

Domain derivative and shape reconstruction for an inverse backscattering problem for the wave equation

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Abstract

We consider an inverse backscattering problem for time-dependent acoustic waves with a compactly supported penetrable scattering obstacle in unbounded three-dimensional free space. Assuming that dynamic backscattering far field data of scattered waves corresponding to a few time-dependent incident plane waves are available, the goal is to reconstruct the shape of the scattering obstacle. We establish Fréchet differentiability of the time-dependent far field pattern with respect to the shape of the scattering obstacle and give a characterization of the associated temporal domain derivative in terms of its Laplace transform. This characterization is then utilized in an efficient implementation of a regularized Gauß-Newton method for the inverse backscattering problem using convolution quadrature and a boundary element method. Numerical examples demonstrate potentials and limitations of the algorithm.

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1 Introduction

While numerical reconstruction algorithms for inverse obstacle scattering problems for time-harmonic acoustic waves have already been thoroughly investigated (see, e.g., [11]), corresponding algorithms for time-dependent scattering data received somewhat less attention so far. However, in practice it is actually very natural to consider time-dependent incident waves and to use remote observations of the associated scattered waves over some finite time interval for reconstruction. In particular dynamic backscattering data can be measured efficiently using just one source and one receiver at the same observation point. Moving this source-receiver combination to different observation points around the obstacle, such backscattering data sets can be obtained for different incident/observation directions. The goal of this work is to establish an efficient numerical reconstruction scheme for such a dynamic backscattering setup.

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We will consider an idealized setting, where a causal incident plane wave interacts with a compactly supported penetrable scattering obstacle that is characterized by its constant wave speed and constant density, both of which may differ from the corresponding parameters of the surrounding unbounded three-dimensional free space. To model remote observations of the scattered wave in the backscattering direction, we assume that the time-dependent far field pattern of the scattered wave is given in the direction opposite to the direction of propagation of the corresponding incident plane wave for some finite time interval. Moreover, we suppose that such a one-dimensional backscattering data set is available for a few incident plane waves with different incident directions around the obstacle.

Since the reconstruction method proposed in this work builds heavily on ideas from the time-harmonic setting, we briefly review the corresponding inverse obstacle scattering problem in the time-harmonic regime to place our results in context. Basically two main classes of reconstruction methods for inverse obstacle scattering problems have emerged over the years. The first class are iterative regularization methods that reformulate the inverse obstacle scattering problem as a nonlinear shape optimization problem and then iteratively update the domain of the unknown scatterer to arrive at a solution. These updates are usually determined using the domain derivative associated to the direct scattering problem (see, e.g., [12, 13, 17, 26, 27, 28, 32, 40]), which requires solving the direct scattering problem at each step of the iteration. We refer, e.g., to [15, 16, 23, 24, 25, 31, 41] for some more recent contributions on iterative reconstruction schemes for time-harmonic waves. An iterative scheme for the inverse backscattering problem has been considered in [36]. The second class of methods are qualitative reconstruction schemes, which are non-iterative and avoid solving direct scattering problems. Those usually require less a priori information on the unknown scattering obstacle but on the other hand use much larger data sets than iterative reconstruction schemes (see, e.g., [6, 7, 33]). Since they typically rely on some sort of sampling strategy for reconstruction, no parametrization of the unknown scatterer is required.

In recent years several qualitative reconstruction methods have been transferred from the frequency domain to the time domain. For instance linear sampling methods have been proposed in [9, 10, 21], factorization methods have been considered in [8, 22], and the enclosure method has been extended in various directions in [29, 30]. In this work we instead consider iterative regularization and develop an efficient reconstruction method that is based on temporal domain derivatives. We generalize a corresponding analysis and an algorithm from [35], where a two-dimensional inverse obstacle scattering problem with a sound-soft obstacle and time-dependent near field scattering data corresponding to a single incident plane wave has been considered. The main novelties compared to [35] are that we consider a three-dimensional instead of a two-dimensional scattering problem, far field backscattering data instead of near field data corresponding to a single incident wave, and a penetrable instead of an impenetrable scattering obstacle. We develop a rigorous characterization of the temporal domain derivative for the associated direct scattering problem in terms of its Laplace transform. To this end, we integrate the variational analysis of transient scattering problems via the Laplace transform, as introduced in [1], with a generalization of the Fréchet differentiability and shape derivative results of [26, 32] to complex frequencies. The time-domain derivative is subsequently incorporated into an iterative Gauss–Newton-type reconstruction algorithm, enabling an efficient implementation based on convolution quadrature and boundary element methods [3, 37]. We note that [14, 43, 44, 45] also consider an iterative reconstruction method for a time-dependent inverse scattering problem. In contrast to our approach, these works first apply a convolution quadrature discretization in time and then perform the shape reconstruction sequentially at dis-

crete Laplace domain frequencies, thereby avoiding an analysis in the time domain.

The outline of this paper is as follows. In Section 2 we introduce the transient acoustic scattering problem that we are going to consider throughout this article and we introduce the corresponding far field expansion of the time-dependent scattered wave. We analyze the direct scattering problem first in the Laplace domain in Section 3 and derive bounds on the domain derivative that are explicit in the Laplace parameter in Section 4. These results are transferred from the Laplace domain to the time domain using a Paley-Wiener argument in Section 5, and Section 6 is devoted to the numerical solution of the inverse backscattering problem. We present numerical results. In the appendix we collect some technical estimates that are used throughout the article.

2 Problem setting

We consider scattering of a time-dependent acoustic incident plane wave

$$u^i(x, t; \theta) := f^i(t - \theta \cdot x), \quad (x, t) \in \mathbb{R}^3 \times \mathbb{R}, \quad (2.1)$$

with direction of propagation $\theta \in S^2$ and for some compactly supported $f^i \in H_c^r(\mathbb{R})$, $r \geq 2$, by a penetrable obstacle supported in a bounded C^2 -domain $D \subseteq \mathbb{R}^3$. We suppose that the wave speed c and the density ρ of the medium are given by the piecewise constant functions

$$c(x) := \begin{cases} c_0, & x \in D, \\ 1, & x \in \mathbb{R}^3 \setminus \overline{D}, \end{cases} \quad \text{and} \quad \rho(x) := \begin{cases} \rho_0, & x \in D, \\ 1, & x \in \mathbb{R}^3 \setminus \overline{D}, \end{cases}$$

where $c_0, \rho_0 > 0$ are the material parameters inside the scatterer. Throughout we denote by $B_R(0)$ a sufficiently large ball around the origin containing D in its interior. The incident wave satisfies

$$\partial_t^2 u^i - \Delta u^i = 0 \quad \text{in } \mathbb{R}^3 \times \mathbb{R}, \quad (2.2a)$$

and assuming that u^i satisfies the causality condition¹

$$u^i = \partial_t u^i = 0, \quad \text{in } B_R(0) \times (-\infty, 0), \quad (2.2b)$$

the scattering problem reads

$$\frac{1}{\rho c^2} \partial_t^2 u - \operatorname{div} \left(\frac{1}{\rho} \nabla u \right) = 0 \quad \text{in } \mathbb{R}^3 \times (0, \infty), \quad (2.3a)$$

$$u(\cdot, 0) = u^i(\cdot, 0), \quad \partial_t u(\cdot, 0) = \partial_t u^i(\cdot, 0) \quad \text{in } \mathbb{R}^3. \quad (2.3b)$$

As usual we call u the total wave, and the scattered wave u^s is defined as

$$u^s(x, t) := u(x, t) - u^i(x, t), \quad (x, t) \in \mathbb{R}^3 \times (0, \infty).$$

Accordingly,

$$\frac{1}{\rho c^2} \partial_t^2 u^s - \operatorname{div} \left(\frac{1}{\rho} \nabla u^s \right) = \left(1 - \frac{1}{\rho c^2} \right) \partial_t^2 u^i - \operatorname{div} \left(\left(1 - \frac{1}{\rho} \right) \nabla u^i \right) \quad \text{in } \mathbb{R}^3 \times (0, \infty), \quad (2.4a)$$

¹In particular this means that $f^i(t) = 0$ for all $t \in (-\infty, R)$.

and we note that (2.2b) implies that u^s is causal, i.e.,

$$u^s(\cdot, 0) = \partial_t u^s(\cdot, 0) = 0 \quad \text{in } \mathbb{R}^3. \quad (2.4b)$$

Our regularity assumptions on f^i imply that $u^i|_{B_R(0)} \in L^2(\mathbb{R}, H^2(B_R(0))) \cap H^1(\mathbb{R}, H^1(B_R(0)))$, and $u^i|_{B_R(0)}$ is compactly supported with respect to time. In particular, the right hand side of (2.4a) belongs to $L^2(\mathbb{R}; L^2(B_R(0)))$. It is well-known (as, e.g., outlined in [34]) that the scattering problem (2.4) possesses a unique weak solution $u^s \in C([0, \infty), H^1(\mathbb{R}^3)) \cap C^1([0, \infty), L^2(\mathbb{R}^3))$ satisfying

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^3} \left(\frac{1}{\rho} \nabla u^s(t) \cdot \nabla \phi(t) - \frac{1}{\rho c^2} \partial_t u^s(t) \partial_t \phi(t) \right) dV dt \\ = \int_0^\infty \int_D \left(\left(1 - \frac{1}{\rho_0}\right) \nabla u^i(t) \cdot \nabla \phi(t) - \left(1 - \frac{1}{\rho_0 c_0^2}\right) \partial_t u^i(t) \partial_t \phi(t) \right) dV dt \end{aligned}$$

for all $\phi \in C_0^\infty([0, \infty), H_c^1(\mathbb{R}^3))$. Since the coefficients c and ρ are piecewise constant, (2.3) can equivalently also be written as a transmission problem for $(u|_D, u^s|_{\mathbb{R}^3 \setminus \overline{D}})$. As usual, we use in the following the notation $D^- := D$ for the interior domain and $D^+ := \mathbb{R}^3 \setminus \overline{D}$ for the complementary exterior domain. We denote the one-sided trace for $D^\pm$ by $\gamma^\pm$, and the normal derivative for $D^\pm$ by $\partial_\nu^\pm$. Therewith, the transmission problem is given by

$$\partial_t^2 u^s - \Delta u^s = 0 \quad \text{in } D^+ \times (0, \infty), \quad (2.5a)$$

$$\frac{1}{c_0^2} \partial_t^2 u - \Delta u = 0 \quad \text{in } D^- \times (0, \infty), \quad (2.5b)$$

$$\gamma^+ u^s - \gamma^- u = -\gamma u^i, \quad \text{on } \partial D \times (0, \infty), \quad (2.5c)$$

$$\partial_\nu^+ u^s - \frac{1}{\rho_0} \partial_\nu^- u = -\partial_\nu u^i, \quad \text{on } \partial D \times (0, \infty), \quad (2.5d)$$

with homogeneous initial conditions $u^s(\cdot, 0) = \partial_t u^s(\cdot, 0) = 0$ in D^+ and $u(\cdot, 0) = \partial_t u(\cdot, 0) = 0$ in D^- .

Following [18, 19, 20], we are now in a position to introduce the definition of the far field pattern of the scattered wave. Throughout, we employ, for any Hilbert space X and $r \in \mathbb{R}$, the notations

$$\begin{aligned} H_c^r(\mathbb{R}; X) &:= \{g \in H^r(\mathbb{R}; X) \mid \text{supp } g \subseteq \mathbb{R} \text{ is compact}\}, \\ H_0^r(0, T; X) &:= \{g|_{(0, T)} \mid g \in H^r(\mathbb{R}; X), g = 0 \text{ in } (-\infty, 0)\}, \\ H_{0, \text{loc}}^r(0, \infty; X) &:= \{g \mid g \in H_0^r(0, T; X) \text{ for all } T > 0\}. \end{aligned}$$

Lemma 2.1. *Suppose that u^i is an incident plane wave as in (2.1) with $f^i \in H_c^r(\mathbb{R})$ for some $r > 5$, which satisfies (2.2b). Then the associated scattered field $u^s|_{D^+} \in H_{0, \text{loc}}^{r-\frac{5}{2}}(0, \infty; H^1(D^+))$ in the exterior of the scatterer has the asymptotic behavior*

$$u^s(x, |x| + t) = \frac{1}{|x|} \left(u^\infty(\xi, t) + O(|x|^{-1}) \right), \quad |x| \rightarrow \infty,$$

uniformly in all directions $\xi = x/|x| \in S^2$ and also in $t \geq 0$ if t is confined to a finite interval. We call $u^\infty : S^2 \times (0, \infty) \rightarrow \mathbb{R}$ the far field pattern of u^s , and we have

$$u^\infty(\xi, t) = \frac{1}{4\pi} \int_{\partial D} \left((\nu_y \cdot \xi) \partial_t u^s(y, t + \xi \cdot y) - \partial_{\nu_y}^+ u^s(y, t + \xi \cdot y) \right) dA_y, \quad \xi \in S^2, t > 0. \quad (2.6)$$

Proof. We will see in Theorem 5.1 below that u^i as in (2.1) with $f^i \in H_c^r(\mathbb{R})$ for some $r > 5$ satisfying (2.2b) implies that $u^s \in H_0^{r-\frac{5}{2}}(0, T; H^1(D^+))$ in the exterior of the scatterer for all $T > 0$. By Sobolev embedding this means that u^s is twice continuously differentiable with respect to the time variable. Using Kirchhoff's representation formula (see, e.g., [4, p. 97] or [38, p. 147]) the scattered field $u^s(x, t)$ with $(x, t) \in D^+ \times (0, \infty)$ in the exterior of the scatterer can be written as the sum of a transient double and single layer potential,

$$\begin{aligned} u^s(x, t) &= \int_{\partial D} \left(\partial_{\nu_y}^+ \left(\frac{u^s(z, t - |x - y|)}{4\pi|x - y|} \right) \Big|_{z=y} - \frac{1}{4\pi|x - y|} \partial_{\nu_y}^+ u^s(y, t - |x - y|) \right) dA_y \\ &= \frac{1}{4\pi} \int_{\partial D} \left(u^s(y, t - |x - y|) \partial_{\nu_y}^+ \frac{1}{|x - y|} - \frac{1}{|x - y|} \partial_t u^s(y, t - |x - y|) \partial_{\nu_y} |x - y| \right. \\ &\quad \left. - \frac{1}{|x - y|} \partial_{\nu_y}^+ u^s(y, t - |x - y|) \right) dA_y. \end{aligned} \quad (2.7)$$

Observing that

$$\begin{aligned} |x - y| &= |x| - \xi \cdot y + O(|x|^{-1}), & |x - y|^{-1} &= |x|^{-1} + O(|x|^{-2}), \\ \partial_{\nu_y} |x - y| &= -\nu_y \cdot \xi + O(|x|^{-1}), & \partial_{\nu_y} (|x - y|^{-1}) &= \nu_y \cdot |x|^{-2} \xi + O(|x|^{-3}), \end{aligned}$$

uniformly for all $y \in \partial D$, and inserting this into (2.7), the result follows from Taylor's theorem. $\square$

We are interested in the following inverse backscattering problem. Suppose we are given the far field patterns $u^\infty(-\theta_k, t; \theta_k)$ corresponding to incident plane waves $u^i(\cdot, \cdot; \theta_k)$ with direction of propagation θ_k for a finite set of incident directions $\theta_k \in S^2$ and on a finite time interval $t \in [0, T]$, can we numerically reconstruct the shape of the scatterer D ?

3 Direct scattering problem in the Laplace domain

We analyze the scattering problem and derive the associated shape derivative first in the Laplace domain. Following [4], we denote by

$$\widehat{g}(s) := \mathcal{L}\{g\}(s) := \int_0^\infty e^{-st} g(t) dt, \quad s \in \mathbb{C}_+ := \{z \in \mathbb{C} \mid \operatorname{Re}(z) > 0\},$$

the Laplace transform of a causal function $g : \mathbb{R} \rightarrow \mathbb{R}$, assuming that it exists. Given any Hilbert space X , the Laplace transform can then be extended to

$$\mathcal{L}'_+(\mathbb{R}; X) := \{g \in \mathcal{D}'_+(\mathbb{R}; X) \mid e^{-\sigma_g t} g(t) \in \mathcal{S}'_+(\mathbb{R}; X) \text{ for some } \sigma_g \geq 0\}.$$

Here, $\mathcal{D}'_+(\mathbb{R}; X)$ and $\mathcal{S}'_+(\mathbb{R}; X)$ denotes the space of causal distributions and of causal tempered distributions with values in X , respectively. If $g \in \mathcal{L}'_+(\mathbb{R}; X)$, then its Laplace transform $\mathcal{L}\{g\}(s)$ is a holomorphic function of s in the half-plane $\operatorname{Re}(s) > \sigma_g$; see, e.g., [42, p. 417]. In particular, the restricted causal incident plane wave $u^i|_{B_R(0)} \in H_c^r(\mathbb{R}; H^2(B_R(0)))$, $r \geq 2$, from (2.1) has a well-defined Laplace transform, which we denote by $\widehat{u}^i|_{B_R(0)}$.

The Laplace transform of the scattering problem (2.4) gives, for all $s \in \mathbb{C}_+$, the equation

$$\operatorname{div} \left(\frac{1}{\rho} \nabla \widehat{u}^s \right) - \frac{s^2}{\rho c^2} \widehat{u}^s = \operatorname{div} \left(\left(1 - \frac{1}{\rho} \right) \nabla \widehat{u}^i \right) - s^2 \left(1 - \frac{1}{\rho c^2} \right) \widehat{u}^i \quad \text{in } \mathbb{R}^3 \quad (3.1)$$

for the Laplace transform of the scattered field denoted by $\widehat{u}^s$. Also this equation has to be understood in weak sense. Since the wave speed c and the density ρ are piecewise constant, (3.1) can equivalently be written as a transmission problem for $(\widehat{v}^-, \widehat{v}^+) = (\widehat{u}|_{D^-}, \widehat{u}^s|_{D^+})$ that is given by

$$\Delta \widehat{v}^+ - s^2 \widehat{v}^+ = 0 \quad \text{in } D^+, \quad (3.2a)$$

$$\Delta \widehat{v}^- - \frac{s^2}{c_0^2} \widehat{v}^- = 0 \quad \text{in } D^-, \quad (3.2b)$$

$$\gamma^+ \widehat{v}^+ - \gamma^- \widehat{v}^- = \widehat{\eta} \quad \text{on } \partial D, \quad (3.2c)$$

$$\partial_\nu^+ \widehat{v}^+ - \frac{1}{\rho_0} \partial_\nu^- \widehat{v}^- = \widehat{\zeta} \quad \text{on } \partial D, \quad (3.2d)$$

with $\widehat{\eta} = -\gamma \widehat{u}^i$ and $\widehat{\zeta} = -\partial_\nu \widehat{u}^i$. In the following, we study the transmission problem (3.2) in a slightly more general form by considering general transmission functions $\widehat{\eta} \in H^{\frac{1}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{-\frac{1}{2}}(\partial D)$.

Following [1, 4], we consider for each $s \in \mathbb{C}_+$ the rescaled H^1 -norm defined by

$$\|\widehat{\phi}\|_{\mathbb{R}^3, s}^2 := \|\nabla \widehat{\phi}\|_{L^2(\mathbb{R}^3)}^2 + \|s\widehat{\phi}\|_{L^2(\mathbb{R}^3)}^2, \quad \widehat{\phi} \in H^1(\mathbb{R}^3).$$

We note that

$$\min(1, |s|) \|\widehat{\phi}\|_{H^1(\mathbb{R}^3)} \leq \|\widehat{\phi}\|_{\mathbb{R}^3, s} \leq \max(1, |s|) \|\widehat{\phi}\|_{H^1(\mathbb{R}^3)}; \quad (3.3)$$

see, e.g., [4, p. 86]. In the next lemma we establish existence and uniqueness of solutions to (3.2) and prove a basic energy estimate.

Lemma 3.1. *For any $s \in \mathbb{C}$ with $\operatorname{Re}(s) > 0$ the transmission problem (3.2) with arbitrary functions $\widehat{\eta} \in H^{\frac{1}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{-\frac{1}{2}}(\partial D)$ has a unique weak solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$, which satisfies*

$$\|\widehat{v}^-\|_{D^-, s} + \|\widehat{v}^+\|_{D^+, s} \leq C_\sigma \frac{|s|^{\frac{3}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad \operatorname{Re}(s) \geq \sigma > 0. \quad (3.4)$$

Proof. The weak formulation we focus on is to find $\widehat{z} \in H^1(\mathbb{R}^3)$ satisfying

$$a(\widehat{z}, \widehat{\phi}) = \ell(\widehat{\phi}) \quad \text{for all } \widehat{\phi} \in H^1(\mathbb{R}^3), \quad (3.5)$$

where

$$\begin{aligned} a(\widehat{z}, \widehat{\phi}) &:= \frac{1}{\rho_0} \int_{D^-} \nabla \widehat{z} \cdot \overline{\nabla \widehat{\phi}} + \frac{s^2}{c_0^2} \widehat{z} \overline{\widehat{\phi}} \, dV + \int_{D^+} \nabla \widehat{z} \cdot \overline{\nabla \widehat{\phi}} + s^2 \widehat{z} \overline{\widehat{\phi}} \, dV, \\ \ell(\widehat{\phi}) &= - \int_{\partial D} \widehat{\zeta} \overline{\gamma \widehat{\phi}} \, dA - \left(\int_{D^+} \nabla(\Lambda \widehat{\eta}) \cdot \overline{\nabla \widehat{\phi}} + s^2(\Lambda \widehat{\eta}) \overline{\widehat{\phi}} \, dV \right), \end{aligned}$$

where $\Lambda \widehat{\eta}$ is any lifting of $\widehat{\eta}$ into D^+ . In this proof we pick $\Lambda \widehat{\eta} = \widehat{w}$, where $\widehat{w}$ is the solution to

$$\begin{aligned} -\Delta \widehat{w} + |s|^2 \widehat{w} &= 0 && \text{in } D^+, \\ \gamma^+ \widehat{w} &= \widehat{\eta} && \text{on } \partial D, \end{aligned}$$

which, by [4, Lmm. 4.4], satisfies

$$\|\widehat{w}\|_{D^+, s} \leq C_\sigma |s|^{\frac{1}{2}} \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}, \quad \operatorname{Re}(s) \geq \sigma > 0. \quad (3.6)$$

Once $\widehat{z} \in H^1(\mathbb{R}^3)$ is shown to be uniquely determined we define

$$(\widehat{v}^-, \widehat{v}^+) = (\widehat{z}|_{D^-}, \widehat{z}|_{D^+}) + (0, \Lambda \widehat{\eta}), \quad (3.7)$$

which is then the unique weak solution of (3.2). Since

$$\begin{aligned} |s| |a(\widehat{z}, \widehat{z})| &\geq \operatorname{Re} \left(\bar{s} \left(\frac{1}{\rho_0} \int_{D^-} |\nabla \widehat{z}|^2 + \frac{s^2}{c_0^2} |\widehat{z}|^2 \, dV + \int_{D^+} |\nabla \widehat{z}|^2 + s^2 |\widehat{z}|^2 \, dV \right) \right) \\ &\geq \min \left(\frac{1}{\rho_0}, \frac{1}{\rho_0 c_0^2} \right) \operatorname{Re}(s) \left(\|\widehat{z}\|_{D^-,s}^2 + \|\widehat{z}\|_{D^+,s}^2 \right), \end{aligned} \quad (3.8)$$

the sesquilinear form a is coercive for all $s \in \mathbb{C}_+$. Hence, existence and uniqueness of a weak solution $\widehat{z} \in H^1(\mathbb{R}^3)$ of (3.5) follows from the lemma of Lax-Milgram. Moreover, combining (3.8) with the weak formulation (3.5) for $\widehat{\phi} = \widehat{z}$, we obtain using the Cauchy-Schwarz inequality together with the bound (3.6) that

$$\begin{aligned} \left(\|\widehat{z}\|_{D^-,s} + \|\widehat{z}\|_{D^+,s} \right)^2 &\leq C \frac{|s|}{\operatorname{Re}(s)} |\ell(\widehat{z})| \\ &\leq C \frac{|s|}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)} \|\gamma \widehat{z}\|_{H^{\frac{1}{2}}(\partial D)} + \|\Lambda \widehat{\eta}\|_{D^+,s} \|\widehat{z}\|_{D^+,s} \right) \\ &\leq C \frac{|s|^{\frac{3}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)} + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)} \right) \left(\|\widehat{z}\|_{D^-,s} + \|\widehat{z}\|_{D^+,s} \right). \end{aligned}$$

Now we use the representation (3.7) together with (3.6) once more to see that

$$\begin{aligned} \|\widehat{v}^-\|_{D^-,s} + \|\widehat{v}^+\|_{D^+,s} &\leq \|\widehat{z}\|_{D^-,s} + \|\widehat{z}\|_{D^+,s} + \|\Lambda \widehat{\eta}\|_{D^+,s} \\ &\leq C_\sigma \frac{|s|^{\frac{3}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad \operatorname{Re}(s) \geq \sigma > 0. \end{aligned}$$

□

To establish an explicit representation of the solution of the transmission problem (3.2) we rely on integral equations. Accordingly, we recall the definitions of the single layer potential and the double layer potential for the partial differential operator $\mathcal{P} := -\Delta + s^2$ with complex $s \in \mathbb{C}_+$,

$$\operatorname{SL}(s) : H^{-\frac{1}{2}}(\partial D) \rightarrow H^1(\mathbb{R}^3), \quad (\operatorname{SL}(s)\varphi)(x) := \int_{\partial D} \varphi(y) \Phi_s(x-y) \, dA_y, \quad (3.9a)$$

$$\operatorname{DL}(s) : H^{\frac{1}{2}}(\partial D) \rightarrow H^1(D^\pm), \quad (\operatorname{DL}(s)\psi)(x) := \int_{\partial D} \psi(y) \partial_{\nu_y} \Phi_s(x-y) \, dA_y. \quad (3.9b)$$

Here,

$$\Phi_s(x) := \frac{e^{-s|x|}}{4\pi|x|}, \quad x \in \mathbb{R}^3 \setminus \{0\},$$

is the fundamental solution for $\mathcal{P}$ in $\mathbb{R}^3$. We have the following pointwise estimates for the single and double layer potential away from D .

Lemma 3.2. For $z \in D^+$ with $\text{dist}(z, \partial D) \geq \delta > 0$ and $s \in \mathbb{C}_+$ with $\text{Re}(s) \geq \sigma > 0$, we have

$$|(\text{SL}(s)\varphi)(z)| \leq C_{\sigma,\delta}|s| \frac{e^{-\text{dist}(z,\partial D)\text{Re}(s)}}{\text{dist}(z,\partial D)} \|\varphi\|_{H^{-\frac{1}{2}}(\partial D)}, \quad \varphi \in H^{-\frac{1}{2}}(\partial D), \quad (3.10a)$$

$$|(\text{DL}(s)\psi)(z)| \leq C_{\sigma,\delta}|s|^{\frac{3}{2}} \frac{e^{-\text{dist}(z,\partial D)\text{Re}(s)}}{\text{dist}(z,\partial D)} \|\psi\|_{H^{\frac{1}{2}}(\partial D)}, \quad \psi \in H^{\frac{1}{2}}(\partial D). \quad (3.10b)$$

Proof. The inequality (3.10a) can be shown as in [3, Lmm. 7]. To establish (3.10b), we follow the same strategy and use [4, Lmm. 4.5] to obtain

$$\begin{aligned} |(\text{DL}(s)\psi)(z)| &\leq \left\| \partial_\nu \frac{e^{-s|z-\cdot|}}{4\pi|z-\cdot|} \right\|_{H^{-\frac{1}{2}}(\partial D)} \|\psi\|_{H^{\frac{1}{2}}(\partial D)} \\ &\leq C \max(1, |s|^{-\frac{1}{2}}) |s|^{\frac{1}{2}} \left\| \frac{e^{-s|z-\cdot|}}{4\pi|z-\cdot|} \right\|_{D,s} \|\psi\|_{H^{\frac{1}{2}}(\partial D)} \\ &\leq C_{\sigma,\delta} |s|^{\frac{3}{2}} \frac{e^{-\text{dist}(z,\partial D)\text{Re}(s)}}{\text{dist}(z,\partial D)} \|\psi\|_{H^{\frac{1}{2}}(\partial D)}. \end{aligned}$$

□

Using Green's representation theorem (see, e.g., [39, Thm. 6.10]), we find that the weak solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ of (3.2) (or equivalently of (3.1)) satisfies

$$\widehat{v}^+ = -\text{SL}(s)(\partial_\nu^+ \widehat{v}^+) + \text{DL}(s)(\gamma^+ \widehat{v}^+) \quad \text{in } D^+, \quad (3.11a)$$

$$\widehat{v}^- = \text{SL}(s_0)(\partial_\nu^- \widehat{v}^-) - \text{DL}(s_0)(\gamma^- \widehat{v}^-) \quad \text{in } D^-, \quad (3.11b)$$

where $s_0 := s/c_0$. Applying the jump relations for the single and double layer potential on ∂D and the associated boundary integral operators

$$\begin{aligned} S(s) : H^{-\frac{1}{2}}(\partial D) &\rightarrow H^{\frac{1}{2}}(\partial D), & (S(s)\varphi)(x) &:= \int_{\partial D} \varphi(y) \Phi_s(x-y) \, dA_y, \\ K(s) : H^{\frac{1}{2}}(\partial D) &\rightarrow H^{\frac{1}{2}}(\partial D), & (K(s)\psi)(x) &:= \int_{\partial D} \psi(y) \partial_{\nu_y} \Phi_s(x-y) \, dA_y, \\ K'(s) : H^{-\frac{1}{2}}(\partial D) &\rightarrow H^{-\frac{1}{2}}(\partial D), & (K'(s)\varphi)(x) &:= \int_{\partial D} \varphi(y) \partial_{\nu_x} \Phi_s(x-y) \, dA_y, \\ T(s) : H^{\frac{1}{2}}(\partial D) &\rightarrow H^{-\frac{1}{2}}(\partial D), & (T(s)\varphi)(x) &:= \partial_{\nu_x} \int_{\partial D} \varphi(y) \partial_{\nu_y} \Phi_s(x-y) \, dA_y, \end{aligned}$$

(see, e.g., [39, Thm. 6.11]) it follows immediately that $(\frac{1}{s}\partial_\nu^+ \widehat{v}^+, -\gamma^+ \widehat{v}^+) \in H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$ satisfies the integral equation

$$\begin{bmatrix} \rho_0 s S(s_0) + s S(s) & K(s_0) + K(s) \\ -K'(s_0) - K'(s) & \frac{1}{\rho_0 s} T(s_0) + \frac{1}{s} T(s) \end{bmatrix} \begin{bmatrix} \frac{1}{s} \partial_\nu^+ \widehat{v}^+ \\ -\gamma^+ \widehat{v}^+ \end{bmatrix} = \begin{bmatrix} -\rho_0 s S(s_0) & -K(s_0) - \frac{1}{2}I \\ K'(s_0) - \frac{1}{2}I & -\frac{1}{\rho_0 s} T(s_0) \end{bmatrix} \begin{bmatrix} -\frac{1}{s} \widehat{\zeta} \\ \widehat{\eta} \end{bmatrix} \quad (3.12)$$

on ∂D .

We define $\mathcal{X} := H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$ with the norm given by

$$\|(\varphi, \psi)\|_{\mathcal{X}}^2 := \|\varphi\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\psi\|_{H^{\frac{1}{2}}(\partial D)}^2, \quad (\varphi, \psi) \in \mathcal{X},$$

and we write $\mathcal{X}' = H^{\frac{1}{2}}(\partial D) \times H^{-\frac{1}{2}}(\partial D)$ for the associated dual space. The corresponding anti-dual form is defined by

$$\langle (\zeta, \eta), (\varphi, \psi) \rangle_{\mathcal{X}', \mathcal{X}} := \langle \bar{\varphi}, \bar{\zeta} \rangle_{H^{-\frac{1}{2}}(\partial D), H^{\frac{1}{2}}(\partial D)} + \langle \eta, \psi \rangle_{H^{-\frac{1}{2}}(\partial D), H^{\frac{1}{2}}(\partial D)}$$

for $\zeta, \varphi \in H^{-\frac{1}{2}}(\partial D)$ and $\eta, \psi \in H^{\frac{1}{2}}(\partial D)$. In Appendix A we show that for any $s \in \mathbb{C}_+$ the boundary integral operator $\mathcal{C}(s) : \mathcal{X} \rightarrow \mathcal{X}'$ defined by

$$\mathcal{C}(s) := \begin{bmatrix} \rho_0 s S(s_0) + s S(s) & K(s_0) + K(s) \\ -K'(s_0) - K'(s) & \frac{1}{\rho_0 s} T(s_0) + \frac{1}{s} T(s) \end{bmatrix} \quad (3.13)$$

has a bounded inverse $\mathcal{C}^{-1}(s) : \mathcal{X}' \rightarrow \mathcal{X}$, which satisfies

$$\|\mathcal{C}^{-1}(s)\|_{\mathcal{X} \leftarrow \mathcal{X}'} \leq C_\sigma \frac{|s|^2}{\operatorname{Re}(s)}, \quad \operatorname{Re}(s) \geq \sigma > 0. \quad (3.14)$$

Moreover, let for any $s \in \mathbb{C}_+$ the boundary integral operator $\mathcal{A} : \mathcal{X} \rightarrow \mathcal{X}'$ be defined by

$$\mathcal{A}(s) := \begin{bmatrix} -\rho_0 s S(s_0) & -K(s_0) - \frac{1}{2} I \\ K'(s_0) - \frac{1}{2} I & -\frac{1}{\rho_0 s} T(s_0) \end{bmatrix}. \quad (3.15)$$

Then we obtain from (3.12) that the solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ of the transmission problem (3.2) with $\widehat{\eta} \in H^{\frac{1}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{-\frac{1}{2}}(\partial D)$ can be written as

$$\widehat{v}^+ = -[s \operatorname{SL}(s) \quad \operatorname{DL}(s)] \mathcal{C}^{-1}(s) \mathcal{A}(s) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta} \\ \widehat{\eta} \end{bmatrix} \quad \text{in } D^+, \quad (3.16a)$$

$$\widehat{v}^- = [\rho_0 s \operatorname{SL}(s_0) \quad \operatorname{DL}(s_0)] \left(\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \mathcal{C}^{-1}(s) \mathcal{A}(s) \right) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta} \\ \widehat{\eta} \end{bmatrix} \quad \text{in } D^-. \quad (3.16b)$$

Applying the representation for $\widehat{v}^+$ in (3.11a), the bounds from Lemma 3.2 and the estimate in Lemma 3.1 yields the next corollary, which gives a pointwise estimate for solutions to (3.2).

Corollary 3.3. *Let $s \in \mathbb{C}_+$ with $\operatorname{Re}(s) \geq \sigma > 0$ and let $\widehat{v}^+$ be as in (3.16a) with $\widehat{\eta} \in H^{\frac{1}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{-\frac{1}{2}}(\partial D)$. Then, for any fixed $z \in D^+$ with $\operatorname{dist}(z, \partial D) \geq \delta > 0$ there holds*

$$|\widehat{v}^+(z)| \leq C_{\sigma, \delta} |s|^3 \frac{e^{-\operatorname{dist}(z, \partial D) \operatorname{Re}(s)}}{\operatorname{dist}(z, \partial D)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \quad (3.17)$$

Regularity results for elliptic equations (see, e.g., [39, Thm. 4.20]) imply that, for every $s \in \mathbb{C}_+$, the weak solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ of (3.2) satisfies $\widehat{v}^- \in H^2(D^-)$ and $\widehat{v}^+ \in H^2(D^+)$. In the following proposition we establish an associated estimate that is explicit in terms of the complex parameter s . This estimate will be required in the derivation of the domain derivative in the Laplace domain in Section 4, and the explicit dependence on s will be required when translating this result back into the time domain in Section 5 below.

Proposition 3.4. *Suppose $s \in \mathbb{C}_+$ with $\operatorname{Re}(s) \geq \sigma > 0$, and let $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ be the unique weak solution to (3.2) with $\widehat{\eta} \in H^{\frac{3}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{\frac{1}{2}}(\partial D)$. Then,*

$$\|\widehat{v}^-\|_{H^2(D^-)} + \|\widehat{v}^+\|_{H^2(D^+)} \leq C_\sigma \frac{|s|^{\frac{5}{2}}}{\operatorname{Re}(s)^{\frac{1}{2}}} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}} \quad (3.18)$$

for $s \in \mathbb{C}_+$ with $\operatorname{Re}(s) \geq \sigma > 0$.

Proof. Proceeding as in the proof of [39, Thm. 4.20], but tracking the dependency on s , we find that, for $\operatorname{Re}(s) \geq \sigma > 0$,

$$\|\widehat{v}^-\|_{H^2(D^-)} + \|\widehat{v}^+\|_{H^2(D^+)} \leq C_\sigma |s| \left(\|\widehat{v}^-\|_{D^-,s} + \|\widehat{v}^+\|_{D^+,s} \right) + C_\sigma |s|^2 \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)} + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)} \right).$$

Substituting (3.4) on the right hand side of this estimate gives (3.18). $\square$

Next we discuss the Laplace transform of the far field pattern from Lemma 2.1. Since the function u^∞ in (2.6) is not causal, we introduce a shifted version $u_R^\infty \in L^2(S^2 \times (0, \infty))$ by

$$u_R^\infty(\xi, t) := u^\infty(\xi, t - R), \quad t \in (0, \infty). \quad (3.19)$$

Here $R > 0$ is as in the causality condition (2.2b). Then u_R^∞ is causal and its Laplace transform satisfies

$$\begin{aligned} \widehat{u}_R^\infty(\xi, s) &= \frac{1}{4\pi} \int_0^\infty e^{-st} \int_{\partial D} \left((\nu_y \cdot \xi) \partial_t (\gamma^+ u^s)(y, t - R + \xi \cdot y) - (\partial_{\nu_y}^+ u^s)(y, t - R + \xi \cdot y) \right) dA_y dt \\ &= \frac{1}{4\pi} \int_{\partial D} e^{-s(R - \xi \cdot y)} \int_0^\infty e^{-s\tau} \left((\nu_y \cdot \xi) \partial_t (\gamma^+ u^s)(y, \tau) - (\partial_{\nu_y}^+ u^s)(y, \tau) \right) d\tau dA_y \\ &= \frac{1}{4\pi} e^{-sR} \int_{\partial D} e^{s\xi \cdot y} \left((\nu_y \cdot \xi) s(\gamma^+ \widehat{u}^s)(y, s) - (\partial_{\nu_y}^+ \widehat{u}^s)(y, s) \right) dA_y. \end{aligned} \quad (3.20)$$

In the second step we used the causality of the scattered field u^s . We denote by

$$\begin{aligned} \text{SL}_R^\infty(s) : H^{-\frac{1}{2}}(\partial D) &\rightarrow L^2(S^2), \quad (\text{SL}_R^\infty(s)\varphi)(x) := \frac{1}{4\pi} e^{-sR} \int_{\partial D} \varphi(y) e^{s\xi \cdot y} dA_y, \\ \text{DL}_R^\infty(s) : H^{\frac{1}{2}}(\partial D) &\rightarrow L^2(S^2), \quad (\text{DL}_R^\infty(s)\psi)(x) := \frac{1}{4\pi} e^{-sR} \int_{\partial D} \psi(y) (\nu_y \cdot \xi) s e^{s\xi \cdot y} dA_y, \end{aligned}$$

the shifted far field patterns of the single and double layer potentials from (3.9). Then we obtain from (3.16) the explicit representation

$$\widehat{u}_R^\infty = - [s \text{SL}_R^\infty(s) \quad \text{DL}_R^\infty(s)] \mathcal{C}^{-1}(s) \mathcal{A}(s) \begin{bmatrix} \frac{1}{s} \partial_\nu \widehat{u}^i \\ -\gamma \widehat{u}^i \end{bmatrix} \quad \text{on } S^2. \quad (3.21)$$

This is also the representation and the associated integral equation that we will use for the numerical simulation of solutions of the direct scattering problem in Section 6.

In order to translate this representation into the time-domain in Section 5 below, we require the following pointwise estimate.

Proposition 3.5. *Suppose $s \in \mathbb{C}_+$, and let*

$$\widehat{v}_R^\infty = - [s \text{SL}_R^\infty(s) \quad \text{DL}_R^\infty(s)] \mathcal{C}^{-1}(s) \mathcal{A}(s) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta} \\ \widehat{\eta} \end{bmatrix} \quad \text{on } S^2, \quad (3.22)$$

be the shifted far field pattern corresponding to the unique solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ of the transmission problem (3.2) with $\widehat{\eta} \in H^{\frac{1}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{-\frac{1}{2}}(\partial D)$. Denoting

$$\delta_D(\xi) := \sup_{x \in D} x \cdot \xi, \quad \xi \in S^2,$$

we have the estimate

$$|\widehat{v}_R^\infty(\xi)| \leq C_\sigma e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \frac{|s|^{\frac{5}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad \xi \in S^2. \quad (3.23)$$

Proof. From (3.20) we immediately obtain that

$$|\widehat{v}_R^\infty(\xi)| \leq C e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \left(|s| \|\gamma^+ \widehat{v}^+\|_{H^{\frac{1}{2}}(\partial D)} + \|\partial_{\nu_y}^+ \widehat{v}^+\|_{H^{-\frac{1}{2}}(\partial D)} \right).$$

Combining this with the continuity of the trace operator $\gamma : H^1(D^+) \rightarrow H^{\frac{1}{2}}(\partial D)$ and [4, Lmm. 4.5] gives

$$|\widehat{v}_R^\infty(\xi, s)| \leq C e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \left(|s| \|\widehat{v}^+\|_{H^1(D^+)} + \max(1, |s|^{-\frac{1}{2}}) |s|^{\frac{1}{2}} \|\widehat{v}^+\|_{D^+, s} \right).$$

Applying (3.3) and (3.4) we obtain

$$|\widehat{v}_R^\infty(\xi, s)| \leq C_\sigma e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \frac{|s|^{\frac{5}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}.$$

This ends the proof. $\square$

4 Domain derivative in the Laplace domain

The domain derivative for the transmission problem for the Helmholtz equation with real wave numbers, i.e., for (3.2) with $s \in i\mathbb{R}$, has been established in [26]. This result including its proof can be transferred to our setting $s \in \mathbb{C}_+$ with minor modifications. However, in contrast to [26] we require explicit knowledge on the dependence of the constants in the associated estimates in terms of the complex parameter s in order to obtain corresponding results for the time-dependent problem via the inverse Laplace transform. These estimates can be shown as worked out in detail in the proof of [35, Prop. 2.3] for the sound-soft scattering problem. Since no new ideas are required, we just comment on the main steps of the proof and refer the reader to [26] and [35] for details.

We consider deformations of the C^2 -boundary ∂D of the obstacle by means of a sufficiently small vector field $h \in C^1(\partial D, \mathbb{R}^3)$ and accordingly we denote by $\partial D_h := \{y \in \mathbb{R}^3 \mid y = x + h(x), x \in \partial D\}$ the boundary of a perturbed domain $D_h \subseteq \mathbb{R}^3$. We always assume that $\|h\|_{C^1(\partial D)} < h_0$ for some $h_0 > 0$ small enough such that $D_h \subset \subset B_R(0)$ and ∂D_h is a C^1 domain. Given an observation point $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$, we study the non-linear operator

$$\widehat{F}_D : \mathcal{D}(\widehat{F}_D) \subset C^1(\partial D, \mathbb{R}^3) \rightarrow \mathbb{C}, \quad \widehat{F}_D(h) := \widehat{u}_h^s(z), \quad (4.1)$$

where $(\widehat{u}_h, \widehat{u}_h^s) \in H^1(D_h) \times H^1(\mathbb{R}^3 \setminus \overline{D_h})$ denotes the solution of the transmission problem (3.2) with D replaced by D_h and with $\widehat{\eta} = -\gamma \widehat{u}^i|_{\partial D_h}$ and $\widehat{\zeta} = -\partial_\nu \widehat{u}^i|_{\partial D_h}$. Here,

$$\mathcal{D}(\widehat{F}_D) := \{h \in C^1(\partial D, \mathbb{R}^3) \mid \|h\|_{C^1(\partial D)} < h_0\}. \quad (4.2)$$

Proposition 4.1. *The operator $\widehat{F}_D$ from (4.1) is Fréchet differentiable at zero. Denoting by $(\widehat{u}, \widehat{u}^s) \in H^1(D^-) \times H^1(D^+)$ the solution to the transmission problem (3.2) with $\widehat{\eta} = -\gamma \widehat{u}^i$ and*

$\widehat{\zeta} = -\partial_\nu \widehat{u}^i$, the Fréchet derivative is given by $\widehat{F}'_D(0)h = \widehat{u}'_h(z)$ for all $h \in C^1(\partial D, \mathbb{R}^3)$, where $\widehat{u}'_h \in H^1(\mathbb{R}^3 \setminus \partial D)$ is the unique solution of the transmission problem

$$\Delta \widehat{u}'_h - s^2 \widehat{u}'_h = 0 \quad \text{in } D^+, \quad (4.3a)$$

$$\Delta \widehat{u}'_h - \frac{s^2}{c_0^2} \widehat{u}'_h = 0 \quad \text{in } D^-, \quad (4.3b)$$

$$\gamma^+ \widehat{u}'_h - \gamma^- \widehat{u}'_h = h_\nu \left(1 - \frac{1}{\rho_0}\right) \partial_\nu^- \widehat{u} \quad \text{on } \partial D, \quad (4.3c)$$

$$\partial_\nu^+ \widehat{u}'_h - \frac{1}{\rho_0} \partial_\nu^- \widehat{u}'_h = -s^2 h_\nu \left(1 - \frac{1}{\rho_0 c_0^2}\right) \gamma^- \widehat{u} + \text{Div} \left(h_\nu \left(1 - \frac{1}{\rho_0}\right) \text{Grad } \gamma^- \widehat{u} \right) \quad \text{on } \partial D. \quad (4.3d)$$

Here $h_\nu := h \cdot \nu$, and Div and Grad denote the surface divergence and the surface gradient on ∂D , respectively. The function $\widehat{u}'_h$ is called the domain derivative of the scattered field in the Laplace domain. We have

$$|\widehat{F}_D(h) - \widehat{F}_D(0) - \widehat{F}'_D(0)h| \leq C_\sigma \frac{e^{-\text{dist}(z, \partial B_R(0)) \text{Re}(s)}}{\text{dist}(z, \partial B_R(0))} \frac{|s|^{\frac{9}{2}}}{\text{Re}(s)^3} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}^2 \quad (4.4)$$

for all $s \in \mathbb{C}_+$ with $\text{Re}(s) \geq \sigma > 0$ and for any $\widetilde{R} > R$.

Proof. Existence and uniqueness of a solution $\widehat{u}'_h \in H^1(\mathbb{R}^3 \setminus \partial D)$ to (4.3) can again be shown by applying the Lemma of Lax-Milgram to the weak formulation of this transmission problem. Below we will give an alternative proof using integral equation techniques.

Let $\chi \in C^\infty(\mathbb{R}^3)$ be a cut-off function with $\chi = 1$ in $B_R(0)$ and $\chi = 0$ in $\mathbb{R}^3 \setminus \overline{B_{\widetilde{R}}(0)}$. Accordingly, we define $\widehat{w} := \widehat{u}^s + \chi \widehat{u}^i \in H^1(\mathbb{R}^3)$. Considering the weak formulation of (3.1), it follows immediately as in the proof of [35, Pro. 2.3] that

$$\|\widehat{w}\|_{\mathbb{R}^3, s} \leq C \frac{|s|}{\text{Re}(s)} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})}.$$

Denoting by $\widehat{u}_h^s \in H^1(\mathbb{R}^3)$ the solution to (3.1) with D replaced by D_h we define $\widehat{w}_h := \widehat{u}_h^s + \chi \widehat{u}^i$. Considering an extension of the boundary perturbation h to $B_R(0)$ that is supported in a neighborhood of ∂D , denoted again by h , we define a diffeomorphism $\varphi : B_R(0) \rightarrow B_R(0)$ by $\varphi(x) := x + h(x)$. This can be used to define the transformed field $\widetilde{w}_h := \widehat{w}_h \circ \varphi$. It follows by combining the analysis from [26] with [35] that

$$\|\widetilde{w}_h - \widehat{w}\|_{\mathbb{R}^3, s} \leq C \frac{|s|^2}{\text{Re}(s)^2} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}.$$

Moreover, it can be shown, following the arguments in [26, 35] that $\widehat{W} := \widehat{u}'_h + h \cdot \nabla \widehat{w}$ fulfills

$$\|\widetilde{w}_h - \widehat{w} - \widehat{W}\|_{\mathbb{R}^3, s} \leq C \frac{|s|^3}{\text{Re}(s)^3} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}^2. \quad (4.5)$$

To establish the pointwise estimate (4.4), we proceed as in the proof of [35, Pro. 2.3]. Using the fact that $\widehat{u}_h(z) - \widehat{u}(z) = \widetilde{w}_h(z) - \widehat{w}(z)$ and that $\widehat{u}'_h(z) = \widehat{W}(z)$ (since $h(z) = 0$) we find using

Green's representation theorem (with single- and double layer potentials on $\partial B_{R-\varepsilon}(0)$ for some $\varepsilon > 0$ sufficiently small such that $\overline{D} \subseteq B_{R-\varepsilon}(0)$) and (3.10) that

$$\begin{aligned} |\widehat{u}_h(z) - \widehat{u}(z) - \widehat{u}'_h(z)| &= |\widetilde{w}_h(z) - \widehat{w}(z) - \widehat{W}(z)| \\ &= |-(\text{SL}(s)(\partial_\nu^+(\widetilde{w}_h - \widehat{w} - \widehat{W}))(z) + (\text{DL}(s)(\gamma^+(\widetilde{w}_h - \widehat{w} - \widehat{W}))(z))| \\ &\leq C_{\sigma,\varepsilon} |s| \frac{e^{-\text{dist}(z, \partial B_R(0)) \text{Re}(s)}}{\text{dist}(z, \partial B_R(0))} \left(\|\partial_\nu^+(\widehat{w}_h - \widehat{w} - \widehat{W})\|_{H^{-\frac{1}{2}}(\partial B_{R-\varepsilon}(0))} \right. \\ &\quad \left. + |s|^{\frac{1}{2}} \|\gamma^+(\widetilde{w}_h - \widehat{w} - \widehat{W})\|_{H^{\frac{1}{2}}(\partial B_{R-\varepsilon}(0))} \right). \end{aligned}$$

Applying [4, Lmm. 4.5], the continuity of the trace operator $\gamma^+ : H^1(\mathbb{R}^3 \setminus \overline{B_{R-\varepsilon}(0)}) \rightarrow H^{\frac{1}{2}}(\partial B_{R-\varepsilon}(0))$ and (3.3) we obtain that

$$\begin{aligned} |\widehat{u}_h(z) - \widehat{u}(z) - \widehat{u}'_h(z)| &\leq C_{\sigma,\varepsilon} \frac{e^{-\text{dist}(x, \partial B_R(0)) \text{Re}(s)}}{\text{dist}(x, \partial B_R(0))} |s|^{\frac{3}{2}} \|\widehat{w}_h - \widehat{w} - \widehat{W}\|_{\mathbb{R}^3 \setminus \overline{D}, s} \\ &\leq C_{\sigma,\varepsilon} \frac{e^{-\text{dist}(x, \partial B_R(0)) \text{Re}(s)}}{\text{dist}(x, \partial B_R(0))} \frac{|s|^{\frac{9}{2}}}{\text{Re}(s)^3} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}. \end{aligned}$$

For the second inequality, we have used (4.5). This shows (4.4). $\square$

Using Green's representation theorem, we can write the weak solution $\widehat{u}'_h \in H^1(D^+)$ of (4.3) as

$$\begin{aligned} \widehat{u}'_h &= -\text{SL}(s)(\partial_\nu^+ \widehat{u}'_h) + \text{DL}(s)(\gamma^+ \widehat{u}'_h) && \text{in } D^+, \\ \widehat{u}'_h &= \text{SL}(s_0)(\partial_\nu^- \widehat{u}'_h) - \text{DL}(s_0)(\gamma^- \widehat{u}'_h) && \text{in } D^-, \end{aligned}$$

where as before $s_0 := s/c_0$. In the following we denote by

$$\widehat{\eta}' := h_\nu \left(1 - \frac{1}{\rho_0}\right) \partial_\nu^- \widehat{u}, \quad (4.6a)$$

$$\widehat{\zeta}' := -s^2 h_\nu \left(1 - \frac{1}{\rho_0 c_0^2}\right) \gamma^- \widehat{u} + \text{Div} \left(h_\nu \left(1 - \frac{1}{\rho_0}\right) \text{Grad} \gamma^- \widehat{u} \right), \quad (4.6b)$$

the right hand sides of the transmission conditions in (4.3). Applying the jump relations for the single and double layer potential on ∂D , we find that $(\frac{1}{s} \partial_\nu^+ \widehat{u}'_h, -\gamma^+ \widehat{u}'_h) \in H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$ satisfies the integral equation

$$\mathcal{C}(s) \begin{bmatrix} \frac{1}{s} \partial_\nu^+ \widehat{u}'_h \\ -\gamma^+ \widehat{u}'_h \end{bmatrix} = \mathcal{A}(s) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta}' \\ \widehat{\eta}' \end{bmatrix} \quad \text{on } \partial D. \quad (4.7)$$

Here, $\mathcal{C}(s)$ and $\mathcal{A}(s)$ are the integral operators introduced in (3.13) and (3.15), respectively. The operator $\mathcal{C}(s)$ has a bounded inverse $\mathcal{C}^{-1} : \mathcal{X}' \rightarrow \mathcal{X}$ for any $s \in \mathbb{C}_+$; see Appendix A. Accordingly, we obtain the following explicit representation of the domain derivative $\widehat{u}'_h \in H^1(\mathbb{R}^3 \setminus \partial D)$ of the scattered field in the Laplace domain,

$$\widehat{u}'_h = -[s \text{SL}(s) \quad \text{DL}(s)] \mathcal{C}^{-1}(s) \mathcal{A}(s) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta}' \\ \widehat{\eta}' \end{bmatrix} \quad \text{in } D^+, \quad (4.8a)$$

$$\widehat{u}'_h = [\rho_0 s \text{SL}(s_0) \quad \text{DL}(s_0)] \left(\mathcal{C}^{-1}(s) \mathcal{A}(s) - \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \right) \begin{bmatrix} -\frac{1}{s} \widehat{\zeta}' \\ \widehat{\eta}' \end{bmatrix} \quad \text{in } D^-. \quad (4.8b)$$

Remark 4.2. For later reference we note that (4.6)–(4.8) and therefore also the transmission problem (4.3) still make sense when we replace $(\widehat{u}, \widehat{u}^s) \in H^1(D^-) \times H^1(D^+)$ by the solution $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ of the transmission problem (3.2) with arbitrary transmission functions $\widehat{\eta} \in H^{\frac{3}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{\frac{1}{2}}(\partial D)$. In this case, one has to use $\partial_\nu^- \widehat{v}^-$ and $\gamma^- \widehat{v}^-$ instead of $\partial_\nu^- \widehat{u}$ and $\gamma^- \widehat{u}$, respectively, in (4.6) for the right hand side of the transmission conditions in (4.3). This generalization will be utilized in Proposition 4.4 and in Theorem 5.2 in order to obtain the continuous extensions in (5.9) and (5.11). $\diamond$

Next we discuss the domain derivative of the shifted far field pattern u_R^∞ from (3.20). Similar to (4.1), we define for any $\xi \in S^2$ the non-linear operator

$$\widehat{F}_{D,R}^\infty : \mathcal{D}(\widehat{F}_{D,R}^\infty) \subset C^1(\partial D, \mathbb{R}^3) \rightarrow \mathbb{C}, \quad \widehat{F}_{D,R}^\infty(h) := \widehat{u}_{R,h}^\infty(\xi), \quad (4.9)$$

where $\widehat{u}_{R,h}^\infty \in L^2(S^2)$ denotes the shifted far field pattern of the solution of the transmission problem (3.2) with D replaced by D_h and with $\widehat{\eta} = -\gamma \widehat{u}^i|_{\partial D_h}$ and $\widehat{\zeta} = -\partial_\nu \widehat{u}^i|_{\partial D_h}$, as defined in (3.20). Here, $\mathcal{D}(\widehat{F}_{D,R}^\infty)$ coincides with $\mathcal{D}(\widehat{F}_D)$ from (4.2).

Corollary 4.3. *The operator $\widehat{F}_{D,R}^\infty$ is Fréchet differentiable at zero. The Fréchet derivative is given by $(\widehat{F}_{D,R}^\infty)'(0)h = (\widehat{u}'_h)_R^\infty(\xi)$, where $(\widehat{u}'_h)_R^\infty \in L^2(S^2)$ denotes the shifted far field pattern*

$$(\widehat{u}'_h)_R^\infty(\xi, s) := \frac{1}{4\pi} e^{-sR} \int_{\partial D} e^{s\xi \cdot y} ((\nu_y \cdot \xi)s(\gamma^+ \widehat{u}'_h)(y, s) - (\partial_\nu^+ \widehat{u}'_h)(y, s)) \, dA_y, \quad (4.10)$$

of the domain derivative in the Laplace domain $\widehat{u}'_h$ from Proposition 4.1. The function $(\widehat{u}'_h)_R^\infty$ is called the domain derivative of the shifted far field pattern in the Laplace domain. We have

$$|\widehat{F}_{D,R}^\infty(h) - \widehat{F}_{D,R}^\infty(0) - (\widehat{F}_{D,R}^\infty)'(0)h| \leq C_\sigma e^{-\varepsilon \operatorname{Re}(s)} \frac{|s|^4}{\operatorname{Re}(s)^3} \|\widehat{u}^i\|_{H^1(B_{\bar{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}^2 \quad (4.11)$$

for all $s \in \mathbb{C}_+$ with $\operatorname{Re}(s) \geq \sigma > 0$ and for any $\widetilde{R} > R$.

Proof. Using (3.20) and (4.10) we find that

$$\begin{aligned} |\widehat{F}_{D,R}^\infty(h) - \widehat{F}_{D,R}^\infty(0) - (\widehat{F}_{D,R}^\infty)'(0)h| &= |\widehat{u}_{h,R}^\infty(\xi) - \widehat{u}_R^\infty(\xi) - (\widehat{u}'_h)_R^\infty(\xi)| \\ &= \left| \frac{1}{4\pi} e^{-sR} \int_{\partial B_{R-\varepsilon}(0)} e^{s\xi \cdot y} \left((\nu_y \cdot \xi)s(\gamma(\widehat{u}_h - \widehat{u} - \widehat{u}'_h))(y) - (\partial_{\nu_y}(\widehat{u}_h - \widehat{u} - \widehat{u}'_h))(y) \right) dA_y \right|. \end{aligned}$$

In the second step we used Green's formula to transfer the integral representations of the far field patterns $\widehat{u}_{h,R}^\infty$, $\widehat{u}_R^\infty$, and $(\widehat{u}'_h)_R^\infty$ from ∂D_h and ∂D , respectively, to $\partial B_{R-\varepsilon}(0)$. Next we use again the notation from the proof of Proposition 4.1. Since $\gamma(\widehat{u}_h - \widehat{u} - \widehat{u}'_h) = \gamma(\widetilde{w}_h - \widehat{w} - \widehat{W})$ on $\partial B_{R-\varepsilon}(0)$, we obtain that

$$\begin{aligned} &|\widehat{u}_{h,R}^\infty(\xi) - \widehat{u}_R^\infty(\xi) - (\widehat{u}'_h)_R^\infty(\xi)| \\ &\leq C e^{-\varepsilon \operatorname{Re}(s)} \left(|s| \|\gamma(\widetilde{w}_h - \widehat{w} - \widehat{W})\|_{H^{\frac{1}{2}}(\partial B_{R-\varepsilon})} + \|\partial_{\nu_y}(\widetilde{w}_h - \widehat{w} - \widehat{W})\|_{H^{-\frac{1}{2}}(\partial B_{R-\varepsilon})} \right). \end{aligned}$$

Applying [4, Lmm. 4.5], the continuity of the trace operator γ^+ , (3.3) as well as (4.5), we obtain similar to the last step in the proof of Theorem 4.1 that

$$|\widehat{u}_{h,R}^\infty(\xi) - \widehat{u}_R^\infty(\xi) - (\widehat{u}'_h)_R^\infty(\xi)| \leq C_\sigma e^{-\varepsilon \operatorname{Re}(s)} \frac{|s|^4}{\operatorname{Re}(s)^3} \|\widehat{u}^i\|_{H^1(B_{\bar{R}}(0) \setminus \overline{B_R(0)})} \|h\|_{C^1(\partial D)}^2.$$

This shows (4.11). $\square$

From (4.8) we immediately obtain the following explicit representation of the shifted far field pattern of the domain derivative,

$$(\widehat{u}'_h)_R^\infty = - [s\text{SL}_R^\infty(s) \quad \text{DL}_R^\infty(s)] \mathcal{C}^{-1}(s)\mathcal{A}(s) \begin{bmatrix} -\frac{1}{s}\widehat{\zeta}' \\ \widehat{\eta}' \end{bmatrix} \quad \text{on } S^2, \quad (4.12)$$

where $\widehat{\eta}'$ and $\widehat{\zeta}'$ are as in (4.6) with $\gamma^-\widehat{u}$ and $\partial_\nu^-\widehat{u}$ denoting the trace and the normal derivative of the solution to the transmission problem (3.2) with $\widehat{\eta} = -\gamma\widehat{u}^i$ and $\widehat{\zeta} = -\partial_\nu\widehat{u}^i$. This representation and the associated integral equation will be used for the numerical implementation of the temporal domain derivative in Section 6 below.

In the next proposition we establish bounds on the domain derivative $\widehat{u}'_h$ and on its shifted far field pattern $(\widehat{u}'_h)_R^\infty$ that are explicit with respect to the parameter s . These will be required to characterize the temporal domain derivative in Theorem 5.2 below. We consider the case of general transmission functions as explained in Remark 4.2.

Proposition 4.4. *Suppose $\text{Re}(s) \geq \sigma > 0$, $h \in C^1(\partial D, \mathbb{R}^3)$, and let $(\widehat{v}^-, \widehat{v}^+) \in H^1(D^-) \times H^1(D^+)$ be the solution of the transmission problem (3.2) with arbitrary transmission functions $\widehat{\eta} \in H^{\frac{3}{2}}(\partial D)$ and $\widehat{\zeta} \in H^{\frac{1}{2}}(\partial D)$. We consider the associated solution $\widehat{u}'_h \in H^1(D^-) \times H^1(D^+)$ of the transmission problem (4.3), where the right hand sides of the transmission conditions are given by (4.6) with $\partial_\nu^-\widehat{v}^-$ and $\gamma^-\widehat{v}^-$ instead of $\partial_\nu^-\widehat{u}$ and $\gamma^-\widehat{u}$, respectively. Then,*

$$\|\widehat{u}'_h\|_{H^1(D^\pm)} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^5}{\text{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad \text{Re}(s) \geq \sigma > 0, \quad (4.13)$$

and

$$\|\widehat{u}'_h\|_{L^2(D^\pm)} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^4}{\text{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad \text{Re}(s) \geq \sigma > 0. \quad (4.14)$$

Furthermore, for any $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ and $\text{Re}(s) \geq \sigma > 0$, we have the pointwise estimate

$$|\widehat{u}'_h(z)| \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{e^{-\text{dist}(x, \partial D) \text{Re}(s)}}{\text{dist}(x, \partial D)} \frac{|s|^{\frac{13}{2}}}{\text{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \quad (4.15)$$

The shifted far field pattern of the domain derivative satisfies, for any $\xi \in S^2$ and $\text{Re}(s) \geq \sigma > 0$,

$$|(\widehat{u}'_h)_R^\infty(\xi)| \leq C_\sigma \|h\|_{C^1(\partial D)} e^{-\text{Re}(s)(R-\delta_D(\xi))} \frac{|s|^6}{\text{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \quad (4.16)$$

Proof. We use again the notations $\widehat{\eta}'$ and $\widehat{\zeta}'$ for the right hand sides of the transmission conditions in (4.3). Proceeding as in the proof of Lemma 3.1 we obtain that

$$\|\widehat{u}'_h\|_{D^-,s} + \|\widehat{u}'_h\|_{D^+,s} \leq C_\sigma \frac{|s|^{\frac{3}{2}}}{\text{Re}(s)} \left(\|\widehat{\zeta}'\|_{H^{-\frac{1}{2}}(\partial D)} + \|\widehat{\eta}'\|_{H^{\frac{1}{2}}(\partial D)} \right). \quad (4.17)$$

Using (4.6) and the continuity of $\partial_\nu^- : H^2(D) \rightarrow H^{\frac{1}{2}}(\partial D)$, we find that

$$\|\widehat{\eta}'\|_{H^{\frac{1}{2}}(\partial D)} = \left\| h_\nu \left(1 - \frac{1}{\rho_0} \right) \partial_\nu^- \widehat{v}^- \right\|_{H^{\frac{1}{2}}(\partial D)} \leq C \|h\|_{C^1(\partial D)} \|\partial_\nu^- \widehat{v}^-\|_{H^{\frac{1}{2}}(\partial D)} \leq C \|h\|_{C^1(\partial D)} \|\widehat{v}^-\|_{H^2(D)}.$$

Applying (3.18) gives

$$\|\widehat{\eta}'\|_{H^{\frac{1}{2}}(\partial D)} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^{\frac{5}{2}}}{\operatorname{Re}(s)^{\frac{1}{2}}} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}} \quad (4.18)$$

for $s \in \mathbb{C}_+$ with $\operatorname{Re}(s) \geq \sigma > 0$. Similarly,

$$\begin{aligned} \|\widehat{\zeta}'\|_{H^{-\frac{1}{2}}(\partial D)} &= \left\| s^2 h_\nu \left(1 - \frac{1}{\rho_0 c_0^2} \right) \gamma \widehat{v}^- + \operatorname{Div} \left(h_\nu \left(1 - \frac{1}{\rho_0} \right) \operatorname{Grad} \gamma \widehat{v}^- \right) \right\|_{H^{-\frac{1}{2}}(\partial D)} \\ &\leq C |s|^2 \|h\|_{C^1(\partial D)} \|\gamma \widehat{v}^-\|_{H^{\frac{1}{2}}(\partial D)} + C \|h\|_{C^1(\partial D)} \|\gamma \widehat{v}^-\|_{H^{\frac{3}{2}}(\partial D)} \\ &\leq C \|h\|_{C^1(\partial D)} (|s|^2 \|\widehat{v}^-\|_{H^1(D^-)} + \|\widehat{v}^-\|_{H^2(D^-)}), \end{aligned}$$

and (3.3), (3.4), and (3.18) give

$$\|\widehat{\zeta}'\|_{H^{-\frac{1}{2}}(\partial D)} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^{\frac{7}{2}}}{\operatorname{Re}(s)} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \quad (4.19)$$

Substituting (4.18) and (4.19) into (4.17) yields

$$\|\widehat{u}'_h\|_{D^-,s} + \|\widehat{u}'_h\|_{D^+,s} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^5}{\operatorname{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}, \quad (4.20)$$

which implies (4.13). The inequality (4.14) also follows immediately from (4.20) by dropping the gradient term in $\|\widehat{u}'_h\|_{D^\pm,s}$ and dividing the resulting inequality by $|s|$.

To show (4.15) we observe that [4, Lmm. 4.5] gives

$$\|\partial_\nu^+ \widehat{u}'_h\|_{H^{-\frac{1}{2}}(\partial D)} \leq C \max(1, |s|^{-\frac{1}{2}}) |s|^{\frac{1}{2}} \|\widehat{u}'_h\|_{D^+,s}. \quad (4.21)$$

We combine (4.21) and (4.20) to see that

$$\|\partial_\nu^+ \widehat{u}'_h\|_{H^{-\frac{1}{2}}(\partial D)} \leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^{\frac{11}{2}}}{\operatorname{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}.$$

Moreover, using the continuity of the trace operator $\gamma^- : H^1(D) \rightarrow H^{\frac{1}{2}}(\partial D)$ and (3.3), and combining the result with (4.20), we obtain

$$\begin{aligned} \|\gamma^+ \widehat{u}'_h\|_{H^{\frac{1}{2}}(\partial D)} &\leq C \|\widehat{u}'_h\|_{H^1(D^+)} \leq C \max(1, |s|^{-1}) \|\widehat{u}'_h\|_{D^+,s} \\ &\leq C_\sigma \|h\|_{C^1(\partial D)} \frac{|s|^5}{\operatorname{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \end{aligned}$$

Using Green's representation theorem and (3.10), we finally arrive at

$$\begin{aligned} |\widehat{u}'_h(z)| &\leq |-(\operatorname{SL}(s)(\partial_\nu^+ \widehat{u}'_h))(z) + (\operatorname{DL}(s)(\gamma^+ \widehat{u}'_h))(z)| \\ &\leq C_\sigma \frac{e^{-\operatorname{dist}(x, \partial D) \operatorname{Re}(s)}}{\operatorname{dist}(x, \partial D)} \frac{|s|^{\frac{13}{2}}}{\operatorname{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \end{aligned}$$

To see (4.16), we use (4.10), [4, Lmm. 4.5], the continuity of the trace operator γ^+ , (3.3), and (4.20) to estimate

$$\begin{aligned} |(\widehat{u}_h')_R^\infty(\xi)| &\leq C e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \left(|s| \|\gamma^+ \widehat{u}_h'\|_{H^{\frac{1}{2}}(\partial D)} + \|\partial_\nu^+ \widehat{u}_h'\|_{H^{-\frac{1}{2}}(\partial D)} \right) \\ &\leq C_\sigma \|h\|_{C^1(\partial D)} e^{-\operatorname{Re}(s)(R-\delta_D(\xi))} \frac{|s|^6}{\operatorname{Re}(s)^2} \left(\|\widehat{\zeta}\|_{H^{\frac{1}{2}}(\partial D)}^2 + \|\widehat{\eta}\|_{H^{\frac{3}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \end{aligned}$$

□

5 Scattering problem and domain derivative in the time domain

To translate the results obtained in Sections 3 and 4 from the Laplace domain into the time domain we recall some basic facts about analytic families of linear operators and their Laplace transform; see, e.g., [4, 37, 42] for further details. Throughout this section, we fix a final observation time $T > 0$.

Suppose that $K(s) : X \rightarrow Y$, $\operatorname{Re}(s) \geq \sigma > 0$, is an analytic family of bounded linear operators between two Hilbert spaces X and Y , which is bounded by

$$\|K(s)\| \leq C_\sigma \frac{|s|^\mu}{\operatorname{Re}(s)^\nu}, \quad \operatorname{Re}(s) \geq \sigma > 0,$$

for some $\mu \in \mathbb{R}$ and $\nu \geq 0$ with respect to the operator norm. Then $K(s)$ is the Laplace transform of a bounded linear convolution operator $K(\partial_t) : H_0^{r+\mu}(0, T; X) \rightarrow H_0^r(0, T; Y)$ for arbitrary $r \in \mathbb{R}$, with

$$\mathcal{L}(K(\partial_t)g)(s) = K(s)(\mathcal{L}g)(s), \quad \operatorname{Re}(s) \geq \sigma > 0.$$

Here we use the usual Heaviside operational notation for the convolution operator in the time domain; see, e.g., [4, 37]. Moreover, the composition rule

$$K_1(\partial_t)K_2(\partial_t)g = (K_1K_2)(\partial_t)g$$

holds for any two such families of operators $K_1(s) : Y \rightarrow Z$ and $K_2(s) : X \rightarrow Y$ with Hilbert spaces X, Y , and Z .

5.1 Scattering problem in the time domain

From the integral representations and estimates developed in Section 3 we immediately infer the following representations and well-posedness results in the time domain.

Theorem 5.1. *Let $r \in \mathbb{R}$, and let u^i be an incident plane wave as in (2.1) with $f^i \in H_c^{r+5}(\mathbb{R})$, which satisfies (2.2). Accordingly, we obtain*

$$(\partial_\nu u^i, \gamma u^i) \in H_0^{r+3}(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D)) \cap H_0^{r+4}(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)).$$

The unique solution of the time-dependent scattering problem (2.5) with homogeneous initial conditions $u^s(\cdot, 0) = \partial_t u^s(\cdot, 0) = 0$ in D^+ and $u(\cdot, 0) = \partial_t u(\cdot, 0) = 0$ in D^- is given by

$$u^s = - [\partial_t \mathcal{S}\mathcal{L}(\partial_t) \quad \mathcal{D}\mathcal{L}(\partial_t)] \mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) \begin{bmatrix} \partial_t^{-1} \partial_\nu u^i \\ -\gamma u^i \end{bmatrix} \quad \text{in } D^+ \times (0, \infty), \quad (5.1a)$$

$$u = [\rho_0 \partial_t \mathcal{S}\mathcal{L}(c_0 \partial_t) \quad \mathcal{D}\mathcal{L}(c_0 \partial_t)] \left(\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) \right) \begin{bmatrix} \partial_t^{-1} \partial_\nu u^i \\ -\gamma u^i \end{bmatrix} \quad \text{in } D^- \times (0, \infty). \quad (5.1b)$$

The operator $\mathcal{F} : (\partial_\nu u^i, \gamma u^i) \mapsto (u, u^s)$ has continuous extensions

$$\mathcal{F} : H_0^{r+4}(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)) \rightarrow H_0^{r+\frac{5}{2}}(0, T; H^1(D^-) \times H^1(D^+)), \quad (5.2a)$$

$$\mathcal{F} : H_0^{r+3}(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D)) \rightarrow H_0^{r+\frac{1}{2}}(0, T; H^2(D^-) \times H^2(D^+)). \quad (5.2b)$$

For any fixed $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$, the operator $\mathcal{F}_z : (\partial_\nu u^i, \gamma u^i) \mapsto u^s(z)$ has a continuous extension

$$\mathcal{F}_z : H_0^{r+4}(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)) \rightarrow H_0^{r+1}(0, T; \mathbb{R}). \quad (5.3)$$

Moreover, the shifted far field pattern in the time-domain from (3.19) can be written as

$$u_R^\infty = - [\partial_t \text{SL}_R^\infty(\partial_t) \quad \text{DL}_R^\infty(\partial_t)] \mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) \begin{bmatrix} \partial_t^{-1} \partial_\nu \widehat{u}^i \\ -\gamma \widehat{u}^i \end{bmatrix} \quad \text{on } S^2 \times (0, \infty), \quad (5.4)$$

and for each $r \in \mathbb{R}$ the operator $\mathcal{F}_\xi^\infty : (\partial_\nu u^i, \gamma u^i) \mapsto u_R^\infty(\xi, \cdot)$ has a continuous extension

$$\mathcal{F}_\xi^\infty : H_0^{r+4}(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)) \rightarrow H_0^{r+\frac{3}{2}}(0, T; \mathbb{R}). \quad (5.5)$$

Proof. This follows from the corresponding explicit representations in the Laplace domain in (3.16) and (3.21), and from the estimates in Lemma 3.1, Corollary 3.3 and the Propositions 3.4 and 3.5. For the continuous extensions in (5.2), (5.3), and (5.5) we use that the estimates (3.4), (3.17), (3.18), and (3.23) hold for arbitrary transmission functions $\widehat{\eta}$ and $\widehat{\zeta}$. $\square$

5.2 Domain derivative in the time domain

Next we consider the well-posedness of the time-domain analog of the transmission problem (4.3), which is then used to characterize the temporal domain derivative in the Theorems 5.3 and 5.4 below. Let $r \in \mathbb{R}$, and let u^i be an incident plane wave as in Theorem 5.1. Then we denote by $(u, u^s) \in H_0^{r+\frac{1}{2}}(0, T; H^2(D^-) \times H^2(D^+))$ the solution of the time-dependent scattering problem (2.5) with initial conditions $u^s(\cdot, 0) = \partial_t u^s(\cdot, 0) = 0$ in D^+ and $u(\cdot, 0) = \partial_t u(\cdot, 0) = 0$ in D^- as in Theorem 5.1. Accordingly, we use the notation

$$\eta' := h_\nu \left(1 - \frac{1}{\rho_0}\right) \partial_\nu^- u, \quad (5.6a)$$

$$\zeta' := -h_\nu \left(1 - \frac{1}{\rho_0 c_0^2}\right) \partial_t^2 \gamma^- u + \text{Div} \left(h_\nu \left(1 - \frac{1}{\rho_0}\right) \text{Grad} \gamma^- u \right). \quad (5.6b)$$

Theorem 5.2. *The unique solution $u'_h \in H_0^{r-2}(0, T; H^1(\mathbb{R}^3 \setminus \partial D))$ of the time-dependent transmission problem*

$$\partial_t^2 u'_h - \Delta u'_h = 0 \quad \text{in } D^+ \times (0, \infty), \quad (5.7a)$$

$$\frac{1}{c_0^2} \partial_t^2 u'_h - \Delta u'_h = 0 \quad \text{in } D^- \times (0, \infty), \quad (5.7b)$$

$$\gamma^+ u'_h - \gamma^- u'_h = \eta' \quad \text{on } \partial D \times (0, \infty), \quad (5.7c)$$

$$\partial_\nu^+ u'_h - \frac{1}{\rho_0} \partial_\nu^- u'_h = \zeta' \quad \text{on } \partial D \times (0, \infty), \quad (5.7d)$$

with homogeneous initial conditions $u'_h(\cdot, 0) = \partial_t u'_h(\cdot, 0) = 0$ in $\mathbb{R}^3$ is given by

$$u'_h|_{D^+} = -[\partial_t \text{SL}(\partial_t) \quad \text{DL}(\partial_t)] \mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) \begin{bmatrix} -\partial_t^{-1} \zeta' \\ \eta' \end{bmatrix} \quad \text{in } D^+ \times (0, \infty), \quad (5.8a)$$

$$u'_h|_{D^-} = [\rho_0 \partial_t \text{SL}(c_0 \partial_t) \quad \text{DL}(c_0 \partial_t)] \left(\mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) - \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \right) \begin{bmatrix} -\partial_t^{-1} \zeta' \\ \eta' \end{bmatrix} \quad \text{in } D^- \times (0, \infty). \quad (5.8b)$$

Moreover, for any observation point $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ the operator $\mathcal{G}_z : (\partial_\nu u^i, \gamma u^i) \mapsto u'_h(z, \cdot)$ has a continuous extension

$$\mathcal{G}_z : H_0^{r+3}(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D)) \rightarrow H_0^{r-\frac{7}{2}}(0, T; \mathbb{R}). \quad (5.9)$$

Similarly, the shifted far field pattern of u'_h as defined in (3.19) can be written as

$$(u'_h)_R^\infty = -[\partial_t \text{SL}_R^\infty(\partial_t) \quad \text{DL}_R^\infty(\partial_t)] \mathcal{C}^{-1}(\partial_t) \mathcal{A}(\partial_t) \begin{bmatrix} -\partial_t^{-1} \zeta' \\ \eta' \end{bmatrix} \quad \text{on } S^2 \times (0, \infty), \quad (5.10)$$

and for any observation direction $\xi \in S^2$ the operator $\mathcal{G}_\xi^\infty : (\partial_\nu u^i, \gamma u^i) \mapsto (u'_h)_R^\infty(\xi, \cdot)$ has a continuous extension

$$\mathcal{G}_\xi^\infty : H_0^{r+3}(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D)) \rightarrow H_0^{r-3}(0, T; \mathbb{R}). \quad (5.11)$$

Proof. This follows from the corresponding explicit representations in the Laplace domain in (4.8) and (4.12) together with the estimates in Proposition 4.4. $\square$

Next we consider the time-domain analog of the operator $\widehat{F}_D$ from (4.1), which is given by

$$F_D : \mathcal{D}(F_D) \subseteq C^1(\partial D, \mathbb{R}^3) \rightarrow H_0^{r+1}(0, T; \mathbb{R}), \quad F_D(h) := u_h^s(z, \cdot), \quad (5.12)$$

where (u_h, u_h^s) denotes the solution of the time-dependent transmission problem (2.5) with D replaced by D_h and with $\eta = -\gamma u^i|_{\partial D_h}$ and $\zeta = -\partial_\nu u^i|_{\partial D_h}$. As before, $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ denotes an arbitrary observation point and $\mathcal{D}(F_D)$ is the same as $\mathcal{D}(\widehat{F}_D)$ in (4.2).

Theorem 5.3. *The operator F_D from (5.12) is Fréchet differentiable at zero. Its Fréchet derivative is given by $F_D'(0)h = u'_h(z, \cdot)$ for all $h \in C^1(\partial D, \mathbb{R}^3)$, where $u'_h \in H_0^{r-2}(0, T; H^1(\mathbb{R}^3 \setminus \partial D))$ is the unique solution of the transmission problem (5.7) with η' and ζ' from (5.6). The function u'_h is called the temporal domain derivative of the scattered wave. We have*

$$\|F_D(h) - F_D(0) - F_D'(0)h\|_{H_0^{r-\frac{1}{2}}(0, T; \mathbb{R})} \leq C_T \|u^i\|_{H_0^{r+4}(0, T; H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)}))} \|h\|_{C^1(\partial D)}^2 \quad (5.13)$$

for any $\widetilde{R} > R$.

Proof. Combining Plancherel's theorem and (4.4), we find that, for $\sigma = 1/T$,

$$\begin{aligned} \|F_D(h) - F_D(0) - F_D'(0)h\|_{H_0^{r-\frac{1}{2}}(0, T; \mathbb{R})}^2 &\leq e^{2\sigma T} \int_{\sigma + i\mathbb{R}} |s|^{2r-1} |\widehat{F}_D(h) - \widehat{F}_D(0) - \widehat{F}_D'(0)h|^2 \, dA \\ &\leq C_T \|h\|_{C^1(\partial D)}^4 \int_{\sigma + i\mathbb{R}} |s|^{2r+8} \|\widehat{u}^i\|_{H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)})}^2 \, dA \\ &\leq C_T \|h\|_{C^1(\partial D)}^4 \|u^i\|_{H_0^{r+4}(0, T; H^1(B_{\widetilde{R}}(0) \setminus \overline{B_R(0)}))}^2 \end{aligned}$$

for any $\widetilde{R} > R$. This shows (5.13), which ends the proof. $\square$

The time-domain analog of the operator $\widehat{F}_{D,R}^\infty$ from (4.9) is given by

$$F_D^\infty : \mathcal{D}(F_D^\infty) \subset C^1(\partial D, \mathbb{R}^3) \rightarrow H_0^{r+\frac{3}{2}}(0, T; \mathbb{R}), \quad F_D^\infty(h) := u_{R,h}^\infty(\xi, \cdot), \quad (5.14)$$

where $u_{R,h}^\infty$ denotes the shifted far field pattern of the solution of the time-dependent transmission problem (2.5) with D replaced by D_h and with $\eta = -\gamma u^i|_{\partial D_h}$ and $\zeta = -\partial_\nu u^i|_{\partial D_h}$. As before, $\xi \in S^2$ denotes an arbitrary observation direction and $\mathcal{D}(F_D^\infty)$ is the same as $\mathcal{D}(\widehat{F}_D)$ in (4.2).

Theorem 5.4. *The operator F_D^∞ from (5.14) is Fréchet differentiable at zero. Its Fréchet derivative is given by $(F_D^\infty)'(0)h = (u_h')^\infty(\xi, \cdot)$ for all $h \in C^1(\partial D, \mathbb{R}^3)$, where $(u_h')^\infty \in H_0^{r-3}(0, T; L^\infty(S^2))$ is the far field pattern of the unique solution of the transmission problem (5.7) with η' and ζ' from (5.6). The function $(u_h')^\infty$ is called the temporal domain derivative of the shifted far field pattern. We have*

$$\|F_D^\infty(h) - F_D^\infty(0) - (F_D^\infty)'(0)h\|_{H_0^r(0, T; \mathbb{R})} \leq C_T \|u^i\|_{H_0^{r+4}(0, T; H^1(B_{\bar{R}}(0) \setminus \overline{B_R(0)}))} \|h\|_{C^1(\partial D)}^2.$$

Proof. After replacing (4.4) by (4.11), the proof is analogous to the proof of Theorem 5.3. $\square$

5.3 Semi-discretization in time using convolution quadrature

For the numerical reconstruction algorithms for the inverse backscattering problem developed in Section 6, we use Runge-Kutta convolution quadrature (RKCQ) based on Radau IIA methods for time discretization and a boundary element method for spatial discretization. In this subsection, we apply the Laplace-domain bounds established in Sections 3 and 4 to derive convergence rates for the resulting semi-discretization with respect to time. We refer the reader to [4, Sec. 5] for an introduction to RKCQ and its numerical implementation.

The Laplace-domain bounds in (3.17), (3.23), (4.15), and (4.16) imply exponential decay of the pointwise Laplace-domain near and far field evaluations as $\text{Re}(s)$ increases. Such bounds have favorable implications for the convergence of RKCQ time discretizations of the associated time-domain convolution-type operators. In particular, [3, Thm. 3] shows that away from the scatterer the Radau IIA-based convolution quadrature considered in this work attains the full classical order of the underlying Runge-Kutta scheme, provided that the incoming wave is sufficiently regular in time.

For a given final time $T > 0$ and fixed $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ and $\xi \in S^2$, we aim to approximate $u^s(z, t)$ and $u_h^s(z, t)$ from (5.1a) and (5.8a), respectively, as well as $u_R^\infty(\xi, t)$ and $(u_h')^\infty(\xi)$ from (5.4) and (5.10), at the discrete time points $t_n = n\tau$, $n = 0, \dots, M$, where $\tau > 0$ denotes the time-step size and, without loss of generality, $M := T/\tau \in \mathbb{N}$. We assume that the temporal approximations are computed using an m -stage Radau IIA RKCQ method. Accordingly, we denote the approximations to $u_h^s(z, t_n)$ and $u_h^s(z, t_n)$ by $(u_{h,\tau}^s(z))_n$ and $(u_{h,\tau}'(z))_n$, respectively, and the approximations to $u_{R,h}^\infty(\xi, t_n)$ and $(u_h')^\infty(\xi, t_n)$ by $(u_{R,h,\tau}^\infty(\xi))_n$ and $((u_h')_{R,\tau}^\infty(\xi))_n$, respectively. For $h = 0$, we omit the index h in $u_{h,\tau}^s$ and $u_{R,h,\tau}^\infty$.

Combining the Laplace-domain bounds established in Corollary 3.3 and Proposition 3.5 with [3, Thm. 3] yields the following convergence result for the solution of the direct scattering problem.

Lemma 5.5. *Let $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ and $\xi \in S^2$ be fixed. The convolution quadrature semi-discretization in time based on a Radau IIA method with m stages used to approximate both $u^s(z, t_n)$ and $u_R^\infty(\xi, t_n)$*

provides the following estimates at $t_n = n\tau$:

$$|u^s(z, t_n) - (u_\tau^s(z))_n| \leq C\tau^{2m-1} \|(\partial_\nu u^i, \gamma u^i)\|_{H_0^r(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D))}, \quad (5.15a)$$

$$|u_R^\infty(\xi, t_n) - (u_{R,\tau}^\infty(\xi))_n| \leq C\tau^{2m-1} \|(\partial_\nu u^i, \gamma u^i)\|_{H_0^{r-\frac{1}{2}}(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D))}, \quad (5.15b)$$

for $(\partial_\nu u^i, \gamma u^i) \in H_0^r(0, T; H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D))$ with $r > 2m + 9/2$.

Proof. Using Corollary 3.3 together with the bound from [3, Thm. 3], applied to the causal function u^i on Γ , immediately yields the estimate

$$|u^s(z, t_n) - (u_\tau^s(z))_n| \leq C\tau^{2m-1} \int_0^{t_n} \|\partial_t^{(\tilde{r}+1)}(\partial_\nu u^i, \gamma u^i)\|_{H^{-\frac{1}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)} dt'$$

for any $\tilde{r} > 2m + 3$. We now use the embedding $H_0^r(0, T; X) \subset C_0^{\tilde{r}+1}([0, T]; X)$, valid for any $r > 3/2 + \tilde{r}$, to obtain (5.15a). The error bound (5.15b) follows similarly. $\square$

Using the same approach, we obtain a temporal error bound for the time semi-discretization of the temporal domain derivative. As before, we derive estimates for both the near and far field, based on [3, Thm. 3] and Proposition 4.4. The proof proceeds analogously to that of Lemma 5.5.

Theorem 5.6. *Let $z \in \mathbb{R}^3 \setminus \overline{B_R(0)}$ and $\xi \in S^2$ be fixed. The convolution quadrature semi-discretization in time based on a Radau IIA method with m stages used to approximate both $u_h'(z, t_n)$ and $(u_h')_R^\infty(\xi, t_n)$ provides the following estimates at $t_n = n\tau$:*

$$\begin{aligned} |u_h'(z, t_n) - (u_{h,\tau}'(z))_n| &\leq C\tau^{2m-1} \|(\partial_\nu u^i, \gamma u^i)\|_{H_0^r(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D))}, \\ |(u_h')_R^\infty(\xi, t_n) - ((u_{h,\tau}')_R^\infty(\xi))_n| &\leq C\tau^{2m-1} \|(\partial_\nu u^i, \gamma u^i)\|_{H_0^{r-\frac{1}{2}}(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D))}, \end{aligned}$$

for $(\partial_\nu u^i, \gamma u^i) \in H_0^r(0, T; H^{\frac{1}{2}}(\partial D) \times H^{\frac{3}{2}}(\partial D))$ with $r > 2m + 8$.

A detailed spatial error analysis and, consequently, a comprehensive assessment of the full discretization error are beyond the scope of this work. To keep the presentation concise, we restrict our discussion to the Galerkin implementation and omit further technical details. In our numerical experiments, we employ the open-source boundary element method library **bempp**; see [5] for further details. Convolution quadrature requires the solution of a large number of scattering problems in the Laplace domain. This applies both to the computation of the direct problem in (3.16) and (3.22) as well as to the evaluation of the domain derivative in (4.8) and (4.12). We use piecewise linear functions for both the trial and the test function space in the Galerkin discretization. For the Galerkin approximation $\gamma^- \hat{u}_h$ of $\gamma^- \hat{u}$ appearing on the right-hand side of (4.6b), the surface gradient $\text{Grad } \gamma^- \hat{u}_h$ is piecewise constant. Consequently, the surface divergence can be assembled weakly according to

$$\int_{\partial D} \text{Div} \left(h_\nu \left(1 - \frac{1}{\rho_0} \right) \text{Grad } \gamma^- \hat{u}_h \right) \hat{y}_h \, dA = - \int_{\partial D} h_\nu \left(1 - \frac{1}{\rho_0} \right) \text{Grad } \gamma^- \hat{u}_h \cdot \text{Grad } \hat{y}_h \, dA$$

for all piecewise linear functions $\hat{y}_h$.

6 Shape reconstruction for time-dependent backscattering data

In this section, we return to the inverse scattering problem and describe an iterative reconstruction algorithm to recover the shape of a three-dimensional penetrable scattering object from observations time-dependent far field backscattering data at finitely many incident/observation directions. We suppose that far field patterns $u^\infty(-\theta_k, t)$ as in (2.6) corresponding to time-dependent incident plane waves $u^i(\cdot, \cdot; \theta_k)$ as in (2.1) with direction of propagation θ_k are available for finitely many $\theta_1, \dots, \theta_K \in S^2$ and all $t \in [0, T]$. Here the observation time $T > 0$ is assumed to be sufficiently large. In the following we use the notation $u^\infty(-\theta_k, \cdot; \theta_k)$, $k = 1, \dots, K$, for such backscattering data obtained with incident direction θ_k and observation direction $-\theta_k$.

Accordingly, we consider the nonlinear operator F^∞ mapping the shape of an obstacle ∂D to the associated far field data $(u^\infty(-\theta_k, \cdot; \theta_k))_{1 \leq k \leq K} \subseteq L^2(0, T)$. We restrict ourselves to boundaries ∂D that are star-shaped with respect to the origin, i.e., ∂D can be represented in the parametric form

$$\partial D = \{x \in \mathbb{R}^3 \mid x = r_D(\xi)\xi, \xi \in S^2\}$$

for some positive, twice continuously differentiable function $r_D : S^2 \rightarrow \mathbb{R}$ representing the radial distance from the origin. For each incident direction θ_k , $k = 1, \dots, K$, the solution of the direct scattering problem defines an operator

$$F_{\theta_k}^\infty : C_+^2(S^2) \rightarrow L^2(0, T),$$

which maps the parametrization r_D of an admissible obstacle boundary ∂D to the associated backscattering data $u^\infty(-\theta_k, \cdot; \theta_k)$. Here, $C_+^2(S^2) := \{r \in C^2(S^2) \mid r > 0\}$. Therewith, we seek a solution ∂D to the nonlinear inverse problem

$$F_{\theta_k}^\infty(r) = u^\infty(-\theta_k, \cdot; \theta_k) \quad \text{for all } k \in \{1, \dots, K\}. \quad (6.1)$$

We consider the solution of (6.1) as the minimum of the associated least squares functional. To handle the ill-conditioning we use a Tikhonov approach, adding an H^2 -penalty term to obtain

$$\Psi_\alpha(r) := \sum_{k=1}^K \|F_{\theta_k}^\infty(r) - u^\infty(-\theta_k, \cdot; \theta_k)\|_{L^2(0, T)}^2 + \alpha \|r\|_{H^2(S^2)}^2, \quad r \in C_+^2(S^2). \quad (6.2)$$

As usual, $\alpha > 0$ denotes a regularization parameter.

We apply the Gauß-Newton (GN) method to obtain a sequence of approximations $(r_n)_n$ to the parametrization of the obstacle boundary r_D , typically using a decreasing sequence $(\alpha_n)_n$ of regularization parameters depending on the relative residual. This is a widely used strategy; see, e.g., [36]. In our numerical implementation, the unknown function r is approximated by a finite linear combination of spherical harmonics of degree at most $L = 5$. Using the composite trapezoidal rule to discretize the $L^2(0, T)$ -norm in (6.2), and Parseval's identity to express the $H^2(S^2)$ -norm in terms of the ℓ^2 -norm of the spherical harmonics coefficients of r , the objective functional Ψ_α can, with a slight abuse of notation, be written as

$$\Psi_\alpha(p) = |\Theta(p)|^2.$$

Here, $p \in \mathbb{R}^{(L+1)^2}$ denotes the parameter vector containing the spherical harmonics coefficients of r , and Θ is a nonlinear vector-valued function of p . Denoting the Jacobian of Θ by J , each GN step

$$p_{n+1} = p_n - (J(p_n)^\top J(p_n))^{-1} J(p_n)^\top \Theta(p_n), \quad n \in \mathbb{N},$$

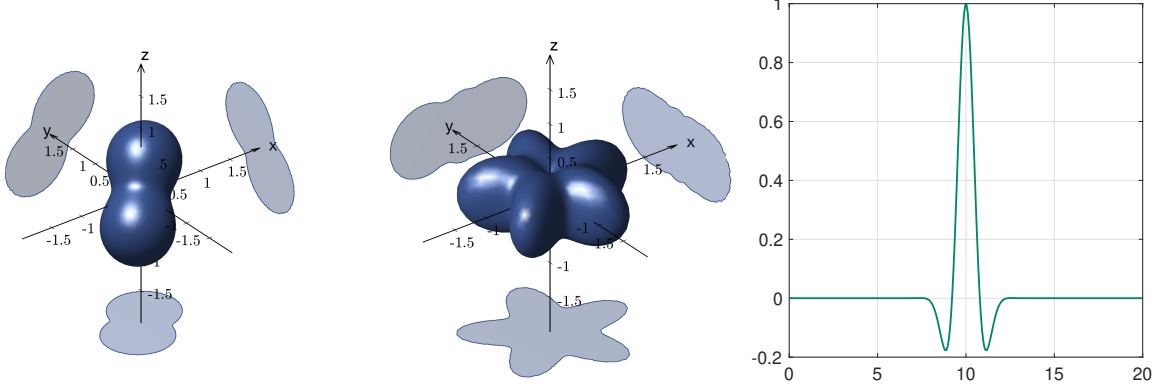


Figure 6.1: Exact shape of the scatterers in Examples 6.1 (left) and 6.2 (middle). Plot of profile f^i of incident plane wave as function of time (right).

requires the computation of the backscattered waves $F_{\theta_k}^\infty(r_n)$ and their temporal domain derivative of $(F_{\theta_k}^\infty)'(r_n)$ for each incident direction θ_k , $k = 1, \dots, K$.

In our numerical examples below we consider the two different obstacles shown in Figure 6.1: a tilted peanut-shape (left) and a sea star with five lobes (middle). We note that these exact shapes do not belong to the finite dimensional shape space that is used for the reconstruction. For both obstacles, the density inside the obstacle is chosen as $\rho_0 = 0.1$ and the wave speed inside the obstacle as $c_0 = 0.05$. The triangular mesh that we use to discretize the boundaries of these obstacles in the numerical solution of the forward problem to generate synthetic forward data has 1610 vertices.

We consider incident plane waves as in (2.1) given by

$$u^i(x, t; \theta_k) = f^i(t - \theta_k \cdot x), \quad (x, t) \in \mathbb{R}^3 \times [0, T],$$

for $k = 1, \dots, K$, where

$$f^i(t) = \chi(t - 10) \cos(-20 + 2t) e^{-(t-10)^2}, \quad t \in \mathbb{R}.$$

Here χ is a smooth cut-off function satisfying $\chi = 1$ in $[-4, 4]$ and $\chi = 0$ in $\mathbb{R} \setminus (-5, 5)$, ensuring that f^i is compactly supported, in accordance with the assumptions stated above. For the final observation time we choose $T = 20$ in both examples, using $M = 300$ equidistant time steps in $[0, T]$ in the numerical discretizations. The choice of this incoming wave is similar as in [2] and represents a plane wave modulated by a Gaussian. A plot of f^i is shown in Figure 6.1 (right). We note that both scattering obstacles are contained in a ball $B_R(0)$ of radius $R = 2$ around the origin. Accordingly, the incident waves $u^i(\cdot, \cdot; \theta_k)$, $k = 1, \dots, K$, clearly satisfy the causality condition (2.2b).

In our examples we choose three different sets of backscattering directions for the reconstruction. These are given by

- (i) $\Theta_6 := \{\pm e_1, \pm e_2, \pm e_3\}$, i.e., $K=6$,
- (ii) $\Theta_8 := \{a_1 e_1 + a_2 e_2 + a_3 e_3 \mid a_l \in \{\pm 1/\sqrt{3}\}, l = 1, 2, 3\}$, i.e., $K=8$,
- (iii) $\Theta_{14} := \Theta_6 \cup \Theta_8$, i.e., $K=14$,

where as usual e_1 , e_2 , and e_3 denote the standard basis vectors in $\mathbb{R}^3$.

For the initial guess in the GN iteration we use a ball of radius 0.3 centered at the origin, as shown in Figure 6.2 (top left). This means $r_0 \equiv 0.3$. The triangular meshes that we use to discretize the boundaries of this initial guess r_0 and all further iterates r_n , $n \in \mathbb{N}$, in the GN iteration, when computing the derivative of the regularized objective functional Ψ_{α_n} in each iteration step, have 1026 vertices.

The stopping rule for the GN iteration is determined by the relative residual

$$\text{Res}(n) := \frac{\left(\sum_{k=1}^K \|F_{\theta_k}^\infty(r_n) - u_{\theta_k}^\infty(-\theta_k, \cdot)\|_{L^2(0,T)}^2 \right)^{\frac{1}{2}}}{\left(\sum_{k=1}^K \|F_{\theta_k}^\infty(r_n)\|_{L^2(0,T)}^2 \right)^{\frac{1}{2}}}, \quad n \in \mathbb{N},$$

and by the relative update

$$\text{Up}(n) := \frac{\|r_{n+1} - r_n\|_{L^2(S^2)}}{\|r_n\|_{L^2(S^2)}}, \quad n \in \mathbb{N},$$

in the n th step of the iteration. We stop the GN iteration, when either the relative residual $\text{Res}(n)$ falls below 0.01 or if the relative update $\text{Up}(n)$ falls below $9 \cdot 10^{-4}$.

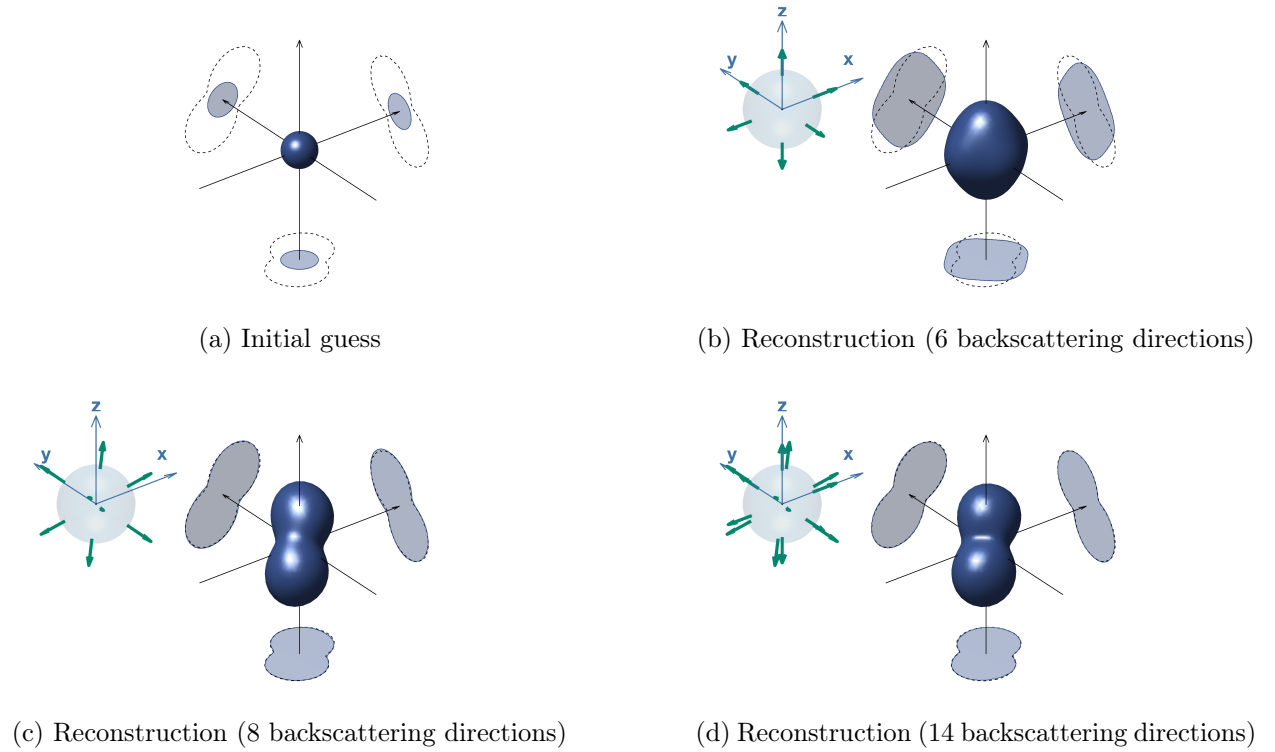


Figure 6.2: Reconstruction of tilted peanut-shape from backscattering data corresponding to 6, 8 and 14 backscattering directions. Spheres and arrows to the left of the plots (b)–(d) indicate incident/backscattering directions.

Example 6.1. In our first example we consider the peanut-shaped scattering object as shown in Figure 6.1 (left). The initial guess used in the GN iteration is shown in Figure 6.2 (top left). During

the GN iteration the regularization parameter is set to $\alpha_n = 5 \cdot 10^{-4}$ as long as $\text{Res}(n) \geq 0.1$. As soon as $\text{Res}(n) < 0.1$, we choose to reduce the regularization by setting the regularization parameter to $\alpha_n = 10^{-5}$. These values were established through trial and error.

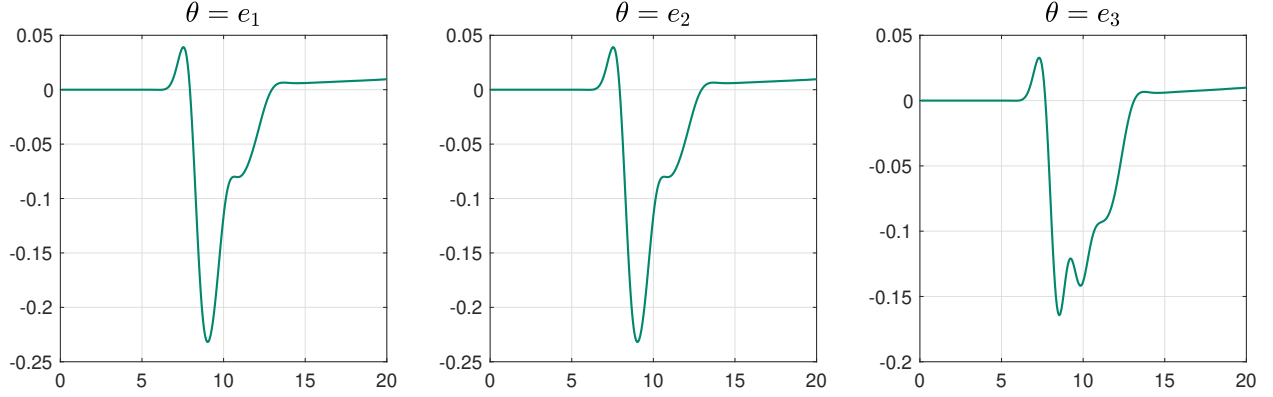


Figure 6.3: Backscattering data as function of time for 3 different backscattering directions in Example 6.1.

We start with the $K = 6$ backscattering directions in Θ_6 from case (i). Plots of the corresponding backscattering data $u^\infty(-e_1, t; e_1)$, $u^\infty(-e_2, t; e_2)$, and $u^\infty(-e_3, t; e_3)$ for $t \in [0, 20]$ are shown in Figure 6.3. Here the left plot and the plot in the middle are the same due to symmetry properties of the scattering obstacle. The initial relative residual satisfies $\text{Res}(0) = 0.78$. The GN iteration terminates after 6 iterations and the corresponding relative residual is at $\text{Res}(6) = 0.17$. The reconstruction is shown in Figure 6.2 (top right). In our second test we use the $K = 8$ backscattering directions in Θ_8 from case (ii). Here, the initial relative residual lies at $\text{Res}(0) = 0.85$. The GN iteration stops after 5 steps, and the corresponding relative residual is at $\text{Res}(5) = 0.01$. The reconstruction is shown in Figure 6.2 (bottom left). When using all $K = 14$ backscattering directions in Θ_{14} from case (iii), we obtain an initial relative residual of $\text{Res}(0) = 0.82$. The GN iteration terminates after 6 steps, and the corresponding relative residual is at $\text{Res}(6) = 0.01$. The reconstruction is shown in Figure 6.2 (bottom right).

Each final reconstruction in Figure 6.2 is shown alongside a sphere and direction vectors (top left of each reconstruction) which visualize the backscattering directions Θ_6 , Θ_8 , and Θ_{14} , respectively, that were used for the reconstruction. Furthermore, the plots include the projections of the reconstructions onto the three coordinate planes. For comparison, the corresponding projections of the exact scatterer are shown as dotted lines.

For this example, we observe that reconstructions using 8 and 14 backscattering directions yield good results. In contrast, 6 backscattering directions appear to be insufficient for achieving a satisfactory reconstruction. $\diamond$

Example 6.2. In our second example we consider the sea star-shaped scattering object, as shown in Figure 6.1 (right). As in the previous Example 6.1, we use a ball of radius 0.3, centered at the origin, shown in Figure 6.4 (top left) for the initial guess. For relative residuals $\text{Res}(n) \geq 0.1$, the regularization parameter is set to $\alpha_n = 9 \cdot 10^{-5}$ in the GN iteration. As soon as $\text{Res}(n) < 0.1$, we switch to $\alpha_n = 10^{-5}$. Again, these values were established through trial and error.

For the $K = 6$ backscattering directions in Θ_6 , the initial relative residual satisfies $\text{Res}(0) = 0.97$. The GN iteration terminates after 15 steps and the corresponding relative residual is at $\text{Res}(15) =$

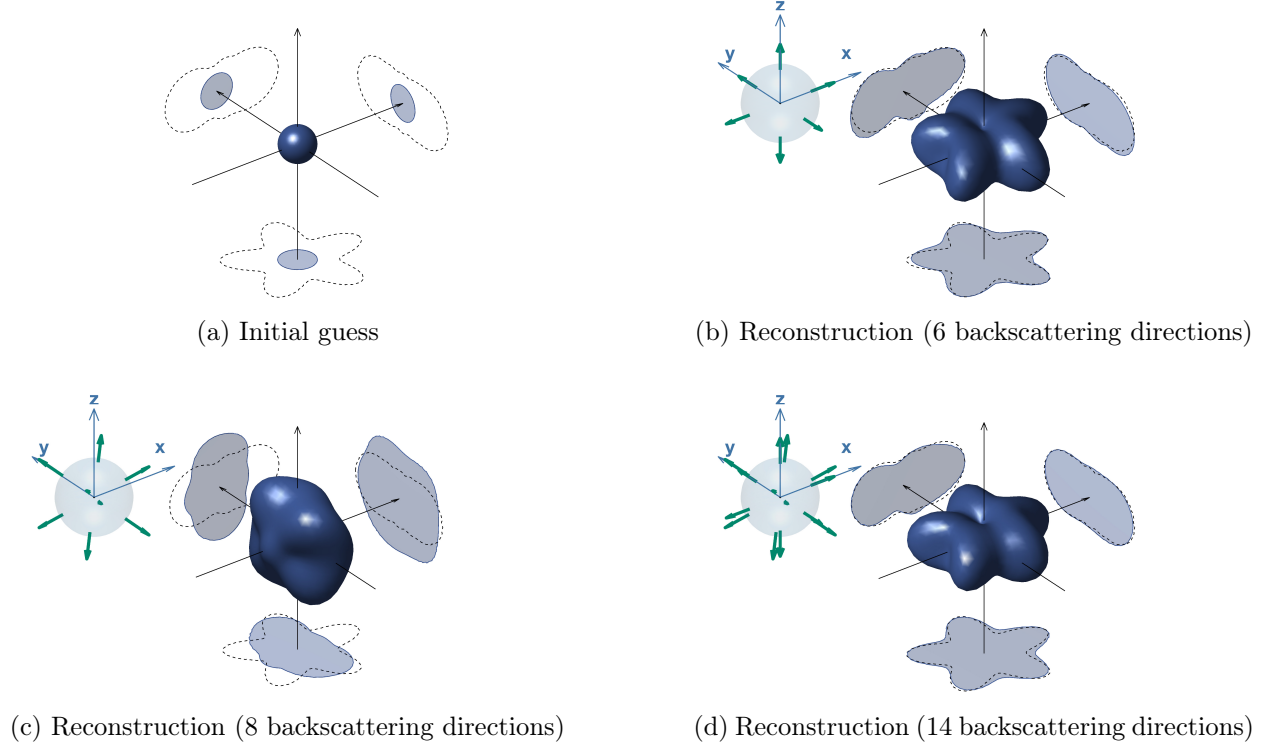


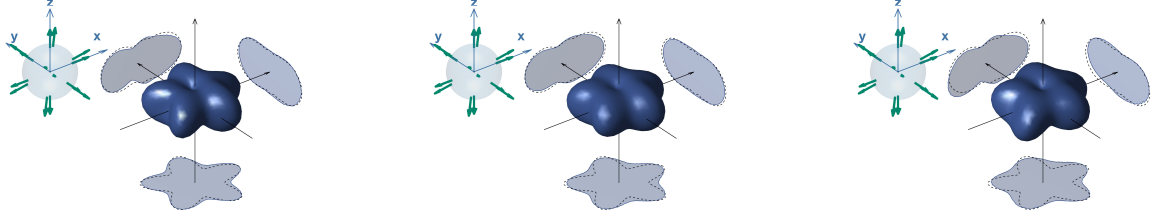
Figure 6.4: Reconstruction of sea star-shape from backscattering data corresponding to 6, 8 and 14 backscattering directions. Spheres and arrows to the left of the plots (b)–(d) indicate incident/backscattering directions.

0.02. The reconstruction is shown in Figure 6.4 (top right). When using the $K = 8$ backscattering directions in Θ_8 , the initial relative residual lies at $\text{Res}(0) = 0.93$. The GN iterations stops after 15 steps, and the corresponding relative residual is at $\text{Res}(15) = 0.05$. The reconstruction is shown in Figure 6.4 (bottom left). When using all 14 directions in Θ_{14} , we obtain an initial relative residual of $\text{Res}(0) = 0.95$. The GN iteration terminates after 11 steps, and the corresponding relative residual is at $\text{Res}(11) = 0.02$. The reconstruction is shown in Figure 6.4 (bottom right).

For this example, only the reconstruction with 14 backscattering directions produces a satisfactory result. In contrast, using 6 or 8 backscattering directions does not provide sufficient information for an accurate reconstruction. $\diamond$

Example 6.3. To assess the sensitivity of the reconstruction method to noise in the data, we repeat the previous examples using the 14 backscattering directions in Θ_{14} . The backscattering data are corrupted with additive uniformly distributed random noise at levels of 5%, 15%, and 30%, respectively. We use the same initial guess and the same regularization parameters as in Examples 6.2.

For a noise-level of 5%, we obtain an initial relative residual of $\text{Res}(0) = 0.95\%$. The GN iteration terminates after 11 steps and the corresponding relative residual is at $\text{Res}(11) = 0.06$. The reconstruction is shown in Figures 6.5 (left). When setting the noise-level to 15%, the initial relative residual lies at $\text{Res}(0) = 0.95$. The GN iteration terminates after 9 steps and the corresponding relative residual is $\text{Res}(9) = 0.16$. The reconstruction is shown in Figures 6.5 (middle). After



(a) Reconstruction (14 backscattering directions and 5% noise) (b) Reconstruction (14 backscattering directions and 15% noise) (c) Reconstruction (14 backscattering directions and 30% noise)

Figure 6.5: Reconstruction of sea star-shape from noisy backscattering data with 14 backscattering directions. Spheres and arrows to the left of the plots indicate incident/backscattering directions.

increasing the noise-level to 30%, we obtain an initial relative residual of $\text{Res}(0) = 0.96$. The GN iteration stops after 9 steps and the corresponding relative residual is at $\text{Res}(9) = 0.29$. The reconstruction is shown in Figures 6.5 (right).

For data contaminated with 5% noise, the reconstruction is almost as accurate as in the case of exact data. Even for noise levels of 15% and 30%, the reconstructions remain satisfactory. These results indicate that the proposed reconstruction method performs reasonably well in the presence of noise. $\diamond$

Appendix

A Estimates for the modified Calderón operator $\mathcal{C}(s)$

In this section we show that the operator $\mathcal{C}(s)$ from (3.13) is boundedly invertible, and we establish (3.14). Since

$$\mathcal{C}(s) = \frac{1}{c_0 \rho_0} \begin{bmatrix} c_0 \rho_0 & 0 \\ 0 & 1 \end{bmatrix} \mathcal{B}(s_0) \begin{bmatrix} c_0 \rho_0 & 0 \\ 0 & 1 \end{bmatrix} + \mathcal{B}(s),$$

where

$$\mathcal{B}(s) := \begin{bmatrix} sS(s) & K(s) \\ -K'(s) & \frac{1}{s}T(s) \end{bmatrix}$$

denotes the Calderón operator (see [4, p. 90]), we can apply [4, Lmm. 4.8] to obtain the following result.

Lemma A.1. *Let $s \in \mathbb{C}_+$, then there exists $C > 0$ such that*

$$\text{Re} \left\langle \mathcal{C}(s) \begin{bmatrix} \varphi \\ \psi \end{bmatrix}, \begin{bmatrix} \varphi \\ \psi \end{bmatrix} \right\rangle_{\mathcal{X}', \mathcal{X}} \geq C \min(1, |s|^2) \frac{\text{Re}(s)}{|s|^2} (\|\varphi\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\psi\|_{H^{\frac{1}{2}}(\partial D)}^2) \quad (\text{A.1})$$

for all $(\varphi, \psi) \in \mathcal{X}$. In particular, the operator $\mathcal{C}(s) : \mathcal{X} \rightarrow \mathcal{X}'$ is coercive.

Accordingly, the operator $\mathcal{C}(s)$ is invertible for all $s \in \mathbb{C}_+$, and a bound for the norm of its inverse can be obtained similarly to [4, Lmm. 7.2].

Lemma A.2. *There exists $C_\sigma > 0$ such that*

$$\|\mathcal{C}^{-1}(s)\|_{\mathcal{X} \leftarrow \mathcal{X}'} \leq C_\sigma \frac{|s|^2}{\text{Re}(s)}, \quad \text{Re}(s) \geq \sigma > 0. \quad (\text{A.2})$$

Proof. Let $(g, h) \in \mathcal{X}'$. Since $\mathcal{C}(S)$ is invertible, we can define

$$\begin{bmatrix} \varphi \\ \psi \end{bmatrix} := \mathcal{C}^{-1}(s) \begin{bmatrix} g \\ h \end{bmatrix}.$$

Using (A.1), we obtain

$$\begin{aligned} C \min(1, |s|^2) \frac{\operatorname{Re}(s)}{|s|^2} \left(\|\varphi\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\psi\|_{H^{\frac{1}{2}}(\partial D)}^2 \right) &\leq \left| \left\langle \mathcal{C}(s) \begin{bmatrix} \varphi \\ \psi \end{bmatrix}, \begin{bmatrix} \varphi \\ \psi \end{bmatrix} \right\rangle_{\mathcal{X}', \mathcal{X}} \right| \\ &= \left| \left\langle \begin{bmatrix} g \\ h \end{bmatrix}, \begin{bmatrix} \varphi \\ \psi \end{bmatrix} \right\rangle_{\mathcal{X}', \mathcal{X}} \right| \leq \left(\|h\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|g\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}} \left(\|\varphi\|_{H^{-\frac{1}{2}}(\partial D)}^2 + \|\psi\|_{H^{\frac{1}{2}}(\partial D)}^2 \right)^{\frac{1}{2}}. \end{aligned}$$

This shows (A.2). □

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