is identical to one that appears in [54], except that here we show results for much higher values of k (in [54] the largest value of k tested was $k=10$).

on is more complicated. In particular, in this case we may see partial illumination of a side of the nonconvex polygon (whereas for a convex polygon a side is either completely illuminated or completely in shadow) and/or rerefections (where a wave that has been re flected from one side of the polygon may be incident on another side of the polygon), as illustrated in Figure 7.

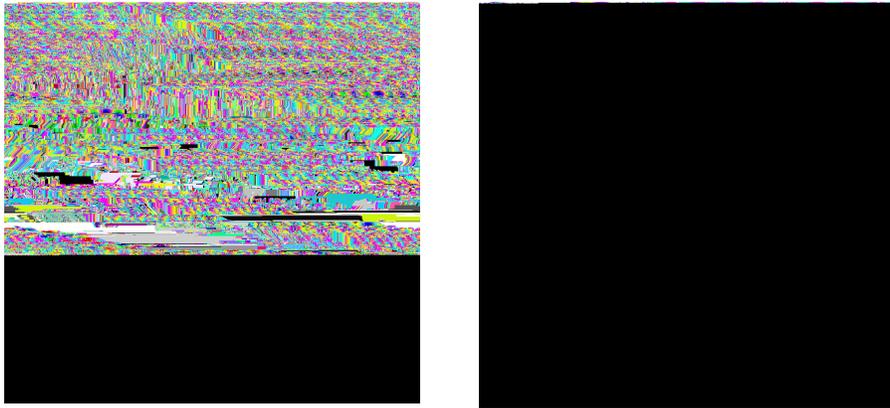


Figure 7: Partial illumination (left) and rere flections (right)

We restrict attention to a particular class of nonconvex polygons that satisfy the following assumptions (a description of how the approach described below can be extended to polygons that do not satisfy these assumptions can be found in [21,x8]):

Assumption 3.12. Each exterior angle θ_j , $j = 1; \dots; n_s$, is either a right angle or greater than $\pi/2$.

Assumption 3.13. At each right angle, the obstacle lies within the dashed lines shown in Figure 8.

Polygons satisfying these criteria may or may not be star-shaped. For each side s_j , $j = 1; \dots; n_s$, if either θ_j or θ_{j+1} is a right angle then we define that side to be a "nonconvex" side, otherwise we say it is a "convex" side, as illustrated for a particular non-star-shaped example in Figure 9. On convex sides, $\phi(u)$ behaves exactly as in the convex case, and the approximation results above hold. However, on nonconvex sides we need to consider the possibilities of partial illumination and/or rere flections. To illustrate our approach, we consider the behaviour at a point $x(s)$ on a nonconvex side s_j , distance s from P_j and r from P_{j-1} , as illustrated in Figure 10. Then s_j will be fully illuminated if $\theta_j < \pi/2$ (where θ_j is the incident angle

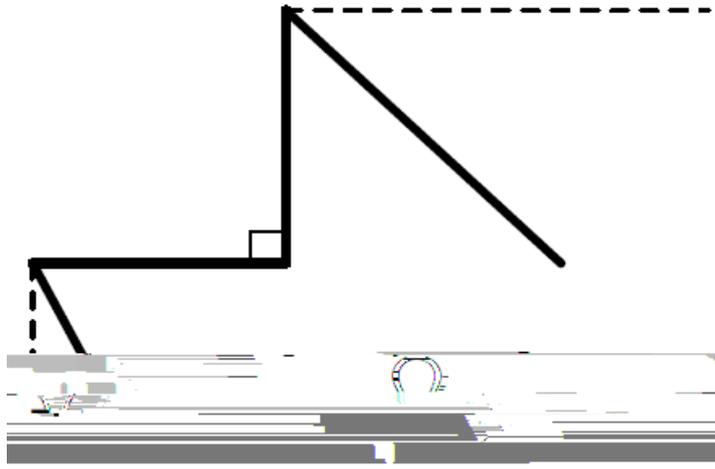


Figure 8: Assumption 3.13 on geometry of nonconvex polygon is that it lies entirely within the semi-infinite dashed lines

shown in Figure 10), P_j will be partially illuminated for some values of θ in the range $2 < \theta < \pi$ (e.g., in the case that $L_j = L_{j-1}$, P_j will be partially illuminated for $3 = 4 < \theta < \pi$), and P_j will be in shadow otherwise. There will be reflections from P_{j-1} onto P_j if $\theta < \pi - 3 = 2$. Whatever the value of θ , there will be diffraction from P_{j-1} and P_{j+1} (either directly from the

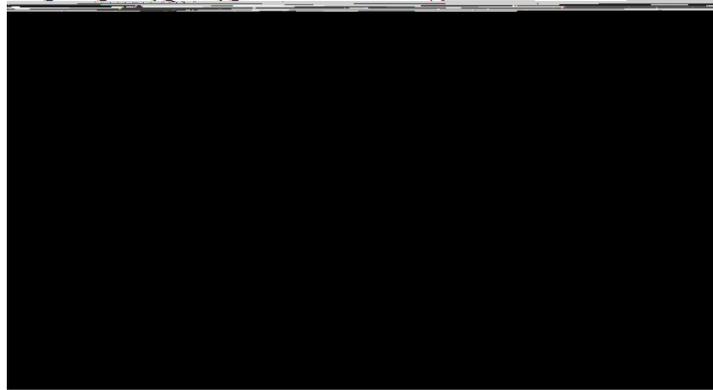


Figure 9: Convex and nonconvex sides, for a non-star-shaped example

where the constant $C > 0$ depends only on k_0 and ϵ .

Here u^d is the known solution of a canonical diffraction problem, namely that of scattering by a semi-infinite "knife edge", precisely scattering of u^i by the semi-infinite sound-soft screen starting at P_{j-1} and extending vertically down through P_j ; for details, see [21, Lemma 35].

Using the representation (66) on each side of the polygon again leads to a representation of the form (55). Our approximation space $\hat{V}_{N;k}$ for

$$v^i(s) := \frac{1}{k} \left(\partial_n u(x(s)) - u^d(x(s)) \right); \quad x(s) \in \Gamma_j; \quad (68)$$

is then identical on each convex side of the polygon to that for the con-

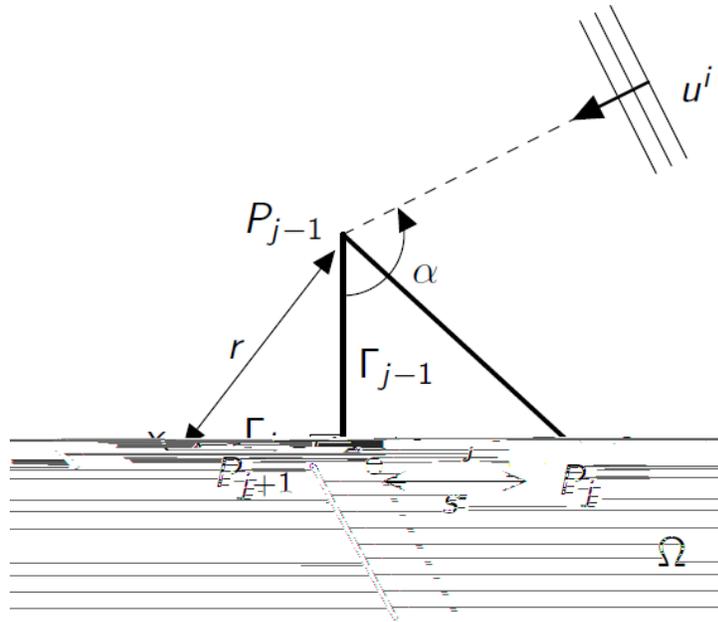


Figure 10: Geometry of a nonconvex side j

depending only on α , k_0 , and ϵ ,

$$\inf_{w_N \in \mathcal{V}_{N,k}} \|u - w_N\|_{L^2(\Omega)} \leq C k^{1-2\alpha} \log^{1-2\alpha}(2 + k/k_0)$$

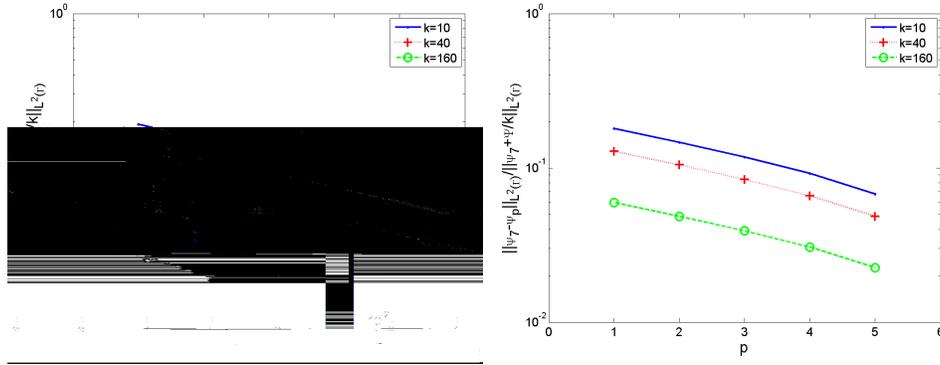


Figure 11: Relative L^2 errors, scattering by a nonconvex polygon, with partial illumination (left) and reflections (right), as in Figure 7.

3.3.4 Transmission scattering problems

Finally we consider the transmission scattering problem (17), for which the behaviour is more complicated still, incorporating as it does multiple internal reflections. To illustrate this, consider the scenario illustrated in Figure 12, in which we show an incident wave striking a penetrable polygonal scatterer. On the left of Figure 12 we show what happens as the incident wave u^I strikes one side of the boundary Γ . Following Snell's Law (see, e.g., [50, Appendix A]), this gives rise to a "reflected" wave u^R (travelling from Ω^- into Ω^+) and a "transmitted" wave u^T that passes into Ω^+ . For the case that the scatterer is impenetrable (as in all the other problems considered earlier in this section), only the reflected wave would be present here. As the transmitted wave passes through Γ it may decay (if $\text{Im}[k^+] > 0$), but if k^+ is constant then its direction does not change. As this transmitted wave

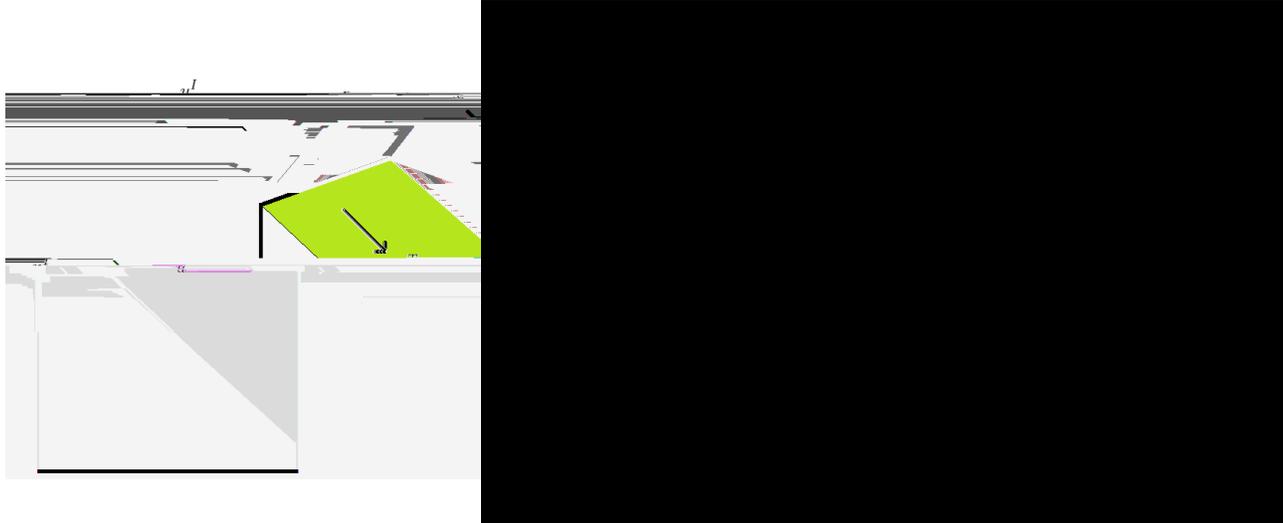


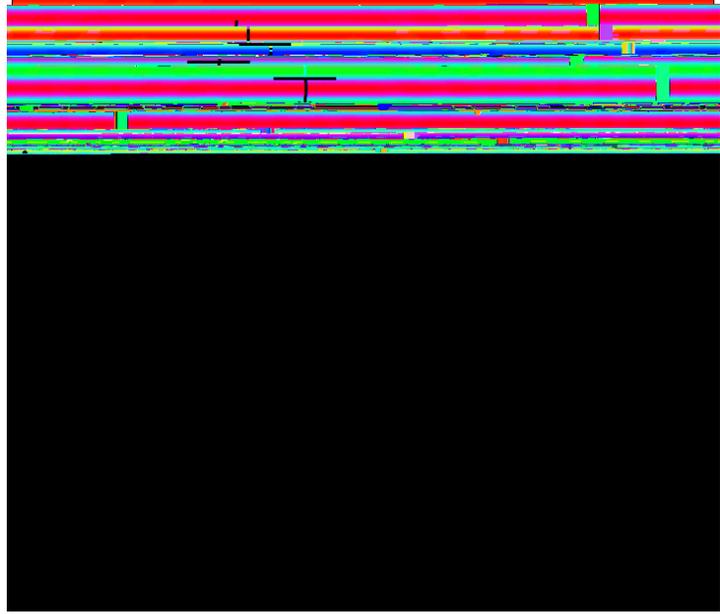
Figure 12: Illustration, for the transmission scattering problem, of incident (u^I), reflected (u^R) and primary transmitted (u^T) field (left), with multiple internal reflections (right)

harder, and we do not discuss such generalisations. Utilising Snell's law, we can write down explicit formulae for each term in the (in general infinite) series of "reflected" waves (the first three of which are illustrated on the right of Figure 12). We refer to [50] for details, but note that these formulae rely on a complete understanding of what happens when a plane wave passes from one (possibly absorbing) homogeneous medium to another, and further that there appear to be some misconceptions in the literature regarding the solution to that canonical problem, which are addressed fully in [50, Appendix A]. Framing this in the context of (55), this corresponds to expressing V_0 as an infinite series of these "reflected" waves, that must be truncated in any numerical algorithm.

The part of the total field that is not represented by this series corresponds primarily to the "diffracted" waves emanating from the corners of the polygon (though other wave components, e.g. lateral waves, may also be present; again we refer to the discussion in [50] for details). These may originate from the incident field (e.g., as illustrated on the left of Figure 13 below), or else they may originate from the waves that travel through the interior of the polygon striking corners that are on the "shadow" side of the polygon (using the same definition as for impenetrable scatterers above). Either way these "diffracted" waves travel through \mathbb{R}^2 with speed deter-

mined by $\text{Re}[k_+]$, and through ω with speed determined by $\text{Re}[k_-]$ (and decay determined by $\text{Im}[k_-]$). These differing wavespeeds in x and z of course imply differing wavelengths, as illustrated in Figure 13. A full consideration of the wave behaviour of the solution would also need to take into

here the phase functions $e^{ik \cdot s}$ capture the oscillations of these "directed" waves, but the amplitudes v are unknown, and are approximated by piecewise polynomials on overlapping graded meshes (due to singularities at the corners) as for the sound-soft convex polygonal scattering problem described above; namely $v_m(s)e^{ik \cdot r_m(s)}$ represents "direction" on Γ_j ; $e^{ik \cdot r_m(s)}$ (or $e^{ik \cdot r_m(s)}$) (from 638 (A) 1289 T27)



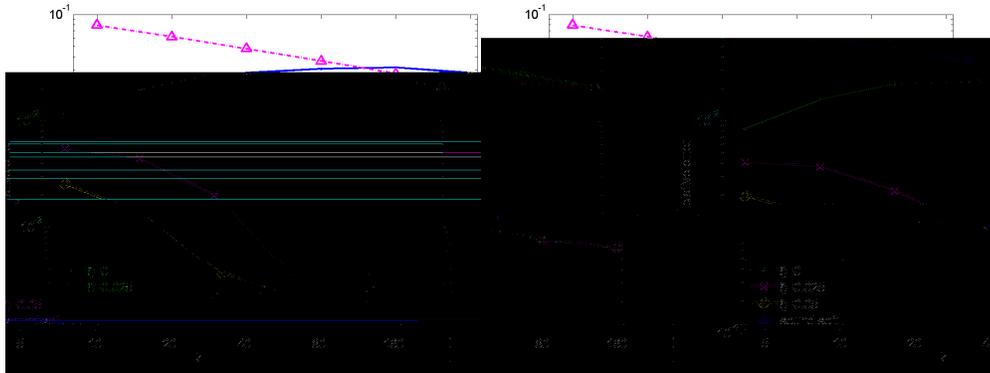


Figure 15: Relative $L^2(\cdot)$ best approximation errors in u (left) and $\|u - u_h\|$ (right) for scattering by a penetrable triangle of varying absorption, and a comparison with the HNA BEM relative errors for scattering by a sound soft polygon.

be achieved for a range of scatterers with different absorptions; as absorption reduces, so the influence of diffraction from non-adjacent corners increases, and we surmise that, in this case, it may be necessary to add additional terms to the ansatz (71) in order to achieve higher levels of accuracy. We note though that results in [50] suggest that the ansatz outlined above is sufficient to achieve 1% relative error in the far-field pattern for any absorption and frequency (for the range of examples tested).

3.3.5 Other boundary conditions and 3D problems

We have focussed mostly in this section on sound soft scattering problems. There is no difficulty in extending the algorithms and much of the analysis to sound hard or impedance scattering problems. In particular, the HNA approach has been very successfully applied to the problem of scattering by convex polygons with impedance boundary conditions (see [23] for details), solving (45) with $\gamma = 0$. We do not include specific details of that case here, but note that the approximation space is very similar to that for scattering by sound-soft convex polygons, as detailed above, and also that a summary of the approach in that case and further numerical results can be found in [19].

Much more challenging is extension to 3D, because of the greater complexity of the high frequency asymptotics of the solution, in particular the much larger number of possible contributing ray paths and associated oscillations.

latory phases. But at least for significant classes of 3D problems it seems

in particular pointing out that one particular implementation (see Theorem 4.2 below), approximating the unknown Neumann data from a space of traces of plane waves, computes precisely the best approximation from that space. We also make additional connections to related methods: the least squares method and the method of fundamental solutions see Remarks 4.3 and 4.4.

The unified transform method, as articulated in §4.1 below and in [78, 76], does not apply to exterior problems for the Helmholtz equation, at any rate to exterior problems set in the exterior of a bounded set Ω , such as the exterior Dirichlet problem (7). The issue is that plane wave (and generalised plane wave) solutions of the Helmholtz equation, which are fundamental to the method (see §4.1) do not satisfy the standard Sommerfeld radiation condition (4) (for more discussion see §4.2 below, and note that [45] does achieve an implementation for a particular exterior problem for the modified Helmholtz equation, i.e., (1) with k pure imaginary). But the unified transform method can be applied to so-called rough surface scattering problems where the scatterer takes the form

$$\Gamma := \{x \in \mathbb{R}^d : x_d < f(x')\}; \quad (72)$$

for some bounded, Lipschitz continuous function $f : \mathbb{R}^{d-1} \rightarrow \mathbb{R}$ so that Γ is the graph of f and the boundary value problem to be solved is posed in the perturbed half-space $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega}$. Generalised plane waves (as defined in §4.1) that propagate upwards or decay in the vertical direction satisfy the appropriate radiation conditions in this case: in 2D these are the so-called Rayleigh expansion radiation condition (80) below, in the case when f is periodic, and the upwards propagating radiation condition [18] more generally.

Not only can the unified transform method be applied to these rough surface scattering problems, it already has been applied in these cases developed independently in papers by DeSanto and co-authors from 1981 onwards [33, 35, 36, 34, 5]. In §4.2 below, we recall this method for the simplest of these problems, the 2D sound soft scattering problem (14) in the particular case when the scatterer Γ is a one-dimensional diffraction grating by which we will mean that $d = 2$ and $f : \mathbb{R} \rightarrow \mathbb{R}$ is periodic (this case considered in particular in [35, 5]). We point out that the so-called spectral-coordinate (SC) and spectral-spectral (SS) methods proposed in [35] correspond to two implementations of the unified transform methods with different choices of approximation space. We note that the SS method proposed in [5], a variant of the SS method, corresponds precisely to the method for the interior

Dirichlet problem (5) analysed in Theorem 4.2 below, and we prove a new result (Theorem 4.6) characterising and proving convergence of this method, sharpening [5, Lemma 4.1]. We also discuss the conditioning of the linear systems that arise from these methods.

4.1 The unified transform method for the interior Dirichlet problem

At the heart of the unified transform method is the so-called global relation. For linear elliptic PDEs with constant coefficients this global relation follows from the divergence theorem. In particular, as described in [78, 76] for the Helmholtz equation (1) (and the Laplace and modified Helmholtz

For $n = 1; \dots; N$ set $x_n := k \cos \theta_n$ and $y_n := k \sin \theta_n$. Suppose, without loss of generality, that $N = 2M$ is even, that $N \geq 4$, and that $\theta_1 = 1$, $\theta_2 = 1$, and $\theta_{2m-1} = \theta_{2m}$, in which case $\theta_{2m-1} = \theta_{2m} \notin 0$, for $m = 2; \dots; M$. Since $v(t; 0) = 0$ for $t \in \mathbb{R}$, it holds that

$$\sum_{m=1}^{M+1} d_m e^{j \theta_m t} = 0; \quad t \in \mathbb{R}; \quad (74)$$

where $d_m := c_m$, $\theta_m := \theta_m$, for $m = 1; 2$, and $\theta_{m+1} := \theta_{2m-1}$, $d_{m+1} := c_{2m-1} + c_{2m}$, for $m = 2; \dots; M$. Since the θ_n , $n = 1; \dots; N$, are distinct, so also are the θ_m , $m = 1; \dots; M+1$. Let $n \in \{1; \dots; M+1\}$ be such that $\text{Im}[\theta_n] = \text{Im}[\theta_m]$, for $m = 1; \dots; M+1$. Then, multiplying (74) by $\exp(-j \theta_n t)$ and integrating it follows that

$$\sum_{m=1}^{M+1} \underline{d_m}$$

this equation overdetermined if $M > N$ in which case it is imposed, e.g., in a least squares sense. Spence [76] tabulates the implementations to date, which vary in the choice of approximation space Q_M and in the choice of

Theorem 4.2. Suppose that k^2 is not a Dirichlet eigenvalue, so that (5) is uniquely solvable, and $h \in H^1(\Omega)$ so that $u := \Delta^{-1} h \in L^2(\Omega)$. Suppose also that $M = N \times N$ and $Q_M := P_N := (P_N)$, where P_N is some N -dimensional subspace of $L^2(\Omega)$. Then (75) has a unique solution which is $u_N = P_N u$, where $P_N : L^2(\Omega) \rightarrow P_N$ is orthogonal projection, so that u_N is the best $L^2(\Omega)$ approximation to u in P_N .

With the choices made in this theorem it holds that

$$u_N = \sum_{n=1}^N c_n v_n; \quad (76)$$

for some complex coefficients c_n , and (75) is equivalent to the linear system

$$\sum_{n=1}^N a_{mn} c_n = \int_{\Omega} h \overline{v_m} ds; \quad m = 1, \dots, N; \quad (78)$$

where $a_{mn} = \int_{\Omega} v_n \overline{v_m} ds$. It is easy to see that the matrix $[a_{mn}]$ is Hermitian and positive semi-definite, indeed positive definite in view of Lemma 4.1(i): see, e.g., the discussion in [5].

4.2 Diffraction gratings and the unified transform method

The previous subsection has described the unified transform method as a numerical method for interior problems, in particular the interior Dirichlet problem (5), but our focus in this paper is acoustic scattering in which we are solving exterior problems. As noted above, we cannot see how the unified transform method, as currently formulated, can be applied to any of the exterior or scattering problems that we have stated in §2, where we need to solve the Helmholtz equation in the exterior of a bounded set Ω , whose boundary is denoted by $\partial\Omega$. In particular, the global

for some complex coefficients c_n , where

$$n := \sum_{j=1}^p (k_j + 2) = (kL) \quad \text{and} \quad n := \begin{cases} p & \text{if } \sum_{j=1}^p \frac{2}{n_j} > 1; \\ i & \text{if } \sum_{j=1}^p \frac{2}{n_j} = 1; \\ j & \text{if } \sum_{j=1}^p \frac{2}{n_j} < 1; \end{cases} \quad (81)$$

The standard Dirichlet problem in this case is then:

$$\begin{aligned} &\text{Given } h \in H^{1/2}(\Gamma_-); \text{ find } u \in C^2(\Gamma_+) \setminus H_{loc}^1(\Gamma_+) \\ &\text{such that (1) holds in } \Gamma_+; u = h \text{ on } \Gamma_-; \\ &\text{and } u \text{ satisfies the RERC (80):} \end{aligned} \quad (82)$$

Here, for $\gamma \in \mathbb{R}$, $H^{1/2}(\Gamma_-)$ is the closure in $H^{1/2}(\Gamma_-)$ of those $\gamma \in C^1(\Gamma_-)$ that satisfy (79) for $x \in \Gamma_-$. That (82) is uniquely solvable is shown in [40].

For $\gamma \in \mathbb{R}$, let

$$R := \{v \in C^2(\Gamma_+) \setminus H_{loc}^1(\Gamma_+) : v \text{ satisfies (1) and (80)}\};$$

and note that $u \in R$ if u is a solution of (82). The numerical schemes in [35] derive from the observation that, if u satisfies (82), then (where \mathbf{n} is the unit normal directed into Γ_+)

$$\int_{\Gamma} \mathbf{n} \cdot \nabla u \, ds = \int_{\Gamma} h \mathbf{n} \cdot \nabla v \, ds; \text{ for all } v \in R; \quad (83)$$

this identity (83) derived by applying Green's second theorem to u and v in $\{x \in \Gamma_+ : x_2 < H\}$, for some $H > f_+$. The identity (83) holds, in particular, for those generalised plane waves $v(\cdot; \mathbf{n})$ that are in the set $P := \{v(\cdot; \mathbf{n}) : \mathbf{n} \in \mathbb{Z}^2\}$; where $\mathbf{n} \in \mathbb{C}$ is defined by

$$(\cos \mathbf{n}; \sin \mathbf{n}) = (\mathbf{n}; \mathbf{n});$$

with \mathbf{n} and \mathbf{n} given by (81). These are the generalised plane waves that are elements of R .

Thus a version of the global relation holds, that

$$\int_{\Gamma} \mathbf{n} \cdot \nabla u \, ds = \int_{\Gamma} h \mathbf{n} \cdot \nabla v \, ds; \text{ where } \mathbf{n} \in \mathbb{Z}^2$$

Numerical experiments with the SC and SS methods are carried out in [35]. The methods are extended to transmission problems in [36], and the SC method to 3D sound soft and sound hard scattering problems for doubly-periodic, diffraction gratings surfaces in [34].

In [5] a variant of the SS method is proposed, the SS method, characterised by the choice $\mathcal{Q}_N = \mathcal{P}_N$, so that $\mathcal{Q}_N = \mathcal{P}_N$, the space spanned by $\{v_n : 1 \leq n \leq N\}$. An attraction of this method, as observed in [5], is that, as with (78), this leads to a coefficient matrix $A_N = [a_{jm}]$, in this case with $a_{jm} = \int_{\Gamma} \overline{v_j} v_m ds$, that is Hermitian and positive definite.

Analogously to (77), (87) can be viewed as a variational formulation problem on $L^2(\Gamma) \times L^2(\Gamma)$: (87) corresponds to (49) with $V = V^0 = L^2(\Gamma)$ and $A = I$, the identity operator. Like (77) this formulation is trivially continuous and coercive, with continuity and coercivity constants, C and α in Lemma 3.2, equal to one. The choice $\mathcal{Q}_N = \mathcal{P}_N$ is a Galerkin method for (87), and by Céa's lemma (Lemma 3.2) one has the following result (cf, Theorem 4.2).

Theorem 4.6. Suppose that $\mathcal{Q}_N = \mathcal{P}_N$. Then u_N , given by (88) and (89), is the best $L^2(\Gamma)$ approximation to u in \mathcal{P}_N .

We note that this result improves on [5, Lemma 4.1] where it is shown, under the assumptions of this theorem, that

$$\|u - u_N\|_{L^2(\Gamma)} \leq 2 \inf_{v \in \mathcal{P}_N} \|u - v\|_{L^2(\Gamma)}.$$

Combining Theorem 4.6 with Lemma 4.5(ii) we obtain the following corollary, guaranteeing convergence of the SS method.

Corollary 4.7. [5, Corollary 4.1] Suppose that the sequence of subspaces $\mathcal{P}_1, \mathcal{P}_2, \dots$, is chosen so that, for every $n \in \mathbb{Z}$, $\mathcal{P}_n \subset \mathcal{P}_{n+1}$, for all sufficiently large N , and that $\mathcal{Q}_N = \mathcal{P}_N$, for all

reliable, but, for some geometries and some angles of incidence, all three methods perform very well, producing highly accurate results with around one degree of freedom per wavelength (see [6] for more details).

Remark 4.9. A potential difficulty with all of the SC, SS, and SS methods is that the linear systems that arise can be very ill-conditioned. For the SS method rigorous upper and lower bounds for $\text{cond}(A_N)$, the condition number of the system matrix A_N , are computed in [5], and the effects of this ill-conditioning on the computed solution are estimated. Regarding the behaviour of $\kappa_N := \text{cond}(A_N)$, the main results are that κ_N remains low as long as P_N contains only plane waves, i.e. $\sqrt{\nu(\cdot; n)}$ with $n \in \mathbb{R}$, but necessarily eventually grows exponentially as $n \rightarrow \infty$.

Remark 4.10. The system matrix in the SS method is the transpose of the matrix to be solved when the same scattering problem is solved by a least squares method: see [5] for more detail, and cf. Remark 4.3.

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