Total wave based fast direct solver for VSP

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Summary of the report. We present a fast direct solver for the volume scattering problem of the Helmholtz equation. The algorithm is faster than existing methods. Moreover, discretization for our method is much simpler and more accurate than that for finite difference, finite elements, and integral equations.

Jacques Hadamard’s work on ill-posedness put us in a box of solving well-posed problems of preferably small condition number. In reformulating elliptic problems, such as the scattering problem for the Helmholtz or Maxwell, by integral equations (IEs) the price we have to pay is the complexity in solution representations and their discretizations, and cost of computation (20 or more, instead of 2 to 4, points per wavelength) for a fast direct solver (FDS). Well-posedness lead us, for example, to reformulating the first order Maxwell equations as second order elliptic PDEs, with symmetries breached and balances of physical quantities disturbed. Additional difficulties will have to be met when the second order equations are formulated by IEs, and as the latter are discretized and solved numerically.

There is another all-embracing box next to that of Hadamard’s. The more capable we become of solving problems, the more we seek challenging and interesting problems, such as a scattering problem. In the present report we propose a different approach to solution of elliptic problems in a compactly supported domain $D$ with inhomogeneous medium, referred to here as the volume scattering problem (VSP). Our method never solves a well-posed or ill-posed problem. Instead it first solves a very simple but not posed problem: PDEs without boundary conditions.

We will construct the total wave solution space (TWSS) for the given PDEs, or more precisely, we will construct the null space of the homogenous PDEs (with zero RHS and of variable coefficients), subject to no boundary or any other conditions. Thus the TWSS consists of general solutions of the PDEs. Constructing the null space seems a non-scattering problem but it may be the easiest way to account for global communications of the linear system, or global multiple scatterings of a scattering problem. It is only after the TWSS is constructed in $D$ that the data, or the incident wave, is incorporated to obtain a specific solution - the specific total wave corresponding to the specified incident wave.

Our method will give rise to a fast direct solver for the elliptic problem in $D$. It does not support an iterative solver. The TWSS will be constructed recursively on a (quadtree for example, in 2-D) hierarchy of domain decomposition, with the TWSS first constructed in each bottom level subdomains. Merging the total waves in the subdomains to those of their parents will end up with the TWSS constructed efficiently for the entire scatterer $D$.

The method will be presented in the scattering context and language, but the prin-
ciples extend to a general boundary value problem for elliptic PDEs, in particular the Maxwell equations. There are 8 first order equations for the 6 unknown $E$ and $B$ for linear material. We can construct the null space of the linear equations in $D$ first, and deal with the boundary conditions latter. Another major benefit of the total wave approach is that it greatly simplifies discretization.

In this report, a total wave refers to a nontrivial solution of the homogenous PDEs with variable coefficients in domain $D$.

1 Introduction

The subject of this report is solution of scattering problem for the Helmholtz equation. There are two standard types of scattering problems. One is for the inhomogeneous medium inside a domain and is referred to here as the volume scattering problem (VSP). The other is for an impenetrable scatterer (such as a perfect conductor for Maxwell), or a penetrable scatterer with constant coefficients inside, and is referred to as surface scattering problem (SSP). When formulated as integral equations (IEs), VSP is related to the Lippmann-Schwinger IE, whereas SSP is related to boundary IEs.

These problems can also be solved by finite element or boundary element methods.

There are fast direct solvers (FDSs) and iterative solver. A FDS is desirable when the condition number of the problem is not small, which occurs, for example, when the problem is near resonance. They are also more efficient for a scattering calculation with multiple incident waves typically required for an inverse scattering problem.

For IEs or finite element methods, discretization has never been made robust, or even easy. For a second kind IE, with all its underlying benefits in conditioning and reduction of dimensionalities, the discretization problem is even more evident. The use of layer potentials makes their discretization extremely unwieldy and difficult. For example, a quadrature to integrate the Coulomb potential $1/r$ near $y$, with $r = |x-y|$ and with $y$ a fixed point on a patch of smooth surface, against smooth functions such as polynomials, is not easy to design due to the strong and non-trivial influence of the curvatures on $1/r$ near the source $y$. Warping a smooth function we get a smooth function. Warping a singular function, we’d better prepared to reap the whirlwinds. So far we have not looked at the frightening situations when these singular kernels meet corners and edges on surfaces or inside inhomogeneous media.

The desirable analytic properties and attractiveness of IE formulation for the scattering problems, or for any elliptic PDEs, or for Maxwell equations, become difficult to exploit the moment they meet discretization. This is because after discretization we have to deal with individual and standing alone poles and dipoles. A pole will not interact well with other nearby poles or singularities unless they are on the same patch of smooth surface. Unfortunately, for many interesting applications, different parts of the surface,
or multiple inclusions, may get very close. On the fly, designing a quadrature will be more difficult than resampling.

We propose a solution method for the scattering problem, also for other elliptic PDEs and the Maxwell equations, which does not require discretization of IEs or PDEs. It requires what we call “sampling” of the original PDEs (as in a collocation method) and their solutions. We don’t call it discretization in the sense that the collocation method may be regarded as sampling, as opposed to discretizing the differential equation. There is a distinction between sampling and discretization. Sampling requires not much of brain, whereas discretization requires too much of it.

Our method does not reformulate the original PDEs as IEs. It works with the PDEs directly. It barely solves those PDEs. Certainly it never solves a well or ill-posed problem for the PDEs. It solves a not posed problem for the PDEs. It solves the PDEs without boundary or other conditions. For scattering problems or other elliptic PDEs formulated as a boundary value problem, the boundary values will be processed only after the general solution space for the PDEs without boundary conditions are constructed. Constructing the general solution space is easier than solving boundary value problems.

The method is a fast direct solver; it cannot be related to and does not support any iterative solver. For a SSP, with the surface not very concave or convoluted, our FDS is faster than existing FDSs. For VSPs, our FDS offers the same asymptotic complexity, with a big reduction on the constant if the inhomogeneous medium occupies a convex domain $D$, such as a square or triangle.

Organization of the report: §2 is a short and informal description of the method. §3 is a full and more formal description of the method. §4 provides formulations of the volume scattering problem and Green’s third identity used as a projector on the boundary of a scatterer. §5 contains background information on layer potential representation for the interior and exterior projectors.

## 2 Our method - Informal description

We will present the method in the context of VSP for the Helmholtz; see §4 for more details on VSP. For a given precision $\epsilon > 0$ and incident wave $u_0$, the algorithm finds the unique solution to the scattering problem in a compactly supported inhomogeneous medium (a variable index of refraction $n(x)$) inside domain $D$. If $v$ denotes the scattered wave, then $u = u_0 + v$ is the total wave, which satisfies the homogeneous Helmholtz with variable coefficients

$$
\Delta u + k^2 n^2(x) u = 0, \quad x \in D
$$

(1)
2.1 Informal description

Our method consists of three parts.

Part I. For the prescribed precision $\epsilon > 0$, a complete set of solutions $\{u_j, j = 1 : N\}$ to the homogeneous Helmholtz (1) are efficiently constructed in $D$ and made available on the boundary $\partial D$. The boundary lies in the free space. See §3 for further details on the size $N$ and how the $N$ solutions are constructed efficiently.

Part II. Each solution $u_j$ thus constructed, being a total wave, can and will be split into two parts on $\partial D$, the incident and scattered waves $u_{0j}$ and $v_j$. This can be accomplished with the third Green’s identity used as a projector on $L^2(\partial D)$. Since the set of total waves $\{u_j\}$ is complete, any total wave, namely a solution of the homogeneous Helmholtz (1), can be represented by linear combination of $\{u_j, j = 1 : N\}$ to precision $\epsilon$. Likewise, any incident wave can be represented by linear combination of $\{u_{0j}, j = 1 : N\}$ to precision $\epsilon$. In particular, our prescribed incident wave $u_0$ can be expressed in terms of $\{u_{0j}, j = 1 : N\}$

$$u_0(x) = \sum_{j=1}^{N} c_j u_{0j}(x), \quad x \in \partial D$$  \hspace{1cm} (2)

Solving (2) for the coefficients $c_j$, we obtain the scattered wave

$$v(x) = \sum_{j=1}^{N} c_j v_j(x), \quad x \in \partial D$$  \hspace{1cm} (3)

corresponding to $u_0$. At this point, we have obtained the scattered wave on $\partial D$ and consequently also outside $D$. For many applications, such as inverse scattering by repeatedly solving forward problems, the scattered wave outside the medium is all that we want.

Part III. Now suppose we also want the scattered wave $v$ inside $D$. It will be obtained efficiently by a downward recursive procedure along a hierarchical structure, such as a quadtree for 2-D domain $D$, which was also used in Part I to efficiently construct the total waves $\{u_j, j = 1 : N\}$ in the first place.

2.2 Discussions

The hierarchical mergings for Part I, and splittings for Part III are universally employed in a typical FDS, although they may not always be presented in a familiar language or structure. It will referred to as domain decomposition.

Definition 2.1 Throughout the report, $D$ is regarded as singly connected. A subdomain is always the result of partitioning $D$ artificially for the domain decomposition.
The method can also be adopted for SSP and scattering problems in layered media, so that no layered Green’s function is required which is necessary for the IE formulation. See §3.3 for more details on the extensions to SSP.

The method solves no scattering problem in order to construct the TWSS. It never solve a well or ill-posed problem for PDEs. In fact one can largely roam in the null space of linear operators without encounter ill-posedness; see §2 for further details. The modern concept of first or second kind IEs seems oxymoron to the primitive kernel hunter-gatherer, and null spaces of IEs or geometric resonances are his trophies to hang up on the walls, not to become his stumbling blocks.

A total wave in a subdomain, such as a square, subject to no condition on the boundary, is only aware of the medium inside the domain. It has no knowledge of what is outside, in particular whether the medium is discontinuous over the boundary, and thus it is unaware of the corners of the domain, unless explicitly informed; see §19. In contrast, a scattered wave is a solution of an inhomogeneous Helmholtz, subject to outgoing radiation conditions in the free space, in which the subdomain must be embedded to set up the scattering problem for the subdomain, on whose solution a scattered wave based FDS relies. Thus the scattered wave sees the manmade discontinuity across the boundary. It is aware of the corners and requires more points there to be represented.

3 Detailed description of the Algorithm

We first present in §3.1 the basic components required by our fast direct solver. We then describe our TWSS based FDS in §3.2. The algorithm is similar to those of [1]-[5] in data structure and complexity; Our method differs from theirs in what solution space to construct and how to merge solution spaces of subdomains; see Remark 3.4.

3.1 The Basic Components and Parameters

For simplicity, we assume that the scatterer $q$ is a smooth function, which vanishes smoothly outside a square domain $D$. In implementation, this requirement can be relaxed to include piecewise smooth scatterers with jumps in a fairly arbitrary, bounded domain $D$ in two dimensions.

A typical fast direct solver for the Helmholtz equation with large wave number $k$ relies on domain decomposition of some sort [1]-[8]. For the Lippmann-Schwinger equation (35), the square domain $D$ is partitioned hierarchically into the balanced quadtree; again for simplicity we will not discuss adaptive partitioning until §3.3.

The size of a scattering problem is measured by the number of wavelengths in each linear dimension, and the number of points required to discretize $D$ is therefore proportional to $k^2$. Let $N = O(k^2)$ be the number of unknowns in the resulting linear system.
of equations to be solved. It is well known, [1], [2], that a fast direct solver requires $O(N^{1.5}) = O(k^3)$ flops to construct general solution space and additional $O(N \log N)$ flops to obtain the specific scattered wave for the prescribed incident wave. Our approach has the same complexity, with a considerable reduction on the constant.

Domain decomposition can be carried out, in principle, before or after the discretization. Our approach will be able to cleanly separate the two issues in a straightforward way, and partition $D$ before discretization. In contrast, existing implementations go the other way around, and have to deal with “subdomains” of mesh points of the discretization. Linear algebra tricks combined with untidy local approximation steps are employed to copy with these “subdomains” and the communications among them. The artificial cuts and corners must still manifest themselves in the “subdomains of points”. For the Lippmann-Schwinger equation, the points are monopoles or dipoles. Strategies have been designed and strifes directed to these issues, to try to mend or heal the cuts and wounds.

Observation 3.1 For a prescribed precision and in a subdomain, typically a square or a rectangle obtained by merging two squares, the number of distinct solutions, whether the incident waves, scattered waves, or total waves, in the subdomain is proportional to the arclength of the subdomain, as measured by the number of wavelengths. This is because these solutions can be determined uniquely by their Dirichlet, or Neumann, or D&N data on the boundary of the subdomain.

Definition 3.2 For a prescribed precision the finite number of distinct solutions form the solution space for the subdomain in question.

Remark 3.3 For simplicity, we will say that the dimension of solution space for a square subdomain, of edge length $L$ and boundary arclength $4L$, is $4L$, instead of proportional to $4L$. Therefore, the dimension of solution space for a rectangle by merging two squares is $6L$.

A necessary step of a fast direct solver is to construct the solution space for the entire $D$ efficiently in a hierarchical order. Once solution space is formed for each subdomain on the same level of the quadtree, two neighbor square subdomains on the level are merged together to form the solution space for the union of two squares, and so on.

Remark 3.4 The main difference between existing methods and our approach is that (i) We merge the total waves whereas they merge the scattered waves (ii) They organize the scattered waves by the incident waves whereas we don’t organize the total waves by the incident waves or any other waves (iii) We merge the total waves by simple continuity conditions whereas they merge the scattered waves via the multiple scattering process
among subdomains. (iv) We deal directly with solutions whereas they deal with operator such as the scattering matrix or the Dirichlet to Neumann map.

Consequently, we never solve a scattering problem in merging; they solve an interesting and difficult scattering problem for each subdomain and in every step of merging.

**Definition 3.5** A total wave in $D$ is a non-trivial solution of the homogeneous, variable coefficient Helmholtz equation (31) in $D$, subject to no boundary conditions. A total wave in a subdomain is a non-trivial solution of (31) in that subdomain, subject to no boundary conditions, other than natural extension to the outside by continuity conditions on the function and its normal derivative on the boundary.

As such, it has a desirable, simple property: A total wave in a subdomain is utterly oblivious to the underlying multiple scattering process among the subdomains. The total waves are much easier to construct and merge to build up the entire solution space for $D$.

**Observation 3.6** As two neighbor square subdomains merge, the two solution spaces, each of dimension $4L$, should merge to the solution space for the rectangle and of dimension $6L$. Indeed, the 2 continuity conditions (on function and its normal derivative) on the common interface of length $L$ of the two squares consist of $2L$ constraints on the $8L$ parameters of the original two solution spaces.

**Remark 3.7** It is important to note that the neighbor subdomains may have different $4L$ as dimensions of solution spaces. Similarly, the number $4L$ does not imply that each edge of a square subdomain bears exactly $L$ parameters. In that case Observation 3.6 still holds: Whatever number of parameters born on the common interface by the Dirichlet, or Neumann, or D&N data (see Observation 3.7) will be eliminated for both subdomains after merging, and thus subtracted from the sum of dimensions of the two solution spaces.

### 3.2 The algorithm

It should be noted that our new algorithm is almost identical to that of [1] in structure and complexity; they differ in solution space and in the merging strategy. The complexities for the old and new differ by a constant multiple, with the new more efficient by a considerable factor.

The main advantage of the new is its simplicity in discretization and merging, two major difficulties still being reckoned with in existing approaches. The total wave based new algorithm never solve any scattering problem in constructing the total wave solution spaces (TWSS) for subdomains and in merging the solution spaces. The new only deals with the total waves in subdomains until the solution space is obtained for the entire
$D$, whereas the old methods solve a local scattering problem every step of the way, and have to deal with the typical corner singularities of the local scattered waves at the four corners of a subdomain. As two scattered wave solution spaces merge, four of the eight singularities at the eight corners of the two subdomains cancel out and disappear. This cancellation would give rise to conditioning problems. The total waves in a subdomain have natural extensions to the outside. They are unaware of the manmade corners of the subdomains, and are easier to sample and merge.

We reiterate that for simplicity in describing our new algorithm, we assume that the scatterer $q$ is a smooth function in $D$, and vanishes smoothly outside square $D$. In actual implementation, we will relax this requirement to include piecewise smooth scatterers with jumps inside and on the boundary of a fairly arbitrary, bounded domain $D$ in two dimensions. We will also deal with jump discontinuities which form corners in the original medium; see §3.3 for more details.

The total wave based fast direct solver is described in the following four subsections.

### 3.2.1 Construct TWSS for bottom level subdomains

Step 1 of the algorithm is to construct total wave solution spaces TWSS for each square subdomains $S$ at the bottom level of the quadtree.

TWSS is obtained by solving the homogeneous, variable coefficient Helmholtz equation (31) in $S$, subject to no boundary conditions. A high order method is provided in §3.3 and also implemented numerically. Here we present a second order method to illustrate the procedure. The square $S$ is discretized $S$ a $m$-by-$m$ uniform mesh $Q$. Five point stencil, to replace the Laplacian of (31) on every point, including those on the

![Figure 1: Uniform mesh on a square $S$](image)
boundary $\partial S$, produces $m^2$ homogeneous equations

$$\Delta_h u(x) + k^2 n(x) u(x) = 0, \quad x \in Q$$

(4)

The equations for the $4(m-1)$ boundary points of the mesh will require $4m$ additional, free variables $u(x)$, with $x$ a step $h$ away from the boundary; see Figure [Figure] for points $x$ outside $S$ marked by $\diamondsuit$. All together, there are $m^2$ equations for $m^2 + 4m$ unknowns $u(x)$, and so the null space of the discrete operator $\Delta_h + k^2 n(x)$ is $4m$ dimensional, namely there are $4m$ nontrivial solutions to the $m^2$ equations.

These $4m$ basis functions for the TWSS in $S$ are collected in a matrix $U_s$ of size $m^2$-by-$4m$. The basis functions are also evaluate at the boundary $\partial S$, and when paired with their normal derivatives, provide the D&N data for the TWSS. For simplicity, we assume that $\partial S$ is sampled with $4m$ points, and that there are $m$ points on each of the four edges of $S$, so that the matrices

$$U = U_s|_{\partial S} = \left[ u^{(1)}, u^{(2)}, \ldots, u^{(4m)} \right], \quad U_n = \left\{ \partial_n U_s \right\}|_{\partial S} = \left[ u_n^{(1)}, u_n^{(2)}, \ldots, u_n^{(4m)} \right],$$

(5)

are each of dimension $4m$-by-$4m$. Let

$$G = \begin{bmatrix} U \\ U_n \end{bmatrix}, \quad \tilde{G} = \begin{bmatrix} -U \\ U_n \end{bmatrix}$$

(6)

so $G$ is of size $8m$-by-$4m$. Our numerical experiment shows that these $4m$ boundary points can be equispaced, as opposed to crowded toward the four corners. Denser sampling points are required near a singularity of the solution (arising from medium discontinuity), or near locations where the total waves have more evanescent modes due to medium complexity.

### 3.2.2 Merging two subdomains

Step 2 of the algorithm is bottom up merging: On each level of the quadtree, merge two neighbor square subdomains, whose TWSS’s are available, to construct TWSS for the resulting rectangular domain. Merge again two neighbor rectangles to form TWSS for the resulting square domain on the higher level. Stop at the highest level which contains only one square domain that is $D$. Merging is achieved by imposing continuity conditions on the D&N data on the common interface of two subdomains; see Observation [3.6]. Let $G_1$ and $G_2$ be the D&N data matrix of the two square subdomains $S_1$ and $S_2$. Let $\Gamma$ be their common interface; see Figure [Figure]. Then merging $G_1$ and $G_2$ to produce D&N data matrix $G$ for $S = S_1 \cup S_2$ requires enforcing the continuity of the D&N data across $\Gamma$, by solution of the homogeneous linear system of $2m$ equations

$$G_1|_\Gamma \tau_1 = -\tilde{G}_2|_\Gamma \tau_2, \quad \text{namely} \quad \begin{bmatrix} G_1|_\Gamma, & \tilde{G}_2|_\Gamma \end{bmatrix} \begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix} = 0$$

(7)
where $G_i|_{\Gamma}$ is the D&N data matrix $G_i$ restricted on $\Gamma$; it is a matrix of size $2m$-by-$4m$. The coefficient matrix $[G_1|_{\Gamma}, G_2|_{\Gamma}]$ is $2m$-by-$8m$ with a null space of dimension $6m$. Let $T_1$ and $T_2$ be matrices of size $4m$-by-$6m$ whose columns consist of the $6m$ solutions $\tau_1$ and $\tau_2$ of $(7)$. The D&N data matrix $G$ on $\partial S = \{\partial S_1 \setminus \Gamma\} \cup \{\partial S_2 \setminus \Gamma\}$ are given by

$$G|_{\{\partial S_1 \setminus \Gamma\}} = G_1|_{\{\partial S_1 \setminus \Gamma\}} T_1, \quad G|_{\{\partial S_2 \setminus \Gamma\}} = G_2|_{\{\partial S_2 \setminus \Gamma\}} T_2$$

(8)

We refer to (7), (8) as the merging formulas, to be used throughout the bottom-up merging process.

In the remainder of this subsection we define and determine splitting. Let $u$ be a total wave-solution of the Helmholtz equation (31) in $S = S_1 \cup S_2$. Let $g, g_1, g_2$ be the D&N data for $u$ on $\partial S, \partial S_1, \partial S_2$, respectively. Thus, there exist coefficients $\gamma, \gamma_1, \gamma_2$ such that

$$g = G\gamma, \quad g_1 = G_1\gamma_1, \quad g_2 = G_2\gamma_2$$

(9)

**Definition 3.8** Splitting is the operation to determine $g_1, g_2$ from $g$, in terms of their coefficients. The linear map $S_p : \gamma \mapsto \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$ is referred to as the splitting operator.

It follows (8) immediately that $S_p$, of size $8m$-by-$6m$, is given by the formula

$$S_p = \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

(10)

**Remark 3.9** All the matrix operations after Step 1 are carried out on the boundaries of the subdomains each with some $4m$ points on the boundary, instead of inside the subdomains each with about $m^2$ points. Therefore, the matrix operations are not nearly as costly. The entire merging step will cost only $O(k^3)$ flops for a $k$-by-$k$ wavelength problem on $D$; see [7] for a complete analysis.
Subsections [3.2.1] and [3.2.2] are about constructing null spaces, and no scattering problem has been solved so far.

### 3.2.3 Decompose TWSS via Green’s formula

Step 3 of the algorithm is to decompose TWSS for the whole scatterer $D$ into the incoming and outgoing parts. Now that the TWSS is constructed for $D$ with the D&N data matrix $G$ available on $\partial D$ which lies in the free space, the Green’s identities apply, with the free space Green’s function. In particular, the D&N data matrix $G$ for the total waves can be split by the projector $P_-$, see [§4.2] for definition and technical details, to obtain the D&N data matrix $G_0$ for the incident parts of the total waves.

Let the incident components of $G$ be denoted by

$$G_0 = \begin{bmatrix} U_0 \\ \partial_n U_0 \end{bmatrix}$$

so that

$$G_0 = P_- G$$  \hfill (11)

Expressing the D&N data of the prescribed incident wave $u_0$ on $\partial D$ by the basis $G_0$

$$G_0 \gamma = \begin{bmatrix} u_0 \\ \partial_n u_0 \end{bmatrix}$$

we solve (12) to obtain the coefficients $\gamma$. Obviously,

$$\begin{bmatrix} u \\ \partial_n u \end{bmatrix} = G \gamma$$

is the D&N data of the total wave corresponding to the prescribed incident wave $u_0$. For many applications, we want the scattered wave, and perhaps also its normal derivative, on $\partial D$. In this case, the D&N data of the scattered wave is obtained by subtracting (12) from (13). This concludes our algorithm if the scattered wave on $\partial D$ is all we want; otherwise continue to the next step.

### 3.2.4 Split a total wave

Step 4 of the algorithm construct the total wave inside $D$. It is a top-down splitting process to propagate recursively along the quadtree the coefficient $\gamma$ from a domain $S$ to its subdomains $S_1$ and $S_2$.

This is the reverse of Step 2 detailed in [3.2.2] see [10] for details. Continue the recursive splitting till $\gamma$ is available for every bottom level square $S$. According to (5), the total wave $u$ in $S$ is obtained by

$$u = U_s \gamma$$

Now the total wave $u$ of (13) is available everywhere inside $D$.

This is the end of our algorithm, and the volume scattering problem for a given incident wave $u_0$ is solved.
3.3 Some implementation details and remarks

There are several very accurate methods to construct TWSS for a small subdomain $S$ on the bottom level of the quadtree. We will present two typical methods: Collocation and the weak formulation.

3.3.1 Collocation method to construct TWSS

The solutions $u$ of (31) in $S$ can be approximated by polynomials or bandlimited functions or some other suitable basis $B_j(x)$. Thus we represent the total waves $u$ in $S$ by

$$u(x) = \sum_j c_j B_j(x), \quad x \in S$$ (15)

The homogeneous, variable coefficient Helmholtz equation (31), with $u$ given above, is evaluated at some $n$ suitable locations in $S$, giving rise to $n$ homogeneous linear equations for $c_j$

$$Ac = 0$$ (16)

The vectors $c$ from the null space of matrix $A$ are then used to construct the total waves $u$ for the TWSS in $S$.

In numerical experiments, we used bandlimited functions of the form

$$B(k, \theta, x) = \exp(ik(x_1 \cos(\theta) + x_2 \sin(\theta))), \quad x \in S, \quad \theta \in [0, 2\pi), \quad k \in [k_1, k_2]$$ (17)

The $n$ collocation points on $S$ are either uniform mesh - see Figure 1 - or a graded mesh such as the tensor legendre points.

3.3.2 Weak formulation for TWSS

The variational formulation for the Helmholtz equation (31) offers more flexibility for an irregular subdomain $S$, and leads to typical finite element solution for (31). Without boundary conditions for (31), the weak formulation assumes the form

$$-\int_S \nabla v \cdot \nabla u dx + \int_{\partial S} vu_n ds + \int_S k^2(x)v(x)u(x)dx = 0$$ (18)

where $u$ and $v$ are both from a function space such as the one spanned by basis in (15), or by a typical finite element basis. In numerical experiments, we used (17) as basis.
3.3.3 Sampling and completeness of TWSS

For the prescribed precision \( \epsilon \), the completeness of TWSS depends only on sampling, specifically the number of points and their distribution in each bottom level subdomain. Sampling rate is determined, as is well known, by the local wave number, by the complexity of the local medium, and by the distance to the nearest singularities arising from (i) the sources of incident wave (ii) the corners (iii) the edges. These sources have different strength of singularities, but if \( \epsilon \) is small it is hardly necessary to treat them differently in sampling rate near them. In the standard case when the medium changes smoothly and slowly relative to wavelength, and if the subdomain is far from a singularity, 2 to 4 points per local wavelength is usually sufficient.

On the other hand, since we always over sample, the TWSS will be unavoidably over complete to the prescribed precision. Once the TWSS space is constructed for a subdomain, particularly the bottom level ones, it may be compressed by SVD, or by pivoted Gram-Schmidt or QR. This will only make the TWSS healthier (because the total waves will be orthonormalized). It will not reduce the level of over-completeness (because smaller singular values of matrix \( G \) of (6) may not correspond to more evanescent waves).

3.3.4 Discontinuities in the medium

If a bottom level subdomain \( S \) contains a smooth interface across which the index of refraction jumps, then \( S \) must be divided into two subdomains. These subdomains of \( S \) become bottom level subdomains.

Let’s assume now that a bottom level subdomain \( S \) contains a corner of the medium over which the index of refraction jumps. Then \( S \) must be partitioned into two subdomains, one contains the corner, the other is the complement. TWSS for each subdomain will contain some regular solutions and some singular solutions because of the corner. The regular ones will be constructed, say, by the collocation method (15). The singular ones will also be constructed by (15), except that the basis functions for them must be chosen to contain the local singular behavior of the total wave near the corner. Finally, the regular and singular solutions are collected together on the boundary and compressed by SVD or QR.

As is well established, near such a corner the solution is spanned by the Bessel-Fourier terms of fractional orders,\[ u(x) \sim \sum_{\nu} c_{\nu} J_{\nu}(kr) e^{i\nu \theta} \] (19)

where \( x \) near the corner is assigned a polar coordinates \((r, \theta)\) centered at the corner.
3.3.5 Equations v.s. solutions

The existing numerical methods for scattering or general elliptic problems can be divided into three categories, according to how much they are involved in building solution space.

1. Our total wave approach deals with the total waves. The differential equations are treated only at the bottom level subdomains, and without boundary conditions. Merging TWSS of subdomains requires no knowledge of the PDEs.

2. Methods based on scattering matrix or related objects [1]-[5] deal with the scattered waves for each subdomain on every level of the hierarchical domain decomposition (such as a quadtree). These methods solve a scattering problem on each bottom level subdomain, and they also need to know the underlying Green’s function in merging two subdomains to construct the scattering matrix for the union of the two subdomains. Each subdomain on the hierarchy has manmade corners, which is visible to the scattered waves and show up as singularities in the scattering matrix.

3. Finite difference, finite elements, or similar methods deals with the differential equations or their variational forms. Continuity conditions over an interface of subdomains are enforced on the equations rather than directly on the solutions, as our method does.

Our total wave approach merges the subdomains directly and cleanly. Existing methods have to avoid dealing directly with the unwieldy analytical issues around the manmade corners arising from the manmade subdomains, by merging two “discretized” subdomains, or two overlapping ones.

3.3.6 All merging formulas

1. Merging two squares $S_1, S_2$ to a rectangle $S$. Let $G_1$ and $G_2$ be the two D&N data matrices to be merged to produce the D&N data matrix $G$ for $S = S_1 \cup S_2$. Denote by $G_{ij}$ the part of $G_j$ restricted to the edge shared with $G_i$, $i \neq j$. Then the merging-splitting matrices $T_1, T_2$ (see (7)) are solutions of the equation

$$
\begin{bmatrix} G_{21} & \tilde{G}_{12} \end{bmatrix}_{2 \times 8} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}_{8 \times 6} = 0_{2 \times 6} \quad (20)
$$

2. Merging two rectangles $S_1, S_2$ to a square $S$. Let $G_1$ and $G_2$ be the two D&N data matrices to be merged to produce the D&N data matrix $G$ for $S = S_1 \cup S_2$. Denote by $G_{ij}$ the part of $G_j$ restricted to the edge shared with $G_i$, $i \neq j$. Then the merging-splitting matrices $T_1, T_2$ are solutions of the equation

$$
\begin{bmatrix} G_{21} & \tilde{G}_{12} \end{bmatrix}_{4 \times 12} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}_{12 \times 8} = 0_{4 \times 8} \quad (21)
$$
3. **Merging four squares** $S_i$, $i = 1 : 4$ **to a square** $S$. Let $G_i$, $i = 1 : 4$ be the four D&N data matrices to be merged to produce the D&N data matrix $G$ for $S = \bigcup_{i=1}^{4} S_i$. Denote by $G_{ij}$ the part of $G_j$ restricted to the edge shared with $G_i$, $i \neq j$. Then the merging-splitting matrices $T_i$, $i = 1 : 4$ are solutions of the equation

\[
\begin{bmatrix}
G_{21} & \tilde{G}_{12} & 0 & 0 \\
0 & G_{32} & \tilde{G}_{23} & 0 \\
0 & 0 & G_{43} & \tilde{G}_{34} \\
\tilde{G}_{41} & 0 & 0 & G_{14}
\end{bmatrix}_{8 \times 16}
\begin{bmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4
\end{bmatrix}_{16 \times 8} = 0_{8 \times 8}
\] (22)

3.4 **Extensions to surface scattering problems**

Our total wave approach for VSP can be extended to a surface scattering problem (SSP). For simplicity, we consider a 2-D SSP off a sound soft (zero Dirichlet for total wave) smooth convex body $D$ such as the unit disc with the sources of the incident wave $u_0$ well separated from $D$. Given $u_0$ on $\partial D$, the SSP is to determine $\partial_n v$, the normal derivative of the scattered wave $v$ on $\partial D$.

The following steps outline a possible extension of the TWSS method to SSP.

1. **The bottom level subdomains.** Dividing the annulus $1 \leq r \leq 1 + h$, for some $h \geq 0$, along the radial direction into sufficient many pieces. Each piece

   \[ A_i = \{(r, \theta), \ 1 \leq r \leq 1 + h, \ \theta_{i-1} \leq \theta \leq \theta_i\}, \quad i = 1 : n \] (23)

   is bounded by four curves: two arcs and two straight radial segments. Remove the arc of $r = 1 + h$. The remaining three curves form the $i$-th subdomain $\Gamma_i$ on the bottom level:

   \[
   \begin{align*}
   \Gamma_{i1} &= \{(1, \theta), \ \theta_{i-1} \leq \theta \leq \theta_i\} \\
   \Gamma_{i2} &= \{(r, \theta_{i-1}), \ 1 \leq r \leq 1 + h\} \\
   \Gamma_{i3} &= \{(r, \theta_i), \ 1 \leq r \leq 1 + h\} \\
   \Gamma_i &= \Gamma_{i1} \cup \Gamma_{i2} \cup \Gamma_{i3}
   \end{align*}
   \] (24-27)

2. **TWSS in bottom level subdomains.** For a prescribed precision construct TWSS in $A_i$ subject to the zero Dirichlet condition (sound soft) on the arc $\Gamma_{i1}$. Let there be $m$ total waves in TWSS of the form $u^{(j)} = u_0^{(j)} + v^{(j)}$, $j = 1 : m$. For each $u^{(j)}$, the TWSS will contain four functions (i) $u^{(j)}$ and $\partial_n u^{(j)}$ restricted on the two radial segments $\Gamma_{i2}, \Gamma_{i3}$ (ii) $u_0^{(j)}$ and $\partial_n v^{(j)}$ on the arc $\Gamma_{i1}$.

3. **Merging.** Merge the subdomains, starting from the bottom level ones $\Gamma_i$, recursively and upward along a hierarchical domain decomposition. Two neighboring
subdomains $C_1, C_2$, separated by a common radial segment, will be merged to form their parent submain $P$ by continuities of total wave and its normal derivative on the interface.

4. *After merging.* The TWSS will contain pairs of functions on $\partial D$, the unit circle. Each pair is of the form

$$u_\ell^{(i)}, \partial_n v^{(i)}, \quad \ell = 1 : N$$

(28)

where $\partial_n v^{(i)}$ is the normal derivative of the scattered wave $v^{(i)}$ off $D$ induced by an incident wave $u_0^{(i)}$; $N$ is proportional to arclength of $\partial D$ measured in wavelength.

5. *Construct $\partial_n v$.* Finally we construct the normal derivative, on $\partial D$, of the scattered wave $v$ off $D$ induced by the prescribed incident wave $u_0$. Spanning $u_0$ by $u_0^{(i)}$

$$u_0 = \sum_\ell \alpha_\ell u_0^{(i)}$$

(29)

we use the coefficients to produce $\partial_n v$

$$\partial_n v = \sum_\ell \alpha_\ell \partial_n v^{(i)}$$

(30)

This is the end of the algorithm. We have constructed the pair $(v, \partial_n v)$ on $\partial D$, with $v = -u_0$, and solved the SSP for sound soft scatterer $D$. The solution of (29) for $\alpha_\ell$ is a bottleneck of the procedure.

4 The Volume Scattering Problem

One of the misfortunes of the 20th Century applied mathematics is that the volume scattering problem (VSP) for the Helmholtz equation was posed and is still being solved today as a boundary value problem for the scattered wave in a domain $D$, and worse yet, for each subdomain of $D$ in a domain decomposition setting. The scattering problem is a very special boundary value problem in that both the Dirichlet and Neumann data of the incident wave are available on the boundary of the whole scatterer $D$. In this section we present the classical formulations for VSP, and special properties useful for the total wave based fast direct solver.

Given index of refraction $n(x) = \sqrt{1 + q(x)}$ in a bounded domain $D$, we consider the volume scattering problem in $k$-space governed by the Helmholtz equation

$$\Delta u + k^2 n^2(x)u = 0, \quad \text{or} \quad \Delta u + k^2(1 + q)u = 0$$

(31)
where \( u \) is the total wave, \( q \) is the scatterer, \( n = 1 \) and \( q = 0 \) outside \( D \). In a typical setting, \( u \) is of the form
\[
 u = u_0 + v, 
\]
where the incident wave \( u_0 \) is given in \( D \) and the scattered wave \( v : \mathbb{R}^2 \rightarrow \mathbb{C} \) is to be determined as a solution of the inhomogeneous Helmholtz equation,
\[
 \Delta v + k^2 v = -k^2 q(u_0 + v) 
\]
subject to the Sommerfeld radiation condition
\[
 \lim_{r \to \infty} \sqrt{r} \left( \frac{\partial v}{\partial r} - ikv \right) = 0 
\]
The scattering problem (33), (34) can also be formulated as the Lippmann-Schwinger equation
\[
 \sigma(x) + k^2 q(x) \int_D G(x, \xi) \sigma(\xi) d\xi = -k^2 q(x)u_0(x) 
\]
for the monopole density \( \sigma \) in \( D \), which is related to \( v \) by
\[
 v(x) = \int_D G(x, \xi) \sigma(\xi) d\xi. 
\]
where \( G = -(i/4)H_0(k|x - \xi|) \) is the free space Green’s function.

4.1 Dirichlet and Neumann Data for \( u_0 \) on \( \partial D \)

For the scattering problem (33) and (34), or (35) and (36), the incident wave \( u_0 \) must be available inside the scatterer \( D \), or better, its sources outside \( D \) are prescribed.

Observation 4.1 For a bounded domain \( D \) with a regular boundary \( \partial D \), the Dirichlet and Neumann data for the incident wave \( u_0 \) are always available on \( \partial D \).

To verify this statement, we observe that more often then not in a typical application, the incident wave \( u_0 \) of a volume scattering problem is specified by its sources outside \( D \), such as a monopole or a plane wave. In that case, the D&N data \( u_0 \) and \( \partial_n u_0 \) can be evaluated directly on the boundary.

Suppose \( u_0 \) is only given in \( D \), as required by (33) or (35). By Green’s third identity, \( u_0 \), being solution of \( \Delta v + k^2 v = 0 \) in \( D \), is given by its D&N data
\[
 u_0(x) = -\int_{\partial D} \left( \partial_n u_0(\xi) \cdot G(x, \xi) - u_0(\xi) \cdot \frac{\partial G(x, \xi)}{\partial n(\xi)} \right) ds(\xi), 
\]
So the D&N data for \( u_0 \) can be recovered by solving (37) as an equation. This solution process can often be simplified if \( u_0 \) is given not only in \( D \), but also on \( \bar{D} \).
4.2 Green’s Third Identity as the Interior Projector \( P_- \)

Let \( W = L^2(\partial D) \times L^2(\partial D) \). Let \( W_\pm \) be two subspaces of \( W \) defined by the formulae

\[
W_- = \{ (v, \partial_nv) \mid \Delta v + k^2v = 0 \text{ in } D \} \tag{38}
\]

\[
W_+ = \{ (v, \partial_nv) \mid \Delta v + k^2v = 0 \text{ outside } \bar{D} \text{ subject to (34)} \} \tag{39}
\]

Therefore, \( W_- \) consists of the D&N data for incident waves in \( D \), and \( W_+ \) consists of the D&N data for outgoing (or scattered) waves outside \( \bar{D} \).

For a bounded domain \( D \) with a regular boundary \( \partial D \), the linear map \( (\phi, \psi) \in W \mapsto v \in L^2(D) \) defined by Green’s third identity

\[
v(x) = -\int_{\partial D} \left( \partial_n \phi(\xi) \cdot G(x, \xi) - \phi(\xi) \cdot \frac{\partial G(x, \xi)}{\partial n(\xi)} \right) \, ds(\xi),
\]

produces \( v \) with \( \Delta v + k^2v = 0 \) in \( D \). Let \( x \) approach \( \partial D \) from \( D \), and denote the limit by \( x_- \) corresponding to \( x \in \partial D \). We thus obtain the linear map \( P_- : (\phi, \psi) \in W \mapsto (v, \partial_nv) \in W_- \)

\[
v(x) = -\int_{\partial D} \left( \partial_n \phi(\xi) \cdot G(x, \xi) - \phi(\xi) \cdot \frac{\partial G(x, \xi)}{\partial n(\xi)} \right) \, ds(\xi),
\]

\[
\partial_nv(x) = -\int_{\partial D} \left( \partial_n \phi(\xi) \cdot \frac{\partial G(x, \xi)}{\partial n(x)} - \phi(\xi) \cdot \frac{\partial^2 G(x, \xi)}{\partial n(x) \partial n(\xi)} \right) \, ds(\xi),
\]

Likewise, using Green’s third identity outside \( D \), we introduce another linear map \( P_+ : (\phi, \psi) \in W \mapsto (v, \partial_nv) \in W_+ \). In terms of the standard layer potential operators \( S, K, K', T \) defined by (56)-(59), the two operators \( P_\pm \) are given by

\[
P_+ \begin{bmatrix} \phi \\ \psi \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & I \\ 0 & I \end{bmatrix} + \begin{bmatrix} -K & S \\ -T & K' \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix},
\]

\[
P_- \begin{bmatrix} \phi \\ \psi \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & I \\ 0 & I \end{bmatrix} - \begin{bmatrix} -K & S \\ -T & K' \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix}.
\]

It follows immediately from Green’s third identity (37) that

**Observation 4.2** The linear map \( P_\pm : W \mapsto W_\pm \) is a projector converting an arbitrary pair of boundary data \( (\phi, \psi) \in W \) to the D&N data for an outgoing/incident wave. In particular, \( P_- \) maps the D&N data of the total wave \( u \) of (32) to those of its incident component \( u_0 \), and \( P_+ \) maps the D&N data of total wave \( u \) to those of its scattered component \( v \).
Remark 4.3 Step 3 of the algorithm splits the D&N data of a total wave on \( \partial D \) for its scattered and incident parts using \( P_- \). Since the D&N data is nearly twice redundant, we only need the D&N data for the incident part evaluated at about half as many discretization points (quadrature nodes for \( P_- \)). We will select these points away from corner and edges to avoid singularities of \( P_- \) there.

In addition, if the wave number \( k \) is not a Dirichlet eigenvalue of the Laplacian in \( D \), namely if \( k \) does not hit a geometric resonance of \( D \), then only the first half of \( G_0 \) in (12) is required to determine \( \gamma \). In other words, the second half of \( P_- \), which involves the hyper singular kernel \( T \), is not necessary for splitting.

5 Layer potential representation for \( P_+, P_- \)

For \( x \) close to the the boundary \( \partial D \), the single and double layer potentials

\[
p(x) = \int_{\partial D} G(x, \xi) \psi(\xi) d\xi, \quad (45)
\]
\[
q(x) = \int_{\partial D} \frac{\partial G(x, \xi)}{\partial n(\xi)} \phi(\xi) d\xi \quad (46)
\]

associated with arbitrary pair of functions \( (\phi, \psi) \), can be rewritten

\[
p(x \pm hn(x)) = \int_{\partial D} G(x \pm hn(x), \xi) \psi(\xi) d\xi, \quad (47)
\]
\[
q(x \pm hn(x)) = \int_{\partial D} \frac{\partial G(x \pm hn(x), \xi)}{\partial n(\xi)} \phi(\xi) d\xi \quad (48)
\]

where \( x \) now is on the boundary \( \partial D \). Taking the directional derivative of \( p, q \) in the normal direction \( n(x) \), we have

\[
\frac{\partial p(x \pm hn(x))}{\partial n(x)} = \int_{\partial D} \frac{\partial G(x \pm hn(x), \xi)}{\partial n(x)} \psi(\xi) d\xi, \quad (49)
\]
\[
\frac{\partial q(x \pm hn(x))}{\partial n(x)} = \int_{\partial D} \frac{\partial^2 G(x \pm hn(x), \xi)}{\partial n(x) \partial n(\xi)} \phi(\xi) d\xi \quad (50)
\]

Therefore, the Dirichlet and Neumann data \( (\phi, \phi_n) \) of (40) are given by

\[
\begin{bmatrix}
\phi \\
\phi_n
\end{bmatrix} = P_- \begin{bmatrix}
\phi \\
\psi
\end{bmatrix} = -\lim_{h \to +0} \left[ \frac{p(x^-) - q(x^-)}{\partial n(x)} \right] \begin{bmatrix}
p(x^-) \\
q(x^-)
\end{bmatrix} \quad (51)
\]
for \( x^- = x - hn(x), x \in \partial D \). The Dirichlet and Neumann data \((\phi, \phi_n)\) of (42) are given by
\[
\begin{bmatrix} \phi \\ \phi_n \end{bmatrix} = P_+ \lim_{h \to +0} \begin{bmatrix} p(x^+) - q(x^+) \\ \partial_{\mathbf{n}(x)}(p(x^+) - q(x^+)) \end{bmatrix}
\] (52)
for \( x^+ = x + hn(x), x \in \partial D \). The use of the jump conditions
\[
\lim_{h \to +0} q(x \pm hn(x)) = \int_{\partial D} \frac{\partial G(x, \xi)}{\partial \mathbf{n}(\xi)} \phi(\xi) d\mathbf{s}(\xi) \mp \frac{1}{2} \phi(x),
\]
(53)
\[
\lim_{h \to +0} \frac{\partial p(x \pm hn(x))}{\partial \mathbf{n}(x)} = \int_{\partial D} \frac{\partial G(x, \xi)}{\partial \mathbf{n}(x)} \psi(\xi) d\mathbf{s}(\xi) \pm \frac{1}{2} \psi(x),
\]
(54)
reduces (51) and (52) to expressions for \( P_\pm \)
\[
P_\pm = \frac{1}{2} \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \pm \begin{bmatrix} -K & S \\ -T & K' \end{bmatrix}
\] (55)
where the layer potential operators \( S, K, K', T \) are defined by
\[
(S\sigma)(x) = \int_{\partial D} G(x, \xi) \cdot \sigma(\xi) \cdot d\mathbf{s}(\xi),
\]
(56)
\[
(K\sigma)(x) = \int_{\partial D} \frac{\partial G(x, \xi)}{\partial \mathbf{n}(\xi)} \cdot \sigma(\xi) \cdot d\mathbf{s}(\xi),
\]
(57)
\[
(K'\sigma)(x) = \int_{\partial D} \frac{\partial G(x, \xi)}{\partial \mathbf{n}(x)} \cdot \sigma(\xi) \cdot d\mathbf{s}(\xi),
\]
(58)
\[
(T\sigma)(x) = \lim_{h \to +0} \int_{\partial D} \frac{\partial^2 G(x \pm hn(x), \xi)}{\partial \mathbf{n}(\xi) \partial \mathbf{n}(x)} \cdot \sigma(\xi) \cdot d\mathbf{s}(\xi)
\] (59)
for \( x \in \partial D \). Obviously, \( P_+ + P_- = I \) implying that the decomposition, of an arbitrary pair of data \((\phi, \psi)\) on boundary into incoming and outgoing parts, is complete.

**Remark 5.1** It is well-known that for a smooth \( \partial D \) the operators \( S, K, K' \) are bounded from \( C(\partial D) \) to \( C(\partial D) \), whereas \( T \) are bounded from \( C^1(\partial D) \) to \( C(\partial D) \).

Define the four linear operators \( S_\pm, K_\pm, K'_\pm, T_\pm \) by the formulae
\[
(S_\pm \psi)(x) = \lim_{h \to +0} p(x \pm hn(x)),
\]
(60)
\[
(K_\pm \phi)(x) = \lim_{h \to +0} q(x \pm hn(x)),
\]
(61)
\[
(K'_\pm \psi)(x) = \lim_{h \to +0} \frac{\partial p(x \pm hn(x))}{\partial \mathbf{n}(x)},
\]
(62)
\[
(T_\pm \phi)(x) = \lim_{h \to +0} \frac{\partial q(x \pm hn(x))}{\partial \mathbf{n}(x)}
\] (63)
for \( x \in \partial D \), and we see that
\[
K_\pm = K \mp \frac{1}{2} I, \quad K'_\pm = K' \mp \frac{1}{2} I, \quad S_\pm = S, \quad T_\pm = T.
\]
(64)

As is well-known, the exterior Green’s formula maps to zero the Dirichlet and Neumann data \((\phi, \phi_n)\) of an outgoing wave \(\phi\) in \(D\). Conversely, the interior Green’s formula maps to zero the Dirichlet and Neumann data \((\psi, \psi_n)\) of an outgoing wave \(\psi\) outside \(D\); therefore,
\[
P_+ \circ P_- = P_- \circ P_+ = 0, \quad W_- \cap W_+ = \{0\}.
\]
(65)

**Lemma 5.2**  
\(P\) is a projector if and only if there exists a unique operator \(Q\) such that
\[
Q^2 = \frac{1}{4} I, \quad P = \frac{1}{2} I + Q
\]
(66)

In particular,
\[
P_\pm = \frac{1}{2} I \pm Q, \quad \text{with} \quad Q = \begin{bmatrix} -K & S \\ -T & K' \end{bmatrix}
\]
(67)

Furthermore, \(Q^2 = I/4\) implies that
\[
ST = -\frac{1}{4} I + K^2, \quad TS = -\frac{1}{4} I + (K')^2, \quad KS = SK', \quad TK = K'T
\]
(68)

Finally, the Dirichlet-to-Neumann maps \(\Lambda_\pm : \phi \mapsto \phi_n\), with \((\phi, \phi_n) \in W_\pm(\partial D)\), are given by the formulae
\[
\Lambda_\pm = \left( K' \mp \frac{1}{2} I \right)^{-1} T = S^{-1} \left( K \pm \frac{1}{2} I \right)
\]
(69)
\[
= T \left( K \mp \frac{1}{2} I \right)^{-1} = \left( K' \pm \frac{1}{2} I \right) S^{-1}
\]
(70)

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