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Volume Integral Equations and Single-Trace Formulations for Acoustic Wave Scattering in an Inhomogeneous Medium

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Abstract

We study frequency domain acoustic scattering at a bounded, penetrable, and inhomogeneous obstacle $\Omega^- \subset \mathbb{R}^d$, $d = 2, 3$. By defining constant reference coefficients, a representation formula for the pressure field is derived. It contains a volume integral operator, related to the one in the Lippmann-Schwinger equation. Besides, it features integral operators defined on $\partial\Omega^-$ and closely related to boundary integral equations of single-trace formulations (STF) for transmission problems with piecewise constant coefficients. We show well-posedness of the continuous variational formulation and asymptotic convergence of Galerkin discretizations. Numerical experiments in 2D validate our expected convergence rates.

1 Introduction

We are interested in solving the frequency domain acoustic wave scattering problem in a medium that is homogeneous outside a bounded region $\Omega^- \subset \mathbb{R}^d$, $d = 2, 3$. We denote the exterior domain $\Omega^+ := \mathbb{R}^d \setminus \bar{\Omega}^-$. Material properties are given by functions $a \in L^\infty(\mathbb{R}^d)$ and $\kappa \in L^\infty(\mathbb{R}^d)$ where

$$a(\mathbf{x}) \equiv 1, \quad \kappa(\mathbf{x}) \equiv \kappa_0 \in \mathbb{C}_+ \quad \text{for } \mathbf{x} \in \Omega^+, \quad (1)$$

and $a_{\max} > a(\mathbf{x}) > a_{\min} > 0$ almost everywhere in \mathbb{R}^d .

The equation governing the problem of finding the total wave $u := u^s + u^{\text{inc}}$ in this inhomogeneous medium is

$$-\operatorname{div}(a(\mathbf{x})\nabla u(\mathbf{x})) - \kappa(\mathbf{x})^2 u(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \mathbb{R}^d, \quad (2)$$

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where u^{inc} is an incident field satisfying the Helmholtz equation in the whole space,

$$-\Delta u^{\text{inc}}(\mathbf{x}) - \kappa_0^2 u^{\text{inc}}(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \mathbb{R}^d, \quad (3)$$

and u^s satisfies radiation conditions [12, Theorem 9.6]

$$\lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u^s}{\partial r} - i\kappa_0 u^s \right) = 0. \quad (4)$$

The problem can be formulated as the following transmission problem: find $u \in H_{\text{loc}}^1(\mathbb{R}^d)$ such that

$$\left\{ \begin{array}{ll} -\Delta u - \kappa_0^2 u = 0 & \text{in } \Omega^+, \\ -\text{div}(a\nabla u) - \kappa^2 u = 0 & \text{in } \Omega^-, \\ \gamma^+ u - \gamma^- u = -\gamma u^{\text{inc}} & \text{in } \Gamma, \\ \partial_n^+ u - \partial_n^- u = -\partial_n u^{\text{inc}} & \text{in } \Gamma, \\ \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u}{\partial r} - i\kappa_0 u \right) = 0, & \end{array} \right. \quad (5)$$

where $\gamma^\pm, \partial_n^\pm$ denote the exterior/interior Dirichlet and Neumann trace operators. We know that there exists a unique solution $u \in H_{\text{loc}}^1(\mathbb{R}^d)$ under certain assumptions on the material parameters. In particular, we need the unique continuation principle to hold. In 2D, this is true for $a \in L^\infty(\Omega)$ with a positive lower bound and real-valued $\kappa \in L^\infty(\Omega)$ [1].

For the general case mentioned above, volume integral equations (VIEs), also known as the Lippmann-Schwinger equation, lead to an integral equation formulation where the problem reduces to finding u in the domain Ω^- . Well-posedness of the equation under different assumptions on the material properties has been studied in [7, 11], with the case of piecewise smooth a the one presenting more complications. The equation is then discretized by a Galerkin method, where different approaches lead to the discrete dipole approximation (DDA) [20] and the partial element equivalent circuit formulation (PEEC) [14], both widely used in the engineering community. A non-exhaustive list of fast solvers for the case of only non-constant κ is also available [3, 4, 19].

Alternatively, a popular choice for problems dealing with exterior unbounded domains arises by writing an expression for the Dirichlet-to-Neumann map, which makes it possible to write a variational formulation that considers the exact radiation conditions. Discretization by a Galerkin method then leads to finite-element-boundary-element coupled schemes. Well-posedness of several discrete formulations can be found in [9].

For the particular case of piecewise constant coefficients, i.e. $a(\mathbf{x}) \equiv a_1, \kappa(\mathbf{x}) \equiv \kappa_1$ for $\mathbf{x} \in \Omega^-$, it is possible to reformulate the problem as a boundary integral equation (BIE) system. First and

second kind single-trace formulations (STFs) can be derived followed by discretization with the boundary element method (BEM) [5]. Its main advantage is that one needs to discretize only function spaces on $\partial\Omega^-$, which leads to smaller (but dense) linear systems. The BEM together with compression techniques such as \mathcal{H} -matrices or the fast multipole method, is a highly efficient approach for this particular case.

Our focus is on the situations where both $a(\mathbf{x})$ and $\kappa(\mathbf{x})$ are discontinuous across the boundary $\Gamma := \partial\Omega^-$ and only piecewise smooth. We present a novel formulation that combines boundary integral representations and volume integral operators. We define appropriate reference coefficients for the interior domain, in a way that the support of volume integrals can potentially be reduced to a minimum. For the particular case of piecewise-constant coefficients, our formulation reduces to the BIE approach. We claim that our formulation can be beneficial in presence of small or locally supported inhomogeneities. Some examples are cases where the parameters are non-constant only in a small region in the interior of Ω^- or close to the boundary Γ . Volume integral operators taking into account these inhomogeneities are shown to be compact for quite general, piecewise-smooth coefficients, contrary to the well-studied Lippmann-Schwinger equation, where the compactness is lost for non-smooth a .

2 Derivation of VIEs

2.1 Preliminaries

Let $\Omega^- \subset \mathbb{R}^d$ be a Lipschitz domain, $\Gamma := \partial\Omega^-$ its Lipschitz boundary with outward unit normal \mathbf{n} . We rely on standard Sobolev spaces $H^s(\Omega^-)$ of order $s > 0$. We also denote as $\widetilde{H}^{-s}(\Omega^-)$ the dual space of $H^s(\Omega^-)$ [12, Section 3]. Sobolev spaces on the boundary Γ are denoted as $H^s(\Gamma)$, which arise naturally as boundary restrictions of elements of $H^{s+1/2}(\Omega^-)$ by the interior trace operator

$$\gamma^- : \begin{cases} H^s(\Omega^-) \rightarrow H^{s-1/2}(\Gamma), \\ u \mapsto u|_{\Omega^-}, \quad u \in C^\infty(\Omega^-), \end{cases} \quad s > \frac{1}{2}.$$

which is a bounded operator [12, Theorem 3.37]. We will use also the interior normal trace operator γ_n [13, Theorem 3.24]

$$\gamma_n^- : \begin{cases} H(\operatorname{div}, \Omega^-) \rightarrow H^{-1/2}(\Gamma), \\ \mathbf{u} \mapsto \mathbf{u}|_\Gamma \cdot \mathbf{n}, \quad \mathbf{u} \in [C^\infty(\Omega^-)]^d, \end{cases}$$

where the space $H(\operatorname{div}, \Omega^-)$ is defined as

$$H(\operatorname{div}, \Omega^-) := \left\{ \mathbf{u} \in [L^2(\Omega^-)]^d : \operatorname{div} \mathbf{u} \in L^2(\Omega^-) \right\}.$$

For $u \in H(\Delta, \Omega^-)$, where

$$H(\Delta, \Omega^-) := \left\{ u \in H^1(\Omega^-) : \Delta u \in L^2(\Omega^-) \right\},$$

we define the Neumann trace operator ∂_n as [15, Theorem 2.8.3]

$$\partial_n^- : \begin{cases} H(\Delta, \Omega^-) \rightarrow H^{-1/2}(\Gamma), \\ u \mapsto \nabla u|_{\Gamma} \cdot \mathbf{n}, \quad u \in C^\infty(\Omega^-). \end{cases}$$

Replacing Ω^- by $\Omega^+ := \mathbb{R}^d \setminus \overline{\Omega^-}$ in the previous definitions, we obtain exterior trace operators: γ^+ , γ_n^+ and ∂_n^+ .

We define jump and average trace operators for elements of $H^1(\mathbb{R}^d \setminus \Gamma)$, $H(\operatorname{div}, \mathbb{R}^d \setminus \Gamma)$ and $H(\Delta, \mathbb{R}^d \setminus \Gamma)$:

$$\llbracket \gamma \rrbracket := \{\gamma^+ - \gamma^-\}, \quad \{\!\!\{ \gamma \}\!\!\} := \frac{1}{2}\{\gamma^+ + \gamma^-\},$$

and similarly for γ_n and ∂_n . We denote the sesqui-linear inner product in $L^2(\Omega^-)$ as $\langle u, v \rangle_{\Omega^-}$. It can be extended to a duality pairing between $\widetilde{H}^{-1}(\Omega^-)$ and $H^1(\Omega^-)$. Similarly, we define the dual product for $H^{1/2}(\Gamma)$ and its dual $H^{-1/2}(\Gamma)$, and denote it as $\langle \cdot, \cdot \rangle_{\Gamma}$.

2.2 Fundamental Solutions and Newton Potential

The fundamental solution for the Helmholtz operator with wavenumber $\kappa \in \mathbb{R}$ is given by $G_\kappa \in L^1_{\text{loc}}(\mathbb{R}^d)$ [18, Section 5.4]:

$$G_\kappa(\mathbf{x}, \mathbf{y}) := \begin{cases} \frac{i}{4} H_0^{(1)}(\kappa|\mathbf{x} - \mathbf{y}|), & d = 2, \\ \frac{\exp(i\kappa|\mathbf{x} - \mathbf{y}|)}{4\pi|\mathbf{x} - \mathbf{y}|}, & d = 3. \end{cases} \quad (6)$$

The Newton potential $N_\kappa : C_c^\infty(\mathbb{R}^d) \rightarrow C^\infty(\mathbb{R}^d)$ is the continuous mapping [15, Section 3.1.1] defined by

$$N_\kappa f(\mathbf{x}) := \int_{\mathbb{R}^d} G_\kappa(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}. \quad (7)$$

The Newton potential can be extended to the following two continuous operators

$$\begin{aligned} N_\kappa &: H_{\text{comp}}^{-1}(\mathbb{R}^d) \rightarrow H_{\text{loc}}^1(\mathbb{R}^d), \\ N_\kappa &: L^2_{\text{comp}}(\mathbb{R}^d) \rightarrow H_{\text{loc}}^2(\mathbb{R}^d) \end{aligned} \quad (8)$$

and more generally, $N_\kappa : H_{\text{comp}}^s(\mathbb{R}^d) \rightarrow H_{\text{loc}}^{s+2}(\mathbb{R}^d)$ is continuous for $s \in \mathbb{R}$ [15, Theorem. 3.12].

Similarly, by extension by zero followed by restriction to Ω^- , it is possible to consider the Newton potential in a bounded domain Ω^- :

$$\begin{aligned} \widetilde{N}_\kappa &: \widetilde{H}^{-1}(\Omega^-) \rightarrow H^1(\Omega^-), \\ \widetilde{N}_\kappa &: L^2(\Omega^-) \rightarrow H^2(\Omega^-). \end{aligned} \quad (9)$$

The following theorem [6, Theorem 8.1] is essential for the derivation of volume integral equations for scattering problems.

Theorem 2.1. *The Newton potential defines a solution operator for the Helmholtz equation on \mathbb{R}^d , i.e. for $f \in L^2_{comp}(\mathbb{R}^d)$ compactly supported in Ω^- , $u := N_\kappa f$ satisfies*

$$-\Delta u - \kappa^2 u = f \quad \text{in } \mathbb{R}^d \quad (10)$$

and the radiation conditions (4).

Theorem 2.1 provides a global representation of the solution of $-\Delta u - \kappa^2 u = f$ in terms of the Newton potential, i.e. u as a solution of the problem in \mathbb{R}^d . Our approach requires a local representation formula. We introduce the transmission problem with piecewise constant coefficients: find $u \in H^1_{loc}(\mathbb{R}^d)$ such that

$$\begin{cases} -\Delta u_0 - \kappa_0^2 u_0 = 0 & \text{in } \Omega^+, \\ -\Delta u_1 - \kappa_1^2 u_1 = f & \text{in } \Omega^-, \\ \gamma^+ u_0 - \gamma^- u_1 = g_1 & \text{in } \Gamma, \\ \partial_n^+ u_0 - \partial_n^- u_1 = g_2 & \text{in } \Gamma, \\ \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u_0}{\partial r} - i\kappa_0 u_0 \right) = 0, \end{cases} \quad (11)$$

where $u_0 = u|_{\Omega^+}$ and $u_1 = u|_{\Omega^-}$. It is possible to write expressions for u_0 and u_1 depending only on their traces and source terms [6, Theorem 2.1]

$$\begin{aligned} u_0 &= D_0(\gamma^+ u_0) - S_0(\partial_n^+ u_0) & \text{in } \Omega^+, \\ u_1 &= S_1(\partial_n^- u_1) - D_1(\gamma^- u_1) + \widetilde{N}_1 f & \text{in } \Omega^-, \end{aligned} \quad (12)$$

where \widetilde{N}_1 is the Newton potential with wavenumber κ_1 , S_j and D_j denote the single layer and double layer potentials with wavenumber κ_j , $j = 0, 1$, [15, Theorem 3.1.16]

$$S_j : H^{-1/2}(\Gamma) \rightarrow H^1_{loc}(\Omega^- \cup \Omega^+), \quad (13)$$

$$D_j : H^{1/2}(\Gamma) \rightarrow H^1_{loc}(\Omega^- \cup \Omega^+), \quad (14)$$

which have the integral representation

$$(S_j \psi)(\mathbf{x}) := \int_{\Gamma} G_{\kappa_j}(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) ds_y, \quad \mathbf{x} \in \mathbb{R}^d \setminus \Gamma, \quad (15)$$

$$(D_j \varphi)(\mathbf{x}) := \int_{\Gamma} \frac{\partial G_{\kappa_j}}{\partial \mathbf{n}_y}(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y}) ds_y, \quad \mathbf{x} \in \mathbb{R}^d \setminus \Gamma, \quad (16)$$

for sufficiently smooth densities φ and ψ . Later we will make use of boundary integral operators. These arise from taking jumps of traces of potentials, which yields the following continuous operators [18, Section 6],[15, Theorem 3.1.16]:

$$V_j := \{\{\gamma S_j\}\} : H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma), \quad (17)$$

$$K_j := \{\{\gamma D_j\}\} : H^{1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma), \quad (18)$$

$$K'_j := \{\{\partial_n S_j\}\} : H^{-1/2}(\Gamma) \rightarrow H^{-1/2}(\Gamma), \quad (19)$$

$$W_j := -\{\{\partial_n D_j\}\} : H^{1/2}(\Gamma) \rightarrow H^{-1/2}(\Gamma). \quad (20)$$

We collect all of them in the Calderón operator

$$A_j := \begin{pmatrix} -K_j & V_j \\ W_j & K'_j \end{pmatrix} : H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma). \quad (21)$$

Layer potentials also satisfy the jump relations [15, Theorem 3.3.1]

$$\begin{aligned} \llbracket \gamma S_j \psi \rrbracket &= 0, & \llbracket \partial_n S_j \psi \rrbracket &= \psi, \\ \llbracket \gamma D_j \varphi \rrbracket &= -\varphi, & \llbracket \partial_n D_j \varphi \rrbracket &= 0. \end{aligned}$$

The representation formula (12) guarantees that u_0 and u_1 satisfy the Helmholtz equation in Ω^+ and Ω^- respectively. Moreover, u_0 satisfies Sommerfeld radiation conditions. Transmission conditions remain to be enforced. This will be presented in the next section.

2.3 Combined Volume-Boundary Integral Representation

Now we consider the case where the interior coefficients are not constant anymore, i.e. vary in space. We write the transmission problem (5) as follows

$$\left\{ \begin{array}{ll} -\Delta u - \kappa_0^2 u = 0, & \text{in } \Omega^+, \\ -\Delta u - \frac{\kappa_1^2}{a_1} u = f, & \text{in } \Omega^-, \\ \gamma^+ u - \gamma^- u = -\gamma u^{\text{inc}}, & \text{in } \Gamma, \\ \partial_n u^+ - a \partial_n^- u = -\partial_n u^{\text{inc}}, & \text{in } \Gamma, \\ \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u}{\partial r} - i\kappa_0 u \right) = 0, & \end{array} \right. \quad (22)$$

where

$$f(\mathbf{x}) := \operatorname{div}(\alpha(\mathbf{x})\nabla u)(\mathbf{x}) + \beta(\mathbf{x})u(\mathbf{x}), \quad \mathbf{x} \in \Omega^-, \quad (23)$$

$$\alpha(\mathbf{x}) := \frac{a(\mathbf{x})}{a_1} - 1, \quad \beta(\mathbf{x}) := \frac{1}{a_1}(\kappa(\mathbf{x})^2 - \kappa_1^2), \quad (24)$$

and $a_1 \in \mathbb{R}_+$, $\kappa_1 \in \mathbb{C}_+$ are conveniently chosen parameters. The representation formula (12) now reads

$$\begin{aligned} u &= D_0(\gamma^+ u) - S_0(\partial_n^+ u), & \text{in } \Omega^+ \\ u &= S_1(\partial_n^- u) - D_1(\gamma^- u) + \widetilde{N}_1(\operatorname{div}(\alpha \nabla u) + \beta u), & \text{in } \Omega^-, \end{aligned} \quad (25)$$

where D_0 and S_0 are the layer potentials with wavenumber κ_0 , and D_1 and S_1 are the layer potentials with wavenumber $\frac{\kappa_1}{\sqrt{a_1}}$. Integration by parts leads to the following expression. For $\mathbf{x} \in \Omega^-$:

$$\begin{aligned} \widetilde{N}_1(\operatorname{div}(\alpha \nabla u))(\mathbf{x}) &= \int_{\Omega^-} G_1(\mathbf{x} - \mathbf{y}) \operatorname{div}(\alpha(\mathbf{y}) \nabla u(\mathbf{y})) \, d\mathbf{y} \\ &= \operatorname{div} \int_{\Omega^-} G_1(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) \nabla u(\mathbf{y}) \, d\mathbf{y} + \int_{\Gamma} G_1(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) \frac{\partial u}{\partial \mathbf{n}_y}(\mathbf{y}) \, ds_y \\ &= \operatorname{div} \widetilde{N}_1(\alpha \nabla u)(\mathbf{x}) + S_1(\alpha \partial_n u)(\mathbf{x}). \end{aligned} \quad (26)$$

Another integration by parts shows:

$$\begin{aligned} \operatorname{div} \widetilde{N}_1(\alpha \nabla u)(\mathbf{x}) &= \operatorname{div} \int_{\Omega^-} G_1(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) \nabla u(\mathbf{y}) \, d\mathbf{y} \\ (\text{Integration by parts}) &= -\operatorname{div} \int_{\Omega^-} \nabla \{G_1(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y})\} u(\mathbf{y}) \, d\mathbf{y} \\ &\quad - \int_{\Gamma} \frac{\partial G_1}{\partial \mathbf{n}_y}(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) u(\mathbf{y}) \, ds_y \\ (\text{Product rule}) &= \int_{\Omega^-} \Delta_y G_1(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) u(\mathbf{y}) \, d\mathbf{y} \\ &\quad - \operatorname{div} \int_{\Omega^-} G_1(\mathbf{y} - \mathbf{y}) u(\mathbf{y}) \nabla \alpha(\mathbf{y}) \, d\mathbf{y} \\ &\quad - \int_{\Gamma} \frac{\partial G_1}{\partial \mathbf{n}_y}(\mathbf{x} - \mathbf{y}) \alpha(\mathbf{y}) u(\mathbf{y}) \, ds_y \\ (\Delta_y G(\mathbf{x} - \mathbf{y}) = -\delta(\mathbf{x} - \mathbf{y}) + \frac{\kappa_1^2}{a_1}) &= -\alpha(\mathbf{x}) u(\mathbf{x}) - \widetilde{N}_1(a_1^{-1} \kappa_1^2 \alpha u)(\mathbf{x}) - \operatorname{div} \widetilde{N}_1(u \nabla \alpha)(\mathbf{x}) \\ &\quad - D_1(\alpha \gamma u)(\mathbf{x}), \end{aligned} \quad (27)$$

for $\mathbf{x} \in \Omega^-$. Combining (26) and (27) we obtain

$$\widetilde{N}_1(\operatorname{div}(\alpha \nabla u)) = S_1(\alpha \partial_n u) - D_1(\alpha \gamma u) - \alpha u - \widetilde{N}_1(a_1^{-1} \kappa_1^2 \alpha u) - \operatorname{div} \widetilde{N}_1(u \nabla \alpha). \quad (28)$$

From (25) and (28) we obtain a new representation formula for the solution of (22) for the interior domain:

$$\tilde{a}u = S_1(\tilde{a} \partial_n^- u) - D_1(\tilde{a} \gamma^- u) + \widetilde{N}_1((\beta - a_1^{-1} \kappa_1^2 \alpha)u) - \operatorname{div} \widetilde{N}_1(u \nabla \alpha) \quad \text{in } \Omega^-, \quad (29)$$

where $\tilde{a}(\mathbf{x}) := \frac{a(\mathbf{x})}{a_1}$.

2.4 STF-VIEs: Operator Form

Let u solve (22) and denote $\varphi := \tilde{a}\gamma^-u$ and $\psi := \tilde{a}\partial_n^-u$. We also write

$$\mathcal{A}w := \widetilde{N}_1((\beta - a_1^{-1}\kappa_1^2\alpha)w) - \operatorname{div}\widetilde{N}_1(w\nabla\alpha). \quad (30)$$

Lemma 2.2. *Let $\alpha \in W^{2,\infty}(\Omega^-)$ and $\beta \in L^\infty(\Omega^-)$. Then, the operator*

$$\mathcal{A} : H^1(\Omega^-) \rightarrow H^1(\Omega^-)$$

as defined in (30) is compact.

Proof. The result follows from the mapping properties of the Newton potential. The operators

$$\widetilde{N}_1((\beta - a_1^{-1}\kappa_1^2\alpha)\cdot) : H^1(\Omega^-) \rightarrow H^2(\Omega^-), \quad (31)$$

$$\operatorname{div}\widetilde{N}_1(\cdot\nabla\alpha) : H^1(\Omega^-) \rightarrow H^{1+s}(\Omega^-), \quad (32)$$

are bounded: (31) follows directly from the mapping properties of the Newton potential in a bounded domain (9). The case of (32) requires more attention: let $u \in H^1(\Omega^-)$ and consider

$$\mathbf{f} := \begin{cases} u\nabla\alpha & \text{in } \Omega^-, \\ 0 & \text{in } \Omega^+. \end{cases}$$

Then $\mathbf{f} \in [H_{\text{comp}}^s(\mathbb{R}^d)]^d$ for $s \in [0, \frac{1}{2})$. By the mapping properties of the Newton potential in the whole space (8), we have $N_1\mathbf{f} \in [H_{\text{loc}}^{2+s}(\mathbb{R}^d)]^d$ and therefore $\widetilde{N}_1(u\nabla\alpha) \in [H^{2+s}(\Omega^-)]^d$. We can conclude that $\operatorname{div}\widetilde{N}_1(u\nabla\alpha) \in H^{1+s}(\Omega^-)$.

The inclusion of $H^{1+s}(\Omega^-)$ into $H^1(\Omega^-)$ for $s > 0$ is compact by Rellich's embedding theorem [15, Theorem 2.5.5]. The result follows by the composition of a bounded operator and a compact operator. \square

We rewrite the representation formula (29) as

$$\tilde{a}u = S_1\psi - D_1\varphi + \mathcal{A}u \quad \text{in } \Omega^- \quad (33)$$

By applying traces γ^- and ∂_n^- to (33) we get

$$\begin{pmatrix} \gamma^- \\ \partial_n^- \end{pmatrix} (\tilde{a}u) = \begin{pmatrix} \gamma^- \\ \partial_n^- \end{pmatrix} (S_1\psi - D_1\varphi) + \begin{pmatrix} \gamma^- \\ \partial_n^- \end{pmatrix} \mathcal{A}u = \left(\frac{1}{2}I + A_1\right) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} + \begin{pmatrix} \gamma^- \\ \partial_n^- \end{pmatrix} \mathcal{A}u. \quad (34)$$

The left-hand side can be equivalently written as

$$\begin{pmatrix} \gamma^- \\ \partial_n^- \end{pmatrix} (\tilde{a}u) = \begin{pmatrix} \tilde{a}\gamma^-u \\ (\partial_n\tilde{a})\gamma^-u + \psi \end{pmatrix} = \begin{pmatrix} \varphi \\ (\mathbf{n} \cdot \nabla\tilde{a})\gamma^-u + \psi \end{pmatrix} \quad (35)$$

Combining (34) and (35) we obtain

$$\left(\frac{1}{2}I - A_1\right) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} + T_\Gamma u + T_{\Omega^-} u = 0, \quad (36)$$

where

$$T_\Gamma u := \begin{pmatrix} 0 \\ -(\mathbf{n} \cdot \nabla \tilde{a}) \gamma^- u \end{pmatrix} \quad \text{and} \quad T_{\Omega^-} u := \begin{pmatrix} \gamma^- \mathcal{A} u \\ \partial_n^- \mathcal{A} u \end{pmatrix}. \quad (37)$$

For the exterior domain it holds

$$\left(\frac{1}{2}I + A_0\right) \begin{pmatrix} \gamma^+ u \\ \partial_n^+ u \end{pmatrix} = 0. \quad (38)$$

The transmission conditions of (22) can be written as

$$\begin{pmatrix} \gamma^+ u \\ \partial_n^+ u \end{pmatrix} - M \begin{pmatrix} \varphi \\ \psi \end{pmatrix} = \begin{pmatrix} \gamma u^{\text{inc}} \\ \partial_n u^{\text{inc}} \end{pmatrix} \quad (39)$$

with a multiplication operator

$$M := \begin{pmatrix} \tilde{a}^{-1} & 0 \\ 0 & a_1 \end{pmatrix}. \quad (40)$$

Combining (38) and (39) leads to

$$\left(\frac{1}{2}I + A_0\right) M \begin{pmatrix} \varphi \\ \psi \end{pmatrix} = \begin{pmatrix} \gamma u^{\text{inc}} \\ \partial_n u^{\text{inc}} \end{pmatrix}, \quad (41)$$

Equations (36) and (41) together amount to first-kind and second-kind variants of the single trace formulation (STF):

$$(M^{-1}A_0M + A_1) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} - T_\Gamma u - T_{\Omega^-} u = M^{-1} \begin{pmatrix} \gamma u^{\text{inc}} \\ \partial_n u^{\text{inc}} \end{pmatrix}, \quad (42)$$

$$(I + M^{-1}A_0M - A_1) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} + T_\Gamma u + T_{\Omega^-} u = M^{-1} \begin{pmatrix} \gamma u^{\text{inc}} \\ \partial_n u^{\text{inc}} \end{pmatrix}. \quad (43)$$

We need an extra equation for our system. This will be the representation formula in the interior domain (33). **For the first-kind variant**, the coupled system reads as follows: find $\varphi \in H^{1/2}(\Gamma)$, $\psi \in H^{-1/2}(\Gamma)$, $u \in H^1(\Omega^-)$ such that

$$\left(\begin{array}{cc|c} M^{-1}A_0M + A_1 & T_\Gamma + T_{\Omega^-} & \\ \hline D_1 & -S_1 & \tilde{a}I - \mathcal{A} \end{array} \right) \begin{pmatrix} \varphi \\ \psi \\ u \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ 0 \end{pmatrix} \quad (44)$$

holds in $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega^-)$.

The second-kind **variant** is: find $\varphi \in H^{1/2}(\Gamma)$, $\psi \in H^{-1/2}(\Gamma)$, $u \in H^1(\Omega^-)$ such that

$$\left(\begin{array}{c|c} I - M^{-1}A_0M + A_1 & -T_\Gamma - T_{\Omega^-} \\ \hline D_1 & -S_1 \end{array} \middle| \begin{array}{c} -T_\Gamma - T_{\Omega^-} \\ \tilde{a}I - \mathcal{A} \end{array} \right) \begin{pmatrix} \varphi \\ \psi \\ u \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ 0 \end{pmatrix} \quad (45)$$

in $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega^-)$. The right hand side is given by

$$\begin{pmatrix} g_1 \\ g_2 \end{pmatrix} = M^{-1} \begin{pmatrix} \gamma u^{\text{inc}} \\ \partial_n u^{\text{inc}} \end{pmatrix}.$$

We call (44) and (45) single-trace volume integral equations (STF-VIE).

Remark 2.3. *We refer to (45) as second-kind, but this formulation fails to be coercive due to the multiplier matrix M . Nevertheless, we include it for our numerical experiments, although we proceed to study the first-kind STF-VIE from (44).*

2.5 First-kind STF-VIE in Special Settings

In this section we will study what (44) boils down to under different assumptions on the functions a and κ .

2.5.1 Piecewise Constant Coefficients

Assuming that $a(\mathbf{x}) \equiv a_{\Omega^-} > 0$ and $\kappa(\mathbf{x}) \equiv \kappa_{\Omega^-} \in \mathbb{C}_+$, an appropriate choice of a_1 and κ_1 leads to:

$$\tilde{a} \equiv 1, \quad \alpha \equiv 0, \quad \beta \equiv 0.$$

Problem (44) now reads: find $\varphi \in H^{1/2}(\Gamma)$, $\psi \in H^{-1/2}(\Gamma)$, $u \in H^1(\Omega^-)$ such that

$$\left(\begin{array}{c|c} M^{-1}A_0M + A_1 & 0 \\ \hline D_1 & -S_1 \end{array} \middle| \begin{array}{c} 0 \\ I \end{array} \right) \begin{pmatrix} \varphi \\ \psi \\ u \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ 0 \end{pmatrix}$$

holds in $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega^-)$. This is equivalent to solving a single-trace BIE and then evaluating the solution u by means of the representation formula. Well-posedness of the formulation has been established in [8].

2.5.2 Piecewise Constant a , Variable κ

Assuming that $a(\mathbf{x}) \equiv a_{\Omega^-} > 0$, an appropriate choice of a_1 leads to:

$$\tilde{a} \equiv 1, \quad \alpha \equiv 0.$$

The volume integral operator \mathcal{A} can be rewritten as $\mathcal{A}u = N_1(\beta u)$. Problem (44) now reads: find $\varphi \in H^{1/2}(\Gamma)$, $\psi \in H^{-1/2}(\Gamma)$, $u \in H^1(\Omega^-)$ such that

$$\left(\begin{array}{c|c} M^{-1}A_0M + A_1 & T_{\Omega^-} \\ \hline D_1 & -S_1 \end{array} \middle| I - \mathcal{A} \right) \begin{pmatrix} \varphi \\ \psi \\ u \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \\ 0 \end{pmatrix}$$

holds in $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega^-)$. In Sections 3 and 4 we will prove well-posedness of the continuous and discrete problems arising in this special case.

2.5.3 Constant Values at the Boundary

Assuming that $a(\mathbf{x}) \equiv a_\Gamma > 0$ for $\mathbf{x} \in \Gamma$, an appropriate choice of a_1 leads to $\tilde{a}(\mathbf{x}) \equiv 1$ for $\mathbf{x} \in \Gamma$. The operator

$$M^{-1}A_0M + A_1 : H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$$

will be injective. The problem reads as usual in (44), but we will be able to give a complete proof of a well-posedness result for the continuous and discrete case.

3 Analysis of first-kind STF-VIE

3.1 Variational Formulations

We now present variational formulations for the coupled systems (44) and (45). We denote by $\langle \cdot, \cdot \rangle_{\Omega^-}$ the duality pairing between $\widetilde{H}^{-1}(\Omega^-)$ and $H^1(\Omega^-)$. On the boundary, $\langle \cdot, \cdot \rangle_\Gamma$ denotes the duality between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$. Moreover, we define

$$\langle \langle \cdot, \cdot \rangle \rangle : \mathcal{H}(\Gamma) \times \mathcal{H}(\Gamma) \rightarrow \mathbb{C}, \quad \langle \langle \boldsymbol{\varphi}, \boldsymbol{\xi} \rangle \rangle := \langle \boldsymbol{\psi}, \boldsymbol{\xi} \rangle_\Gamma + \langle \boldsymbol{\eta}, \boldsymbol{\varphi} \rangle_\Gamma,$$

for all $\boldsymbol{\varphi} = (\varphi, \psi) \in \mathcal{H}(\Gamma)$, $\boldsymbol{\xi} = (\xi, \eta) \in \mathcal{H}(\Gamma)$ and $\mathcal{H}(\Gamma) := H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$.

Problem 3.1 (First kind STF-VIE variational formulation). *Given $\mathbf{g} \in \mathcal{H}(\Gamma)$, we seek $(\boldsymbol{\varphi}, u) \in \mathcal{H}(\Gamma) \times H^1(\Omega^-)$ such that the variational formulation*

$$\begin{aligned} \mathbf{a}_1(\boldsymbol{\varphi}, \boldsymbol{\xi}) + \mathbf{b}(u, \boldsymbol{\xi}) &= \langle \langle \mathbf{g}, \boldsymbol{\xi} \rangle \rangle, \\ \mathbf{c}(\boldsymbol{\varphi}, v) + \mathbf{d}(u, v) &= 0, \end{aligned} \tag{46}$$

holds for all $(\boldsymbol{\xi}, v) \in \mathcal{H}(\Gamma) \times \widetilde{H}^{-1}(\Omega^-)$, where we denote

$$\begin{aligned} \mathbf{a}_1(\boldsymbol{\varphi}, \boldsymbol{\xi}) &:= \langle\langle (M^{-1}A_0M + A_1)\boldsymbol{\varphi}, \boldsymbol{\xi} \rangle\rangle, & \mathbf{b}(u, \boldsymbol{\xi}) &:= \langle\langle T_\Gamma u, \boldsymbol{\xi} \rangle\rangle + \langle\langle T_{\Omega^-} u, \boldsymbol{\xi} \rangle\rangle, \\ \mathbf{c}(\boldsymbol{\varphi}, v) &:= \langle D_1\boldsymbol{\varphi} - S_1\boldsymbol{\psi}, v \rangle_{\Omega^-}, & \mathbf{d}(u, v) &:= \langle \tilde{a}u - \mathcal{A}u, v \rangle_{\Omega^-}. \end{aligned} \quad (47)$$

with A_0 and A_1 defined as in (21), \tilde{a} in (29), T_Γ and T_{Ω^-} in (37), M in (40).

Problem 3.2 (Second kind STF-VIE variational formulation). *Given $\mathbf{g} \in \mathcal{H}(\Gamma)$, we seek $(\boldsymbol{\varphi}, u) \in \mathcal{H}(\Gamma) \times H^1(\Omega^-)$ such that the variational formulation*

$$\begin{aligned} \mathbf{a}_2(\boldsymbol{\varphi}, \boldsymbol{\xi}) - \mathbf{b}(u, \boldsymbol{\xi}) &= \langle\langle \mathbf{g}, \boldsymbol{\xi} \rangle\rangle, \\ \mathbf{c}(\boldsymbol{\varphi}, v) + \mathbf{d}(u, v) &= 0, \end{aligned} \quad (48)$$

holds for all $(\boldsymbol{\xi}, v) \in \mathcal{H}(\Gamma) \times \widetilde{H}^{-1}(\Omega^-)$, where we denote

$$\mathbf{a}_2(\boldsymbol{\varphi}, \boldsymbol{\xi}) := \langle\langle (I - M^{-1}A_0M + A_1)\boldsymbol{\varphi}, \boldsymbol{\xi} \rangle\rangle, \quad (49)$$

besides the notations from Problem 3.1.

3.2 Coercivity

Proposition 3.3 (Coercivity of \mathbf{a}_1 , [8, Theorem 5.3]). *Let $\Gamma := \partial\Omega^-$ be the boundary of a Lipschitz domain $\Omega^- \subset \mathbb{R}^d$. Let $a \in W^{1,\infty}(\Omega^-)$, $\kappa \in L^\infty(\Omega^-)$ and set $a_1 \in \mathbb{R}_+$, $\kappa_1 \in \mathbb{C}_+$. Then, for \mathbf{a}_1 as defined in (47), there exists a compact operator $T_A : \mathcal{H}(\Gamma) \rightarrow \mathcal{H}(\Gamma)$ and a constant $c_{\mathbf{a}_1} > 0$ such that*

$$\operatorname{Re} \{ \mathbf{a}_1(\boldsymbol{\varphi}, \boldsymbol{\varphi}) + \langle\langle T_A \boldsymbol{\varphi}, \boldsymbol{\varphi} \rangle\rangle \} \geq c_{\mathbf{a}_1} \|\boldsymbol{\varphi}\|_{\mathcal{H}(\Gamma)}^2$$

for all $\boldsymbol{\varphi} \in \mathcal{H}(\Gamma)$.

Proposition 3.4 (inf-sup condition for \mathbf{d}). *Let $\Gamma := \partial\Omega^-$ be the boundary of a Lipschitz domain $\Omega^- \subset \mathbb{R}^d$. Let $a \in W^{1,\infty}(\Omega^-)$, $\kappa \in L^\infty(\Omega^-)$ and set $a_1 \in \mathbb{R}_+$, $\kappa_1 \in \mathbb{C}_+$. Let $\mathcal{A} : H^1(\Omega^-) \rightarrow H^1(\Omega^-)$ be the volume integral operator defined in (30). There exists a compact operator $T_A : H^1(\Omega^-) \rightarrow H^1(\Omega^-)$ and a constant $c_d > 0$ such that*

$$c_d \leq \inf_{u \in H^1(\Omega^-)} \sup_{v \in \widetilde{H}^{-1}(\Omega^-)} \frac{\mathbf{d}(u, v) - \langle T_A u, v \rangle_{\Omega^-}}{\|u\|_{H^1(\Omega^-)} \|v\|_{\widetilde{H}^{-1}(\Omega^-)}},$$

Proof. Consider the linear operator

$$G : H^1(\Omega^-) \rightarrow \widetilde{H}^{-1}(\Omega^-)$$

such that $Gu := -\Delta u + u$. There also exists a bounded inverse for G . For every $v \in \widetilde{H}^{-1}(\Omega^-)$, there exists a unique solution of the variational formulation: find $u \in H^1(\Omega^-)$ such that

$$\langle Gu, w \rangle_{\Omega^-} = (\nabla u, \nabla w)_{\Omega^-} + (u, w)_{\Omega^-} = \langle v, w \rangle_{\Omega^-} \quad \text{for all } w \in H^1(\Omega^-).$$

We know that

$$\|v\|_{\widetilde{H}^{-1}(\Omega^-)} = \|Gu\|_{\widetilde{H}^{-1}(\Omega^-)} = \sup_{w \in H^1(\Omega^-)} \frac{\langle Gu, w \rangle_{\Omega^-}}{\|w\|_{H^1(\Omega^-)}} = \sup_{w \in H^1(\Omega^-)} \frac{(\nabla u, \nabla w)_{\Omega^-} + (u, w)_{\Omega^-}}{\|w\|_{H^1(\Omega^-)}} = \|u\|_{H^1(\Omega^-)}.$$

Now, for any arbitrary $0 \neq u \in H^1(\Omega^-)$ consider $v^* = \frac{1}{\tilde{a}}Gu \in \widetilde{H}^{-1}(\Omega^-)$ and $T_{\mathcal{A}} = -\mathcal{A}$. We know that $\frac{1}{\tilde{a}} \in W^{1,\infty}(\Omega^-)$ and therefore

$$\|v^*\|_{\widetilde{H}^{-1}(\Omega^-)} \leq \left\| \tilde{a}^{-1} \right\|_{W^{1,\infty}(\Omega^-)} \|u\|_{H^1(\Omega^-)}.$$

Then

$$\begin{aligned} \sup_{0 \neq v \in \widetilde{H}^{-1}(\Omega^-)} \frac{\mathbf{d}(u, v) - \mathbf{t}_{\mathcal{A}}(u, v)}{\|v\|_{\widetilde{H}^{-1}(\Omega^-)}} &\geq \frac{\langle v^*, \tilde{a}u \rangle_{\Omega^-}}{\|v^*\|_{\widetilde{H}^{-1}(\Omega^-)}} = \frac{1}{\left\| \tilde{a}^{-1} \right\|_{W^{1,\infty}(\Omega^-)}} \frac{\langle \frac{1}{\tilde{a}}G(u), \tilde{a}u \rangle_{\Omega^-}}{\|u\|_{H^1(\Omega^-)}} \\ &= c_d \frac{\langle Gu, u \rangle_{\Omega^-}}{\|u\|_{H^1(\Omega^-)}} = c_d \|u\|_{H^1(\Omega^-)}. \end{aligned}$$

Taking the infimum over $u \in H^1(\Omega^-)$ concludes the proof. \square

3.3 Uniqueness

In order to show uniqueness of Problem 3.1, we will need to make the following assumption.

Assumption 3.5. *Let $\Omega^- \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Consider $a \in C^2(\Omega^-)$, with*

$$0 < a_{\min} < a(\mathbf{x}) < a_{\max},$$

for all $\mathbf{x} \in \Omega^-$. Let $\kappa_0, \kappa_1 \in \mathbb{R}_+$. Then, the trivial solution is the only solution to the problem

$$\left\{ \begin{array}{l} -\Delta u_0 - \kappa_0^2 u_0 = 0 \quad \text{in } \Omega^-, \\ -\Delta u_1 - \kappa_1^2 u_1 = 0 \quad \text{in } \mathbb{R}^d \setminus \Omega^-, \\ \gamma^+ u_0 - a \gamma^- u_1 = 0 \quad \text{in } \Gamma, \\ \partial_n^+ u_0 - \partial_n^- u_1 = 0 \quad \text{in } \Gamma. \\ \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u_0}{\partial r} - i \kappa_0 u_0 \right) = 0, \end{array} \right. \quad (50)$$

Remark 3.6. *Assumption 3.5 is satisfied for the case where $a|_{\Gamma} \equiv a_1$ is a constant. In this case a simple rescaling $\tilde{u}_1 = a_1 u_1$ leads to*

$$\left\{ \begin{array}{l} -\Delta u_0 - \kappa_0^2 u_0 = 0 \quad \text{in } \Omega^-, \\ -\operatorname{div} \left(\frac{1}{a_1} \nabla \tilde{u}_1 \right) - \frac{\kappa_1^2}{a_1} \tilde{u}_1 = 0 \quad \text{in } \mathbb{R}^d \setminus \Omega^-, \\ \gamma^+ u_0 - \gamma^- \tilde{u}_1 = 0 \quad \text{in } \Gamma, \\ \partial_n^+ u_0 - \frac{1}{a_1} \partial_n^- \tilde{u}_1 = 0 \quad \text{in } \Gamma. \\ \lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u_0}{\partial r} - i \kappa_0 u_0 \right) = 0, \end{array} \right. \quad (51)$$

Uniqueness of solutions for (51) then follows from the uniqueness of solutions of Helmholtz transmission problems with constant coefficients. It is not clear if the result holds for the general case. This remains as an open problem, therefore the need of Assumption 3.5.

Lemma 3.7 (Uniqueness). *Provided that Assumption 3.5 holds, there exists at most one solution to Problem 3.1.*

Proof. We will prove the result for the first-kind formulation in Problem 3.1. We study the operator equation

$$\left(\begin{array}{c|c} M^{-1}A_0M + A_1 & T_{\Gamma} + T_{\Omega^-} \\ \hline D_1 & \tilde{a}I - \mathcal{A} \end{array} \right) \begin{pmatrix} \varphi \\ \psi \\ u \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (52)$$

We want to show that the unique solution in $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma) \times H^1(\Omega^-)$ is $\varphi = 0, \psi = 0, u = 0$.

(I) From the last equation we have

$$\tilde{a}u = S_1\psi - D_1\varphi + \mathcal{A}u \quad \text{in } \Omega^-. \quad (53)$$

It is possible to go back using integration by parts (26) and (27) and obtain

$$u = S_1(\psi - \tilde{a}\partial_n^- u) - D_1(\varphi - \tilde{a}\gamma^- u) + N_1(\operatorname{div}(\alpha \nabla u) + \beta u), \quad (54)$$

which shows that u satisfies

$$-\Delta u - \frac{\kappa_1^2}{a_1} u = \operatorname{div}(\alpha \nabla u) + \beta u \quad \text{in } \Omega^-,$$

and therefore

$$-\operatorname{div}(a \nabla u) + \kappa^2 u = 0 \quad \text{in } \Omega^-. \quad (55)$$

Let us define

$$u_0 = \begin{pmatrix} D_0 & -S_0 \end{pmatrix} M \begin{pmatrix} \varphi \\ \psi \end{pmatrix}. \quad (56)$$

By definition, u_0 satisfies

$$\Delta u_0 + \kappa_0^2 u_0 = 0 \quad \text{in } \mathbb{R}^d \setminus \Omega^-. \quad (57)$$

Taking interior traces of (53), exterior traces of (56), we obtain

$$\begin{pmatrix} \gamma^-(\tilde{a}u) \\ \tilde{a}\partial_n^-(u) \end{pmatrix} = \left(\frac{1}{2}I + A_1\right) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} + T_\Gamma u + T_{\Omega^-} u, \quad (58)$$

$$\begin{pmatrix} \gamma^+ u_0 \\ \partial_n^+ u_0 \end{pmatrix} = \left(\frac{1}{2}I - A_0\right) M \begin{pmatrix} \varphi \\ \psi \end{pmatrix}. \quad (59)$$

Multiplying (59) by M^{-1} , subtracting from (58) and using (52)

$$M^{-1} \begin{pmatrix} \gamma^+ u_0 \\ \partial_n^+ u_0 \end{pmatrix} - \begin{pmatrix} \gamma^-(\tilde{a}u) \\ \tilde{a}\partial_n^-(u) \end{pmatrix} = 0, \quad (60)$$

which is equivalent to

$$\begin{pmatrix} \gamma^+ u_0 \\ \partial_n^+ u_0 \end{pmatrix} - \begin{pmatrix} \gamma^- u \\ a\partial_n^-(u) \end{pmatrix} = 0. \quad (61)$$

Combining (55), (57) and (61), we know that

$$U = \begin{cases} u & \text{in } \Omega^-, \\ u_0 & \text{in } \mathbb{R}^d \setminus \Omega^-, \end{cases} \quad (62)$$

must be the unique solution of a homogeneous transmission problem. Therefore, $U \equiv 0$ in \mathbb{R}^d . We conclude that $u = 0$ in Ω^- , $u_0 = 0$ in $\mathbb{R}^d \setminus \Omega^-$.

(II) This implies

$$0 = \left(\frac{1}{2}I + A_1\right) \begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \quad 0 = \left(\frac{1}{2}I - A_0\right) M \begin{pmatrix} \varphi \\ \psi \end{pmatrix}. \quad (63)$$

Now, note that $M = a_1 \tilde{M} := a_1 \begin{pmatrix} a^{-1} & 0 \\ 0 & 1 \end{pmatrix}$. Therefore, using (52) and the fact that $u = 0$ in Ω^- ,

$$(M^{-1}A_0M + A_1) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} = (\tilde{M}^{-1}A_0\tilde{M} + A_1) \begin{pmatrix} \varphi \\ \psi \end{pmatrix} = 0. \quad (64)$$

Define

$$v := \begin{pmatrix} -D_0 & S_0 \end{pmatrix} \tilde{M} \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \quad \text{in } \Omega^-, \quad (65)$$

$$v_0 := \begin{pmatrix} D_1 & -S_1 \end{pmatrix} \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \quad \text{in } \mathbb{R}^d \setminus \Omega^-. \quad (66)$$

Taking traces, we derive

$$\begin{pmatrix} \gamma^- v \\ \partial_n^- v \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I + A_0 \end{pmatrix} \tilde{M} \begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \quad \begin{pmatrix} \gamma^+ v_0 \\ \partial_n^+ v_0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - A_1 \end{pmatrix} \begin{pmatrix} \varphi \\ \psi \end{pmatrix}.$$

By (64), we get

$$\begin{pmatrix} \gamma^+ v_0 \\ \partial_n^+ v_0 \end{pmatrix} - \tilde{M}^{-1} \begin{pmatrix} \gamma^- v \\ \partial_n^- v \end{pmatrix} = 0.$$

We conclude that

$$\begin{aligned} -\Delta v - \kappa_0^2 v &= 0 \quad \text{in } \Omega^-, \\ -\Delta v_0 - \frac{\kappa_1^2}{a_1} v_0 &= 0 \quad \text{in } \mathbb{R}^d \setminus \Omega^-, \\ \gamma^+ v_0 - a \gamma^- v &= 0 \quad \text{in } \Gamma, \\ \partial_n^+ v_0 - \partial_n^- v &= 0 \quad \text{in } \Gamma. \end{aligned}$$

There is a unique solution by Assumption 3.5. Therefore, we know that

$$V = \begin{cases} v & \text{in } \Omega^-, \\ v_0 & \text{in } \mathbb{R}^d \setminus \Omega^-, \end{cases}$$

must be zero. This implies $v = 0$ in Ω^- , $v_0 = 0$ in $\mathbb{R}^d \setminus \Omega^-$, and

$$0 = \begin{pmatrix} \frac{1}{2}I + A_0 \end{pmatrix} \tilde{M} \begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \quad 0 = \begin{pmatrix} \frac{1}{2}I - A_1 \end{pmatrix} \begin{pmatrix} \varphi \\ \psi \end{pmatrix}. \quad (67)$$

Combining (63) and (67) we conclude that $\varphi = 0, \psi = 0$.

□

Remark 3.8. *It is worth noting that Assumption 3.5 ensures uniqueness for the traces $\varphi \in H^{1/2}(\Gamma), \psi \in H^{-1/2}(\Gamma)$. Uniqueness holds for the solution $u \in H^1(\Omega^-)$ of Problem 3.1 without Assumption 3.5.*

Theorem 3.9 (Well-posedness of Problem 3.1). *Under Assumption 3.5, there exists a unique solution $(\varphi^*, u^*) \in \mathcal{H}(\Gamma) \times H^1(\Omega^-)$ to Problem 3.1, that satisfies*

$$\|\varphi^*\|_{H^{1/2}(\Gamma)} + \|\psi^*\|_{H^{-1/2}(\Gamma)} + \|u^*\|_{H^1(\Omega^-)} \leq C \left(\|g_1\|_{H^{1/2}(\Gamma)} + \|g_2\|_{H^{-1/2}(\Gamma)} \right).$$

Proof. Lemma 3.7 shows that the block operator is injective. Proposition 3.3 shows coercivity of the first-kind single-trace operator. Layer potentials are bounded operators and $\tilde{a}I - \mathcal{A}$ satisfies an inf-sup condition up to a compact operator, according to Proposition 3.4. Therefore, Assumption A.1 holds and the result follows from Proposition A.2, see Appendix A. \square

4 Galerkin Discretization

4.1 Finite Element and Boundary Element Spaces

Let $\{\mathcal{T}_h\}_{h>0}$ be a globally quasi-uniform and shape-regular family of triangular meshes of Ω^- . Let $\{\Sigma_h\}_{h>0}$ be the induced family of meshes of Γ . We choose finite element spaces $V_h := V_h(\mathcal{T}_h) \subset H^1(\Omega^-)$ of piecewise linear functions on \mathcal{T}_h . We also use the same finite dimensional space V_h as a conforming subspace of $\tilde{H}^{-1}(\Omega^-)$. We consider boundary element spaces $U_h := U_h(\Sigma_h) \subset H^{1/2}(\Gamma)$ of piecewise linear functions. For the first-kind formulation we will use $W_h := W_h(\Sigma_h) \subset H^{-1/2}(\Gamma)$ of piecewise constant functions, while the second-kind formulation requires $U_h \subset H^{-1/2}(\Gamma)$.

4.2 Asymptotic Quasi-Optimality

The first result needed is a discrete version of Lemma 3.4.

Proposition 4.1 (Discrete inf-sup condition for d). *There exists $\tilde{c}_d > 0$ such that*

$$\tilde{c}_d \leq \inf_{u_h \in V_h} \sup_{v_h \in V_h} \frac{\langle v_h, \tilde{a}u_h \rangle_{\Omega^-}}{\|u_h\|_{H^1(\Omega^-)} \|v_h\|_{\tilde{H}^{-1}(\Omega^-)}}.$$

Proof. We start by denoting as $\langle \cdot, \cdot \rangle_{\tilde{a}}$ the weighted L^2 inner product and by $\|\cdot\|_{\tilde{a}}$ the induced weighted L^2 -norm. This norm is equivalent to $\|\cdot\|_{L^2(\Omega^-)}$, due to $\tilde{a} \in W^{1,\infty}(\Omega^-)$ being bounded below by a positive constant. Moreover,

$$c_{\min} \|w\|_{H^1(\Omega^-)} \leq \|\tilde{a}w\|_{H^1(\Omega^-)} \leq c_{\max} \|w\|_{H^1(\Omega^-)} \quad \text{for all } w \in H^1(\Omega^-),$$

because $\tilde{a} \in W^{1,\infty}(\Omega^-)$ and $\frac{1}{\tilde{a}} \in W^{1,\infty}(\Omega^-)$. We know ([17, Section 2.1]) that there exists an L^2 -orthogonal projection operator $Q_h : H^1(\Omega^-) \rightarrow V_h \subset H^1(\Omega^-)$ such that

$$\langle Q_h u, w_h \rangle_{\Omega^-} = \langle u, w_h \rangle_{\Omega^-}, \quad \text{for all } w_h \in V_h,$$

with

$$\|Q_h u\|_{H^1(\Omega^-)} \leq c_S \|u\|_{H^1(\Omega^-)}, \quad \text{for all } u \in H^1(\Omega^-), \quad (68)$$

$$\|u - Q_h u\|_{L^2(\Omega^-)} \leq c_1 h |u|_{H^1(\Omega^-)}, \quad (69)$$

where c_S, c_1 depend only on the shape-regularity and quasi-uniformity measure of \mathcal{T}_h , but not on the parameter h . Similarly, we can define $Q_h^{\tilde{a}} : H^1(\Omega^-) \rightarrow V_h$ as

$$\langle Q_h^{\tilde{a}} u, w_h \rangle_{\tilde{a}} = \langle u, w_h \rangle_{\tilde{a}}, \quad \text{for all } w_h \in V_h.$$

First, we show that $Q_h^{\tilde{a}}$ also satisfies properties similar to (68) and (69). Note that

$$\begin{aligned} \|u - Q_h^{\tilde{a}} u\|_{\tilde{a}} &\leq \|u - Q_h u + (Q_h u - Q_h^{\tilde{a}} u)\|_{\tilde{a}} \\ &\leq \|u - Q_h u\|_{\tilde{a}} + \|(Q_h u - Q_h^{\tilde{a}} u)\|_{\tilde{a}} \\ &\leq \|u - Q_h u\|_{\tilde{a}} + \|Q_h^{\tilde{a}}(Q_h u - u)\|_{\tilde{a}} \\ &\leq 2 \|u - Q_h u\|_{\tilde{a}} \leq 2\tilde{a}_{\max} \|u - Q_h u\|_{L^2(\Omega^-)} \leq \tilde{c}_1 h |u|_{H^1(\Omega^-)}, \end{aligned}$$

for all $u \in H^1(\Omega^-)$, with $\tilde{c}_1 > 0$. Now, we can show that with $\tilde{c}_S > 0$

$$\begin{aligned} \|Q_h^{\tilde{a}} u\|_{H^1(\Omega^-)} &\leq \|Q_h u + (Q_h^{\tilde{a}} u - Q_h u)\|_{H^1(\Omega^-)} \\ &\leq \|Q_h u\|_{H^1(\Omega^-)} + \|(Q_h^{\tilde{a}} u - Q_h u)\|_{H^1(\Omega^-)} \\ &\leq \|Q_h u\|_{H^1(\Omega^-)} + \|Q_h(Q_h^{\tilde{a}} u - u)\|_{H^1(\Omega^-)} \\ &\leq c_S \|u\|_{H^1(\Omega^-)} + c_G h^{-1} \|Q_h(Q_h^{\tilde{a}} u - u)\|_{L^2(\Omega^-)} \\ &\leq c_S \|u\|_{H^1(\Omega^-)} + c_G h^{-1} \|Q_h^{\tilde{a}} u - u\|_{L^2(\Omega^-)} \leq \tilde{c}_S \|u\|_{H^1(\Omega^-)}, \end{aligned}$$

appealing to global quasi-uniformity of the mesh for the inverse inequality. We proceed to show the main result. Using the adjoint projection operator $(Q_h^{\tilde{a}})^* : \tilde{H}^{-1}(\Omega^-) \rightarrow V_h$, and definition of the dual norm:

$$\begin{aligned} c_{\min} \|u_h\|_{H^1(\Omega^-)} &\leq \|\tilde{a} u_h\|_{H^1(\Omega^-)} = \sup_{v \in \tilde{H}^{-1}(\Omega^-)} \frac{\langle v, \tilde{a} u_h \rangle_{\Omega^-}}{\|v\|_{\tilde{H}^{-1}(\Omega^-)}} = \sup_{v \in \tilde{H}^{-1}(\Omega^-)} \frac{\langle v, u_h \rangle_{\tilde{a}}}{\|v\|_{\tilde{H}^{-1}(\Omega^-)}} \\ &= \sup_{v \in \tilde{H}^{-1}(\Omega^-)} \frac{\langle (Q_h^{\tilde{a}})^* v + (v - (Q_h^{\tilde{a}})^* v), u_h \rangle_{\tilde{a}}}{\|v\|_{\tilde{H}^{-1}(\Omega^-)}} = \sup_{v \in \tilde{H}^{-1}(\Omega^-)} \frac{\langle (Q_h^{\tilde{a}})^* v, u_h \rangle_{\tilde{a}}}{\|v\|_{\tilde{H}^{-1}(\Omega^-)}} \\ &\leq \tilde{c}_S \sup_{v \in \tilde{H}^{-1}(\Omega^-)} \frac{\langle (Q_h^{\tilde{a}})^* v, u_h \rangle_{\tilde{a}}}{\|(Q_h^{\tilde{a}})^* v\|_{\tilde{H}^{-1}(\Omega^-)}} \leq \tilde{c}_S \sup_{v_h \in V_h} \frac{\langle v_h, u_h \rangle_{\tilde{a}}}{\|v_h\|_{\tilde{H}^{-1}(\Omega^-)}} \end{aligned}$$

which completes the proof with $\tilde{c}_d := \frac{c_{\min}}{\tilde{c}_S}$.

□

Now, we are able to establish the main result on the Galerkin discretization of Problem 3.1.

Theorem 4.2. *Provided that Assumption 3.7 holds, there is $h_0 > 0$ and a constant $c_{qo} > 0$ independent of h such that there exists a unique Galerkin solution $(\varphi_h, u_h) \in (U_h \times W_h) \times V_h$ of Problem 3.1 for all $h < h_0$. The solution satisfies*

$$\|(\varphi - \varphi_h, u - u_h)\| \leq c_{qo} \inf_{\substack{\lambda_h \in U_h \times W_h, \\ w_h \in V_h}} \|(\varphi - \lambda_h, u - w_h)\|.$$

Similarly, there is \tilde{h}_0 and $\tilde{c}_{qo} > 0$ independent of h such that there exists a unique Galerkin solution $(\tilde{\varphi}_h, \tilde{u}_h) \in (U_h \times U_h) \times V_h$ of Problem 3.2 for all $h < \tilde{h}_0$. The solution satisfies

$$\|(\varphi - \tilde{\varphi}_h, u - \tilde{u}_h)\| \leq c_{qo} \inf_{\substack{\lambda_h \in U_h \times U_h, \\ w_h \in V_h}} \|(\varphi - \lambda_h, u - w_h)\|.$$

Proof. We need to show that our system satisfies Assumption A.1. By Assumption 3.7 we have injectivity. By Propositions 3.3, 3.4, and 4.1 we can comply with the inf-sup condition for the principal part given in Proposition A.3. Then, by Proposition A.4 we obtain the result. \square

If the solution (φ, ψ, u) of Problem (3.1) enjoys some extra regularity, we can use best approximation estimates for finite elements and boundary elements [15, Section 4] to predict convergence rates for the Galerkin discretization. Let $k \in \mathbb{N}$ be the polynomial degree of approximation in the finite/boundary element spaces, then

$$\begin{aligned} \inf_{\eta_h \in U_h} \|\varphi_h - \eta_h\|_{H^{1/2}(\Gamma)} &\leq c_1^{\text{ba}} h^{\min\{s-\frac{1}{2}, k\}} \|\varphi\|_{H^s(\Gamma)}, \quad \forall \varphi \in H^s(\Gamma), \\ \inf_{\tau_h \in W_h} \|\psi_h - \tau_h\|_{H^{-1/2}(\Gamma)} &\leq c_2^{\text{ba}} h^{\min\{s+\frac{1}{2}, k\}} \|\psi\|_{H^s(\Gamma)}, \quad \forall \psi \in H^s(\Gamma), \\ \inf_{w_h \in V_h} \|u_h - w_h\|_{H^1(\Omega^-)} &\leq c_3^{\text{ba}} h^{\min\{s-1, k\}} \|u\|_{H^s(\Omega^-)}, \quad \forall u \in H^s(\Omega). \end{aligned}$$

5 Numerical Experiments in 2D

In this section we will show numerical experiments for different cases. The parameters a_1, κ_1 will be chosen as

$$a_1 = a_\Gamma := \int_{\Gamma} a(\mathbf{x}) ds_x, \quad \kappa_1 = \kappa_\Gamma := \int_{\Gamma} \kappa(\mathbf{x}) ds_x. \quad (70)$$

This particular choice reduces problems with constant coefficients to boundary integral equation formulations. Moreover, it reduces to a minimum the support of functions α, β in our examples.

We refer to multiple formulations in our experiments¹. In particular, the Lippman-Schwinger equation [11] is denoted as **LS**; Costabel’s coupled formulation [7] is denoted as **CVIE**; Johnson-Nedelec FEM-BEM coupling [10, 16] is denoted as **FEM-BEM**; Problem 3.1 is denoted as **STF-VIE**, while Problem 3.2 is denoted as **2STF-VIE**.

5.1 Case $\alpha \equiv 0$: Constant Coefficient a in Ω^-

We are interested to solve the transmission problem (5) with $a(\mathbf{x}) \equiv 1$ for all $\mathbf{x} \in \mathbb{R}^2$. The incident field u^{inc} is given by

$$u^{\text{inc}}(\mathbf{x}) := \exp(i\kappa_0 \mathbf{x} \cdot \mathbf{d}), \quad \mathbf{d} := (\cos(\theta), \sin(\theta)), \quad \theta \in [-\pi, \pi].$$

5.1.1 Validation: Artificial Domain

We consider a domain $\Omega^- \subset \mathbb{R}^2$ consisting of a: (a) unit disk centered at the origin; (b) square of length 2 centered at the origin. The wavenumber $\kappa = 4$ is the same for both interior and exterior domains. The solution for the interior field corresponds to $u(\mathbf{x}) = u^{\text{inc}}(\mathbf{x})$.

Figure 1 shows convergence results. We observe expected convergence rates for the Galerkin discretization.

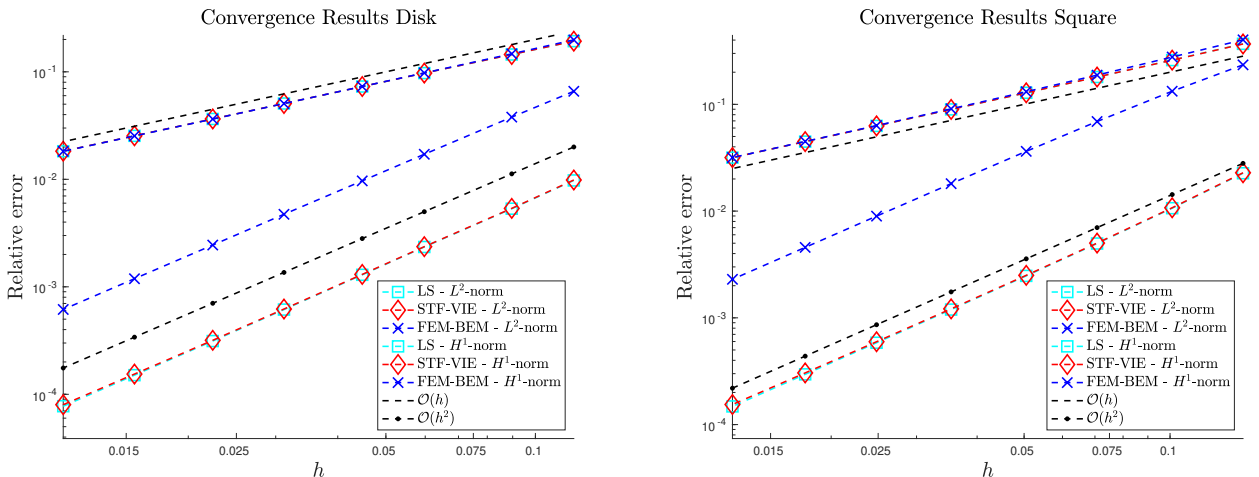


Figure 1: Plots of error norms vs. meshwidth h : plane-wave solution. (a) Unit disk; (b) Square $[-1, 1] \times [-1, 1]$.

¹Finite element and boundary element implementation were done based on GYPSILAB [2]. Regularization for volume integral operators was implemented using semi-analytic formulas. The MATLAB code is available in the Github repository www.github.com/ilabarca/stf-vie

5.1.2 Scattering at a Unit Disk

This section considers a problem in a domain $\Omega^- \subset \mathbb{R}^2$ consisting of a unit disk centered at the origin. The smoothly spatially varying wavenumber is defined as

$$\kappa(\mathbf{x}) := \begin{cases} 4, & \mathbf{x} \notin \Omega^-, \\ 8 + 2\eta(s|\mathbf{x}|), & \mathbf{x} \in \Omega^-, \end{cases}$$

where $s = 1.5$ and

$$\eta(t) := \begin{cases} \exp\left(-\frac{t^2}{1-t^2}\right), & |t| < 1 \\ 0, & |t| > 1. \end{cases}$$

We solve Problem 3.1 and measure errors in the $H^1(\Omega^-)$ norm using the numerical solution on a mesh obtained by one additional refinement step as reference. The results are shown in Figure 2. We observe expected convergence rates for the Galerkin discretization.

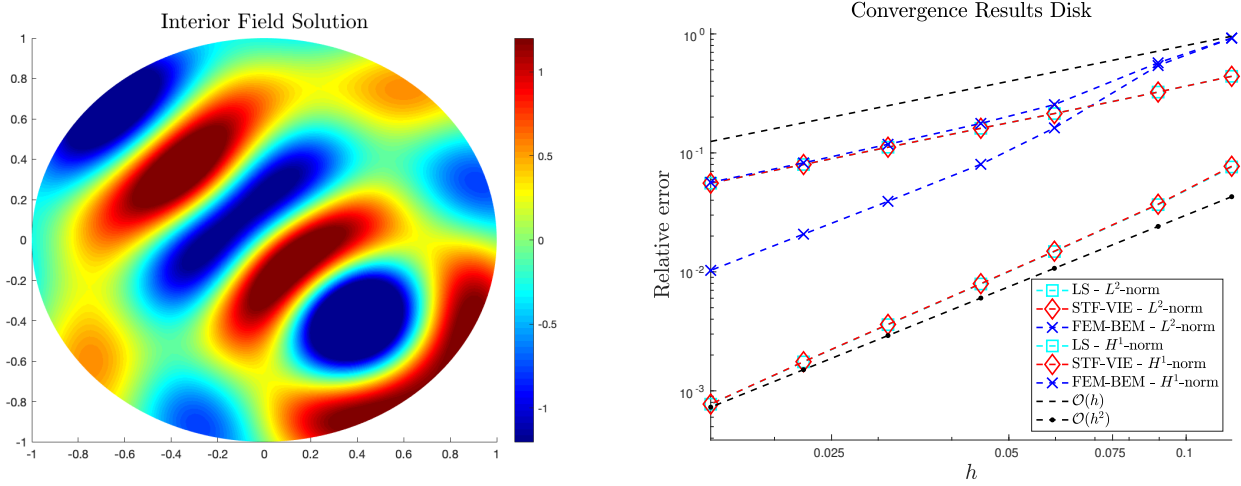


Figure 2: Scattering at a disk: problem in Section 5.1.2. Real part of the interior field solution and plot of error norms vs meshwidth.

5.1.3 Scattering at a Square (Case $\alpha|_{\Gamma} \equiv 0$)

The wavenumber is defined as

$$\kappa(\mathbf{x}) := \begin{cases} 2, & \mathbf{x} \notin \Omega^-, \\ 4 + 2\eta(s|\mathbf{x}|), & \mathbf{x} \in \Omega^-, \end{cases}$$

where $s = 1.5$ and

$$a(\mathbf{x}) := \begin{cases} 1, & \mathbf{x} \notin \Omega^-, \\ 2 + \frac{1}{2}\eta(x)\eta(y), & \mathbf{x} \in \Omega^-. \end{cases}$$

Note that for this experiment $a(\mathbf{x}) \equiv a_\Gamma > 0$ for all $\mathbf{x} \in \Gamma$. The results are shown in Figure 3. We observe the expected convergence rates.

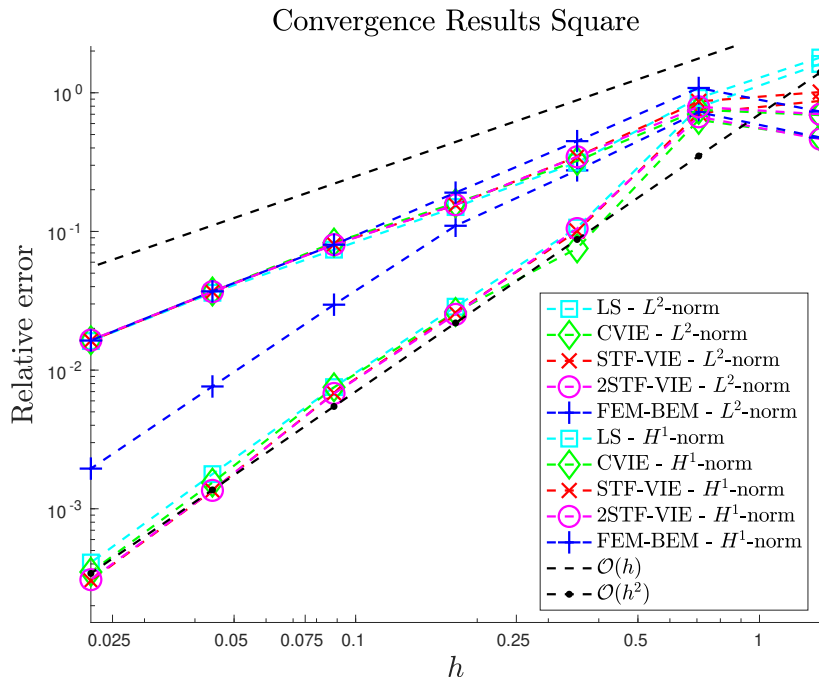


Figure 3: Scattering at a square: problem of Section 5.1.3. Error norms as functions of h .

5.1.4 Scattering at a Square (Case $\alpha|_\Gamma \neq 0$)

The wavenumber is defined as

$$\kappa(\mathbf{x}) := \begin{cases} 2, & \mathbf{x} \notin \Omega^-, \\ 4 - 2\eta(x)\eta(y), & \mathbf{x} \in \Omega^-, \end{cases}$$

and

$$a(\mathbf{x}) := \begin{cases} 1, & \mathbf{x} \notin \Omega^-, \\ 1 - \frac{1}{4}(x^2 + y^2), & \mathbf{x} \in \Omega^-. \end{cases}$$

Note that for this experiment $\alpha|_\Gamma \neq 0$. The results are shown in Figure 4. We observe that expected convergence rates are obtained after a preasymptotic regime.

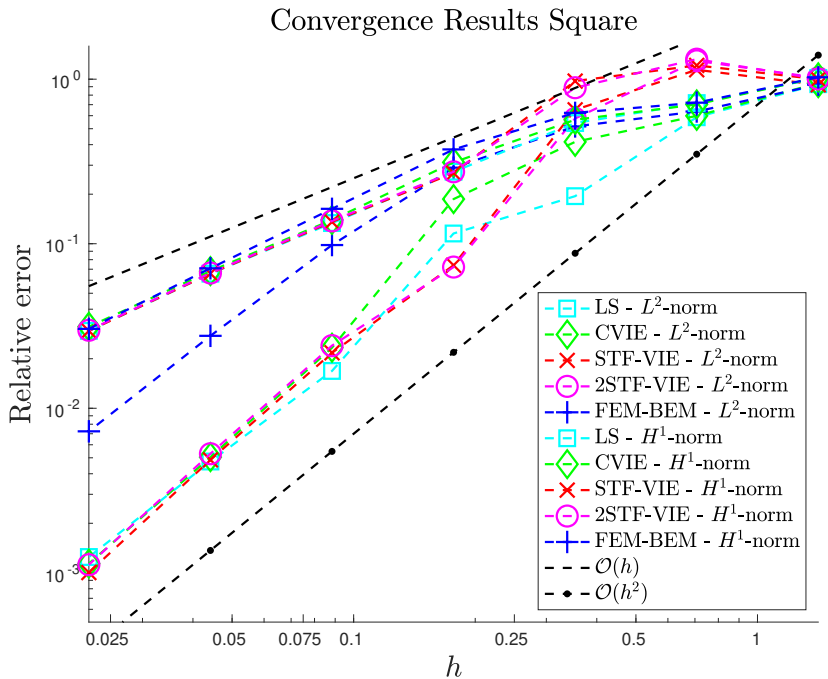


Figure 4: Scattering at a square: problem of Section 5.1.4. Error norms as functions of h .

6 Conclusion

We derived new coupled VIE-BIE formulations for the acoustic transmission problem in frequency domain, relying on new representation formulas and volume integral operators. In particular, first and second-kind single-trace formulations are coupled with a volume integral operator, similar to the ones studied in the Lippmann-Schwinger equation. Well-posedness of the continuous and discrete problem is established for the first-kind STF-VIE, provided that an assumption on uniqueness of solutions of a special transmission problem holds. Verifying this assumption remains as an open problem.

Galerkin discretizations of the formulation was studied, with a result on the quasi-optimality of solutions. Numerical experiments in two dimensions demonstrate that the theoretical predictions are sharp. Convergence rates are obtained according to our theoretical results.

Future work has to address the efficiency of the proposed method. Compression and acceleration techniques become even more important when the volume integral operators are involved, especially for 3D problems. Spectral methods for volume integrals are also worth considering.

Extending the methodology to electromagnetic scattering is work in progress. Although the idea seems straightforward to apply, there are particular challenges related to the theory of boundary integral equations for electromagnetic problems.

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A Block Operators

A.1 Fredholm Equation

Let X, Π be Hilbert spaces and X', Π' their duals. Consider the operators

$$\begin{aligned} A : X &\rightarrow X', & B : \Pi &\rightarrow X', \\ C : X &\rightarrow \Pi', & D : \Pi &\rightarrow \Pi'. \end{aligned}$$

All of them linear bounded operators. We study the system

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}. \tag{71}$$

Assumption A.1. *The operator*

$$\mathbf{T} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} : X \times \Pi \rightarrow X' \times \Pi'$$

is injective. Moreover, A and D are coercive operators. B is a compact operator.

Proposition A.2. *Under assumption A.1, there exists a unique solution $(u^*, p^*) \in X \times \Pi$ to the system in (71). Moreover, the solution satisfies*

$$\|u^*\|_X + \|p^*\|_\Pi \leq C \|f\|_{X'}.$$

Proof. This is a consequence of A and D being coercive, B being compact and the Fredholm Alternative. We know there exist compact operators

$$T_A : X \rightarrow X', \quad T_D : \Pi \rightarrow \Pi',$$

such that $A = A_0 + T_A$, $D = D_0 + T_D$, with A_0 and D_0 elliptic operators. We can write (71) as

$$\begin{pmatrix} A_0 & 0 \\ C & D_0 \end{pmatrix} + \begin{pmatrix} T_A & B \\ 0 & T_D \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

We denote

$$\mathbf{A} := \begin{pmatrix} A_0 & 0 \\ C & D_0 \end{pmatrix}, \quad \mathbf{K} := \begin{pmatrix} T_A & B \\ 0 & T_D \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

Then, \mathbf{A} has a bounded inverse, \mathbf{K} is a compact operator and $\mathbf{T} = \mathbf{A} + \mathbf{K}$ is injective. By the Fredholm Alternative we know that

$$(\mathbf{A} + \mathbf{K})\mathbf{u} = \mathbf{f},$$

has a unique solution $\mathbf{u}^* = (u^*, p^*) \in X \times \Pi$ with

$$\|u^*\|_X + \|p^*\|_\Pi \leq c \|f\|_{X'}.$$

□

A.2 Galerkin Discretization

Next, we consider the Galerkin discretization of (71). Choose finite dimensional subspaces $X_h \subset X$ and $\Pi_h \subset \Pi$. We study the following variational problem: find $(u_h, p_h) \in X_h \times \Pi_h$ such that

$$\begin{aligned} \langle Au_h, v_h \rangle_X + \langle Bp_h, v_h \rangle_X &= \langle f, v_h \rangle, & \text{for all } v_h \in X_h, \\ \langle Cu_h, q_h \rangle_\Pi + \langle Dp_h, q_h \rangle_\Pi &= 0, & \text{for all } q_h \in \Pi_h, \end{aligned}$$

which can be rewritten as

$$\mathfrak{t}((u_h, p_h), (v_h, q_h)) = \langle f, v_h \rangle, \quad \text{for all } v_h \in X_h, q_h \in \Pi_h, \quad (72)$$

where

$$\mathfrak{t}((u_h, p_h), (v_h, q_h)) = \langle Au_h, v_h \rangle_X + \langle Bp_h, v_h \rangle_X + \langle Cu_h, q_h \rangle_\Pi + \langle Dp_h, q_h \rangle_\Pi. \quad (73)$$

Proposition A.3 (inf-sup condition). *The bilinear form $\mathfrak{t}_0 : (X \times \Pi) \times (X \times \Pi) \rightarrow \mathbb{C}$ given by*

$$\mathfrak{t}_0((u, p), (v, q)) = \langle A_0 u, v \rangle_X + \langle C u, q \rangle_\Pi + \langle D_0 p, q \rangle_\Pi$$

satisfies the discrete inf-sup condition

$$c_1^{\mathfrak{t}_0} \leq \inf_{(u_h, p_h) \in X_h \times \Pi_h} \sup_{(v_h, q_h) \in X_h \times \Pi_h} \frac{\Re\{\mathfrak{t}_0((u_h, p_h), (v_h, q_h))\}}{\|(u_h, p_h)\|_{X \times \Pi} \|(v_h, q_h)\|_{X \times \Pi}} \quad (74)$$

Proof. For any arbitrary $(u_h, p_h) \in X_h \times \Pi_h$, we write

$$\sup_{(v_h, q_h) \in X_h \times \Pi_h} \frac{\Re\{\mathfrak{t}_0((u_h, p_h), (v_h, q_h))\}}{\|(v_h, q_h)\|_{X \times \Pi}} \geq \frac{\Re\{\mathfrak{t}_0((u_h, p_h), (v_h^*, q_h^*))\}}{\|(v_h^*, q_h^*)\|_{X \times \Pi}} \quad (75)$$

for some $(v_h^*, q_h^*) \in X_h \times \Pi_h$. We choose conveniently

$$\begin{pmatrix} v_h^* \\ q_h^* \end{pmatrix} = \begin{pmatrix} u_h + w_h \\ p_h \end{pmatrix} \quad (76)$$

where $w_h \in X_h$ satisfies the variational problem:

$$\langle A_0 w_h', w_h \rangle_X = -\langle C w_h', p_h \rangle \quad \text{for all } w_h' \in X_h, \quad (77)$$

which is well-posed by the Lax-Milgram lemma:

$$\|w_h\|_X \leq \frac{c_2^C}{c_1^{A_0}} \|p_h\|_\Pi, \quad (78)$$

where $c_2^C > 0$ is the continuity constant of the operator C , and $c_1^{A_0}$ is the ellipticity constant of A_0 . Using (78) we also know that

$$\|(v_h^*, q_h^*)\| \leq \left(1 + \frac{c_2^C}{c_1^{A_0}}\right) \|(u_h, p_h)\|_{X \times \Pi}. \quad (79)$$

Now, we compute

$$\begin{aligned}
\mathbf{t}_0((u_h, p_h), (v_h^*, q_h^*)) &= \left\langle \mathbf{A} \begin{pmatrix} u_h \\ p_h \end{pmatrix}, \begin{pmatrix} u_h + w_h \\ p_h \end{pmatrix} \right\rangle \\
&= \langle A_0 u_h, u_h + w_h \rangle_X + \langle C u_h, p_h \rangle_\Pi + \langle D_0 p_h, p_h \rangle_\Pi \\
&= \langle A_0 u_h, u_h \rangle_X + \langle A_0 u_h, w_h \rangle_X + \langle C u_h, p_h \rangle_\Pi + \langle D_0 p_h, p_h \rangle_\Pi \\
&= \langle A_0 u_h, u_h \rangle_X - \langle C u_h, p_h \rangle_\Pi + \langle C u_h, p_h \rangle_\Pi + \langle D_0 p_h, p_h \rangle_\Pi \\
&= \langle A_0 u_h, u_h \rangle_X + \langle D_0 p_h, p_h \rangle_\Pi.
\end{aligned}$$

Therefore, by the ellipticity of A_0 and D_0 we obtain

$$\Re\{\mathbf{t}_0((u_h, p_h), (v_h^*, q_h^*))\} \geq \min(c_1^{A_0}, c_1^{D_0}) \|(u_h, p_h)\|_{X \times \Pi}^2. \quad (80)$$

We conclude by combining (79) and (80) into (75) and taking the infimum over $(u_h, p_h) \in X_h \times \Pi_h$. \square

Proposition A.4 (Asymptotic quasi-optimality). *Provided that Assumption A.1 holds, there is $h_0 > 0$ and a constant $c_{\text{qo}} > 0$ independent of h such that there exists a unique Galerkin solution $(u_h, p_h) \in X_h \times \Pi_h$ of (72) for all $h < h_0$. The solution satisfies*

$$\|(u, p) - (u_h, p_h)\|_{X \times \Pi} \leq c_{\text{qo}} \inf_{(\eta_h, \tau_h) \in X_h \times \Pi_h} \|(u, p) - (\eta_h, \tau_h)\|_{X \times \Pi}. \quad (81)$$

Proof. The result follows from Proposition A.3 and $\mathbf{t} = \mathbf{t}_0 + \mathbf{t}_{\mathbf{K}}$, with $\mathbf{t}_{\mathbf{K}}$ being the bilinear form associated to the compact operator \mathbf{K} . \square

B Neumann Trace of Volume Integral Operators

In this section we show how to compute the duality pairing

$$\mathbf{b}_N(u, \eta) = \langle \partial_n \operatorname{div} \widetilde{N}_1(u \nabla \alpha), \eta \rangle, \quad u \in H^1(\Omega^-), \eta \in H^{1/2}(\Gamma). \quad (82)$$

This is important for the variational formulations presented in Problem 3.1 and Problem 3.2. Let us denote $\underline{w} := \widetilde{N}_1(u \nabla \alpha)$. This is a solution of

$$-\Delta \underline{w} - \frac{\kappa_1^2}{a_1} \underline{w} = u \nabla \alpha,$$

which can be rewritten as

$$\operatorname{curl}^2 \underline{w} - \nabla \operatorname{div} \underline{w} - \frac{\kappa_1^2}{a_1} \underline{w} = u \nabla \alpha. \quad (83)$$

By using (83), we obtain

$$\nabla \operatorname{div} \widetilde{N}_1(u \nabla \alpha) = \operatorname{curl}^2 \underline{w} - \frac{\kappa_1^2}{a_1} \underline{w} - u \nabla \alpha.$$

Therefore, we have the following expression for (82)

$$\begin{aligned} \mathbf{b}_N(u, \eta) &= \langle \mathbf{n} \cdot \{ \operatorname{curl}^2 \underline{w} - \frac{\kappa_1^2}{a_1} \underline{w} - u \nabla \alpha \} |_{\Gamma}, \eta \rangle \\ &= \langle \gamma_{\mathbf{n}} \operatorname{curl}^2 \underline{w}, \eta \rangle - \frac{\kappa_1^2}{a_1} \langle \gamma_{\mathbf{n}} \underline{w}, \eta \rangle - \langle (\mathbf{n} \cdot \nabla \tilde{a}) \gamma^- u, \eta \rangle \\ &= \langle \operatorname{div}_{\Gamma} \{ \gamma_t \operatorname{curl} \underline{w} \}, \eta \rangle - \frac{\kappa_1^2}{a_1} \langle \gamma_{\mathbf{n}} \underline{w}, \eta \rangle - \langle (\mathbf{n} \cdot \nabla \tilde{a}) \gamma^- u, \eta \rangle \\ &= \langle \gamma_t \operatorname{curl} \underline{w}, \nabla_{\Gamma} \eta \rangle - \frac{\kappa_1^2}{a_1} \langle \gamma_{\mathbf{n}} \underline{w}, \eta \rangle - \langle (\mathbf{n} \cdot \nabla \tilde{a}) \gamma^- u, \eta \rangle, \end{aligned} \tag{84}$$

which contains only weakly singular kernels. Note that the last term in the right hand side of (84) cancels with the operator T_{Γ} in (37).