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Boundary element methods for control problems subject to the exterior Helmholtz equation

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Abstract

In this thesis we consider Dirichlet and Neumann boundary control problems subject to the Helmholtz equation, which has to be solved in three dimensional unbounded exterior domains. In case of the Dirichlet boundary control problem, the $\mathrm{H}^{1/2}(\Gamma_C)$-norm is used for regularization and in case of the Neumann boundary control problem the $\mathrm{H}^{-1/2}(\Gamma_C)$-norm is used. The observation takes place on volumes, two dimensional manifolds, curves or finitely many points. In case of the Dirichlet boundary control problem, control constraints are used. As we have to solve the Helmholtz equation in unbounded exterior domains, we use boundary integral equations and the corresponding boundary element method. Another motivation for using boundary integral equations is given by the fact that the control takes place on the boundary of the domain. For special wave numbers it is well known for boundary integral equations that spurious modes can appear. Therefore, modified boundary integral equations are used to circumvent this phenomenon. For the numerical approximation a symmetric boundary element approach is used. Due to control constraints in case of the Dirichlet boundary control problem, the first order optimality condition is given by a variational inequality. To solve the corresponding discrete variational inequality, a semi-smooth Newton method is used. In case of the Neumann boundary control problem, the first order optimality condition is given by a boundary integral equation. Therefore, a standard linear solver can be used to solve the corresponding system of linear equations. Eventually, numerical examples verify the proven theoretical results.

Zusammenfassung

In dieser Arbeit werden Dirichlet und Neumann Randsteuerungsprobleme betrachtet. Die zugehörige Nebenbedingung ist gegeben durch die Helmholtzgleichung, welche im dreidimensionalen unbeschränkten Außenraum gelöst wird. Im Falle der Dirichlet Randsteuerung wird die $\mathrm{H}^{1/2}(\Gamma_C)$-Norm zur Regularisierung verwendet und im Falle der Neumann Steuerung die $\mathrm{H}^{-1/2}(\Gamma_C)$-Norm. Die Beobachtung findet auf dreidimensionalen Objekten, zweidimensionalen Mannigfaltigkeiten, Kurven oder auf endlich vielen Punkten statt. Im Falle der Dirichlet Randsteuerung können zusätzlich Steuerbeschränkungen verwendet werden. In dieser Arbeit werden Randintegralgleichungen und die dazugehörige Randelementmethode verwendet. Ein großer Vorteil dieser Methode besteht darin, dass das Lösen von partiellen Differentialgleichungen im unbeschränkten Außenraum nicht schwieriger ist, als im beschränkten Innenraum. Durch die Verwendung von Randintegralgleichungen ist es möglich, das Außenraumproblem auf den Rand zu reduzieren. Daher sind Randintegralgleichungen für die Behandlung von Randsteuerungsproblemen besonders geeignet. Um Wohldefiniertheit für beliebige Wellenzahlen gewährleisten zu können, werden modifizierte Randintegralgleichungen verwendet. Bezüglich der Diskretisierung wird eine symmetrische Formulierung gewählt. Im Falle von Steuerbeschränkungen wird die Optimalitätsbedingung durch eine Variationsungleichung beschrieben. Die zugehörige diskrete Variationsungleichung wird unter Zuhilfenahme der semiglatten Newton Methode gelöst. Falls keine Steuerbeschränkungen vorliegen, wird die Optimalitätsbedingung durch eine Randintegralgleichung charakterisiert. Das zugehörige lineare Gleichungssystem kann daher mit üblichen Methoden gelöst werden. Für beide Randsteuerungsprobleme werden numerische Beispiele herangezogen, um die theoretischen Aussagen zu überprüfen. Es stellt sich heraus, dass die Theorie in den numerischen Beispielen sehr gut widergespiegelt wird.

Contents

1 Introduction

Motivation

The wave equation plays an important role in many branches of engineering. For linear acoustics the wave equation can be used to model the propagation of acoustic waves, see [27]. In applications of acoustics time harmonic excitations arise quite often. When dealing with time harmonic excitations, it is possible to transform the time and spatial dependent wave equation into a partial differential equation which depends only on the spatial variables, see [40]. The resulting complex valued equation

$$-\Delta u - \kappa^2 u = 0$$

is named after the German physician and physicist Hermann von Helmholtz. κ is called the wave number and the scalar function u can describe e.g. the alternating part of the acoustic pressure. In this thesis, the Helmholtz equation plays a central role. Unbounded domains arise quite often in practical applications. However, solving the Helmholtz equation in unbounded domains is a challenging task and radiation conditions have to be considered. A widespread radiation condition is named after the German theoretical physicist Arnold Sommerfeld, see [54].

In many applications direct simulations are not sufficient and optimal control problems or inverse problems have to be considered, see [14, 35]. In this thesis we want to discuss and analyze optimal control problems, where we minimize a cost functional subject to the Helmholtz equation in unbounded exterior domains. The control takes place on the boundary of the domain, hence this kind of minimization problem is called boundary control problem. Dirichlet as well as Neumann boundary control problems are considered in this thesis, see [38, 66]. The corresponding cost functional turns out to be quadratic and

strictly convex. Such kind of problems are analyzed in e.g. [64]. Applications can be found in acoustics, where the aim is to control on the boundary, such that a desired behavior of the pressure is obtained in some part of the domain. Sound source reconstruction could be another possible application.

In most cases analytic solutions are not known and one has to use numerical methods. Over the years the finite difference method [62], the finite element method [5], the finite volume method [18] and the boundary element method [39] turned out to be quite useful tools to approximate the solution of partial differential equations. As unbounded domains are considered in this thesis, the boundary element method will be used. Of course, the coupling of different numerical tools can be advantageous. E.g. the coupling of finite elements and boundary elements turned out to be a quite successful concept [24]. However, coupling of different methods is out of the scope of this thesis. The main idea of the boundary element method consists in the reduction of the partial differential equation to a problem which is defined on the boundary. The resulting equations are called boundary integral equations. As in most applications the boundaries of unbounded domains are bounded, unbounded domains can be used in a quite natural way. Furthermore, it turns out that the solution automatically satisfies the desired radiation condition. The boundary element method requires the knowledge of a so-called fundamental solution. In case of the Helmholtz equation, the fundamental solution is well known. Further details about the theory of boundary integral equations can be found in e.g. [14, 25, 39, 40, 50, 57].

Outline

In the second chapter the already mentioned Helmholtz equation will be discussed in more detail. Afterwards, some basics from functional analysis as well as Sobolev spaces will be discussed. Boundary integral equations for the Helmholtz equations will be derived. Approximation methods will be analyzed for two kinds of problems. The discretization of boundary integral equations leads to the boundary element method, which will be discussed in the last part of chapter two.

"Exterior Dirichlet boundary control problems" is the main topic of the third chapter. At first, the minimization problem will be introduced. Afterwards, unique solvability and first order optimality conditions will be discussed. The main result is the derivation of the so-called optimality system, which consists of a primal problem, a dual problem, a point evaluation and an optimality condition. Boundary integral equations will be the major ingredient in this chapter. Due to control constraints, the optimality condition is given by a variational inequality. The discretization of the optimality system and the derivation of error estimates for the control is the next issue. To handle discrete variational inequalities, a semi-smooth Newton method will be used. Eventually, numerical examples will be shown and the proven theory will be validated.

In the forth chapter, exterior Neumann boundary control problems will be analyzed. The procedure is similar to the previous chapter. Therefore, an optimality system will be derived and discretized. For the Neumann boundary control problem no control constraints are used. Hence, the resulting optimality condition results in an equation which is defined on the boundary. Again, numerical examples will be shown. It will turn out that the theory and the numerical results fit together very well.

2 Preliminaries

In the first part of this chapter we focus on the Helmholtz equation to model the propagation of acoustic waves. We are interested in linear acoustics with time harmonic excitations. For such kind of problems the Helmholtz equation is a popular and widespread model, see [14] or [27] for more details.

In the second part we will consider functional analytic basics. The used references are [2, 36, 39, 67, 71]. The main result will be the well known Fredholm alternative.

Next, some Sobolev spaces, see [1, 39, 69], will be introduced. As boundary integral equations will be used, Sobolev spaces defined on the boundary are the relevant ones.

In the forth section, boundary integral equations are discussed for the Helmholtz equation in unbounded exterior domains, see [25, 44, 57]. Using the Fredholm alternative, it will be shown that critical wave numbers and corresponding spurious modes exist. For such critical wave numbers, the standard boundary integral equation is not uniquely solvable, although the boundary value problem is uniquely solvable. Therefore, modified boundary integral equations will be introduced, which are robust in these critical wave numbers, see [56, 60, 61, 68].

Finally, general approximation methods will be discussed, see [21, 57]. One special approximation method is given by the boundary element method, which will be introduced at the end of this chapter.

2.1 Helmholtz equation

In this thesis we consider acoustic phenomena in homogeneous isotropic media. Furthermore, we are interested in linear acoustics. Therefore, the wave equation is a good model to describe the propagation of acoustic waves. For a given bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ with corresponding boundary Γ and a given constant $T > 0$ we want to solve the wave equation

$$-\Delta U + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}U = 0 \quad \text{in } \Omega \times (0,T)$$

with Dirichlet boundary conditions

$$U = G_d \quad \text{on } \Gamma \times (0,T)$$

or Neumann boundary conditions

$$\frac{\partial}{\partial \boldsymbol{n}}U = G_n \quad \text{on } \Gamma \times (0,T)$$

and initial conditions

$$\begin{aligned} U &= U_0 \quad \text{in } \Omega \times \{0\}, \\ \frac{\partial}{\partial t}U &= U_1 \quad \text{in } \Omega \times \{0\}. \end{aligned}$$

The function $U(\boldsymbol{x}, t)$ describes the alternating part of the acoustic pressure and the given constant c is called the speed of sound. In case of a Dirichlet boundary value problem, the function G_d defined on $\Gamma \times (0,T)$ is given and in case of a Neumann boundary value problem, the function G_n is given. In acoustics Dirichlet conditions are used to describe sound-soft obstacles and Neumann conditions are used to describe sound-hard obstacles.

The wave equation can be derived by using Euler's equations, the equation of continuity and the state equation, which describes the relation between pressure and density. To obtain the wave equation, it is assumed that all thermodynamic processes are adiabatic. Finally, it is assumed that all occurring quantities are small perturbations of the static state. Therefore, linearization is justified and we obtain the wave equation. For more details see [14] or [27] and the references therein.

In the following we are interested in time harmonic excitations, i.e. in case of a Dirichlet boundary value problem the Dirichlet datum is given by

$$G_d(\boldsymbol{x}, t) = \Re\left(e^{-i\omega t} g_d(\boldsymbol{x})\right)$$

and in case of a Neumann boundary value problem the Neumann datum is given by

$$G_n(\boldsymbol{x}, t) = \Re\left(e^{-i\omega t} g_n(\boldsymbol{x})\right),$$

respectively. The given data g_d and g_n depend only on the spatial variable $\boldsymbol{x}$ and the used constant ω is called the angular frequency. Therefore, the frequency f is given by $f = \frac{\omega}{2\pi}$. This motivates the time harmonic ansatz

$$U(\boldsymbol{x}, t) = \Re\left(e^{-i\omega t} u(\boldsymbol{x})\right).$$

No initial conditions are considered anymore. Hence, this approach is not correct for the transient state. Only for the steady state this is justified.

Next we define the wave number κ as $\kappa := \frac{\omega}{c}$. When we insert the time harmonic ansatz into the wave equation, we end up with the Helmholtz equation, i.e. we have to solve

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega, \\ u &= g_d \quad \text{on } \Gamma, \end{aligned}$$

in case of a Dirichlet boundary value problem and

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega, \\ \frac{\partial}{\partial \boldsymbol{n}} u &= g_n \quad \text{on } \Gamma, \end{aligned}$$

in case of a Neumann boundary value problem, respectively.

In many applications the spatial domain of interest is unbounded. In this case we denote the unbounded domain by Ω^c, i.e. $\Omega^c = \mathbb{R}^3 \setminus \bar{\Omega}$. For unbounded Dirichlet and Neumann problems we have to introduce a suitable radiation condition for the alternating part of the acoustic pressure. One possibility would be to use the well known Sommerfeld radiation condition

$$\lim_{|\boldsymbol{x}|=R\to\infty} R\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u\right) = 0,$$

see [54]. When dealing with boundary integral equations, it turns out that there is a related, more practical radiation condition. In the following we will claim that the function u satisfies the radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \mathrm{d}\mu = 0,$$

see [39, Theorem 9.6] or [47].

To motivate these conditions, we look at the following example. The function

$$U(\boldsymbol{x}, t) = \frac{\cos\left(\omega\left(-t + \frac{1}{c}|\boldsymbol{x}|\right)\right)}{|\boldsymbol{x}|}$$

and the corresponding time independent function $u(\boldsymbol{x}) = \frac{e^{i\kappa|\boldsymbol{x}|}}{|\boldsymbol{x}|}$ satisfy the Sommerfeld radiation condition and therefore also the radiation condition of Rellich. Obviously the function $U(\boldsymbol{x}, t)$ is an outgoing wave with speed c satisfying the wave equation. For the incoming wave

$$U(\boldsymbol{x}, t) = \frac{\cos\left(\omega\left(t + \frac{1}{c}|\boldsymbol{x}|\right)\right)}{|\boldsymbol{x}|}$$

the radiation condition is not satisfied.

In the following we always assume that all assumptions concerning linear acoustics are satisfied. Furthermore, we assume that the time domain is apart from the transient state. Therefore, the time harmonic ansatz is justified and we only have to deal with time independent problems.

As we are interested in unbounded domains, we sum up the results for this case. The appearing quantities depend only on the spatial variable $\boldsymbol{x}$, hence the following notation should not be misleading. In the following, the Dirichlet datum is denoted by g and the Neumann datum by t. In case of a Dirichlet boundary value problem we have to solve

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega^c, \\ u &= g \quad \text{on } \Gamma, \end{aligned}$$

where the unknown function u has to satisfy

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \mathrm{d}\mu = 0.$$

In case of a Neumann boundary value problem we have to solve

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega^c, \\ \frac{\partial}{\partial \boldsymbol{n}} u &= t \quad \text{on } \Gamma. \end{aligned}$$

Again u has to satisfy the radiation condition of Rellich, i.e.

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \mathrm{d}\mu = 0.$$

In the next section we focus on the functional analytic basics.

2.2 Functional analytic basics

In this section, the main focus is on the functional analytic basics which are used in this thesis.

As we have seen in Section 2.1, the solution of the Helmholtz equation is a complex valued function. Hence all Sobolev spaces which are introduced later and their corresponding inner products have to be defined in a complex setting. Primarily we use the notation from [39]. More about functional analytic results can be found in e.g. [2, 36, 39, 67, 71].

Let X be a Hilbert space. The dual space is then denoted by X^* and is defined as the set of all bounded and linear functionals from X to $\mathbb{C}$. The following notation is used: for $(u, f) \in X \times X^*$ we define

$$\langle f, u \rangle_{X^* \times X} := f(u).$$

The used norm is given by

$$\|f\|_{X^*} := \sup_{0 \neq u \in X} \frac{|\langle f, u \rangle_{X^* \times X}|}{\|u\|_X}.$$

The dual space of X^* is denoted by X^{**} and is identified by X. Therefore it is possible to define

$$\langle u, f \rangle_{X \times X^*} := \langle f, u \rangle_{X^* \times X}.$$

In case that the conjugate complex is defined in X, we can define the conjugate complex of $f \in X^*$ by:

$$\langle \bar{f}, u \rangle_{X^* \times X} := \overline{\langle f, \bar{u} \rangle_{X^* \times X}}.$$

In this definition, the conjugate complex of X and $\mathbb{C}$ is used. Later we will use the space $\mathrm{H}^s(\Gamma), s \geq 0$, where the conjugate complex is well defined. Using the above definition of the conjugate complex of the dual space, we can therefore extend this to the space $\mathrm{H}^{-s}(\Gamma)$. Therefore it is possible to define the real part and the imaginary part of f:

$$\Re f := \frac{1}{2}(f + \bar{f}), \quad \Im f := -\frac{i}{2}(f - \bar{f}).$$

In the following we do not use $\langle \cdot, \cdot \rangle_{X^* \times X}$ and $\langle \cdot, \cdot \rangle_{X \times X^*}$. Instead we use

$$(f, u)_{X^* \times X} := \langle \bar{f}, u \rangle_{X^* \times X} \quad \text{and} \quad (u, f)_{X \times X^*} := \langle \bar{u}, f \rangle_{X \times X^*}.$$

Therefore there holds

$$(u, f)_{X \times X^*} = \overline{(f, u)_{X^* \times X}}.$$

In the following we are interested in linear operators, mapping from X to its dual X^* or more general from X to another Hilbert space Y.

Definition 2.1 (Adjoint operator)**.** *Let X, Y be two Hilbert spaces. The adjoint operator of the linear operator $A\colon X \to Y$ is the mapping $A^*\colon Y^* \to X^*$ which satisfies*

$$(A^* v, u)_{X^* \times X} = (v, Au)_{Y^* \times Y}$$

for all $u \in X$ and $v \in Y^*$.

In the special case $A\colon X \to X^*$ it is more convenient to use the following definition for the adjoint operator.

Definition 2.2 (Adjoint operator)**.** *Let X be a Hilbert space and $A\colon X \to X^*$ be a linear operator. The adjoint operator is the mapping $A^*\colon X \to X^*$ which is characterized by*

$$(A^* v, u)_{X^* \times X} = (v, Au)_{X \times X^*} = \overline{(Au, v)_{X^* \times X}},$$

for all $u, v \in X$.

In the following the second definition of the adjoint operator is used, as the bi-dual space can be omitted. Bounded operators which are X-elliptic or X-coercive play an important role in the theory of partial differential equations. Therefore they will be introduced in the following definitions:

Definition 2.3 (Bounded operator)**.** *Let X, Y be two Hilbert spaces. A linear operator $A\colon X \to Y$ is called bounded, if there exists a constant $c \geq 0$ such that*

$$\|Au\|_Y \leq c\|u\|_X$$

is satisfied for all $u \in X$.

If the operator A is a mapping form X to X^* we obtain

$$|\,(Au, v)_{X^* \times X}\,| \leq c\|u\|_X \|v\|_X,$$

for all $u, v \in X$.

Definition 2.4 (X-elliptic operator)**.** *Let X be a Hilbert space. A linear operator $A\colon X \to X^*$ is called X-elliptic, if there exists a constant $c > 0$ such that*

$$\Re\,(Au, u)_{X^* \times X} \geq c\|u\|_X^2,$$

for all $u \in X$.

Definition 2.5 (X-coercive operator)**.** *Let X be a Hilbert space. A linear operator $A\colon X \to X^*$ is called X-coercive, if there exists a constant $c > 0$ and a compact operator $C\colon X \to X^*$ such that the Gårding inequality*

$$\Re\,((A + C)\,u, u)_{X^* \times X} \geq c\|u\|_X^2$$

is satisfied for all $u \in X$.

Using the same idea, we can also define U-elliptic and U-coercive operators for subspaces U of X.

A more general characterization of operators is the concept of Fredholm operators with index n.

Definition 2.6 (Fredholm operator and index)**.** *Let X, Y be two Hilbert spaces. A bounded and linear operator $A\colon X \to Y$ is said to be Fredholm with index n if*

- *the subspace* $\mathrm{Im}A$ *is closed in* Y*,*
- *the subspaces* $\mathrm{Ker}A$ *and* $Y \setminus \mathrm{Im}A$ *are finite-dimensional.*

The index n is then defined by

$$n := \mathrm{ind}A := \dim \mathrm{Ker}A - \dim\left(Y \setminus \mathrm{Im}A\right).$$

In case of a bounded and X-elliptic operator $A\colon X \to X^*$, the well known Lax-Milgram Lemma [33] states, that A is a Fredholm operator with index zero.

Using [39, Theorem 2.33] we can show that a bounded and X-coercive operator is a Fredholm operator with index zero. This is due to the fact that a X-coercive operator is a X-elliptic operator which is disturbed by a compact operator.

The following theorem is a very important statement about Fredholm operators with index zero, which can be applied onto X-coercive operators.

Theorem 2.7 (Fredholm alternative)**.** *Let X, Y be two Hilbert spaces and $A\colon X \to Y$ be a Fredholm operator with index zero. There are two mutually exclusive possibilities:*

- *A is injective:*
  In this case, the operator equation $Au = v$ has a unique solution $u \in X$ for a given $v \in Y$. Additionally, the adjoint equation $A^*g = f$, where $f \in X^*$ is given, has a unique solution $g \in Y^*$.
- *A is not injective:*
  In this case a $p \in \mathbb{N} \setminus \{0\}$ exists, such that the homogeneous equation $Au = 0$ has p linear independent solutions $u_1, \cdots, u_p \in X$. The same is true for the adjoint homogeneous equation, i.e. there exist p linear independent solutions $g_1, \cdots, g_p \in Y^*$ of the equation $A^*g = 0$. The inhomogeneous equation $Au = v$ is solvable if and only if the right-hand side satisfies $(g_i, v)_{Y^* \times Y} = 0$ for all $i \in \{1, \cdots, p\}$. Analogously, the inhomogeneous adjoint equation $A^*g = f$ is solvable if and only if the right-hand side satisfies $(f, u_i)_{X^* \times X} = 0$ for all $i \in \{1, \cdots, p\}$.

The proof is based on the closed range theorem and can be found in e.g. [39, Theorem 2.27].

Therefore we get, that for an injective, bounded and X-coercive operator $A\colon X \to X^*$ and for a given right-hand side $f \in X^*$, the equation

$$Au = f$$

has a unique solution. Due to the bounded inverse theorem, see [67, Corollary IV.3.4] or [48, Corollary 2.12], there holds the stability estimate

$$\|u\|_X \leq c\|f\|_{X^*}.$$

Finally we will discuss a result for variational inequalities. For a non-empty, bounded, closed and convex set $X_{ad} \subset X$ we are now interested in finding $u \in X_{ad}$ such that

$$\Re\,(Au, v-u)_{X^*\times X} \geq \Re\,(f, v-u)_{X^*\times X}\,, \tag{2.1}$$

for all $v \in X_{ad}$ instead of the equation $Au = f$. Again f is assumed to be a given element in the dual of X.

Theorem 2.8. *Let X be a Hilbert space and $A\colon X \to X^*$ a bounded and X-elliptic operator. The X-ellipticity constant is denoted by c_1. Furthermore let X_{ad} be a non-empty, bounded, closed and convex subset of X. There exists a unique solution $u \in X_{ad}$ of the variational inequality*

$$\Re\,(Au, v-u)_{X^*\times X} \geq \Re\,(f, v-u)_{X^*\times X}\,,$$

for all $v \in X_{ad}$, for any given right hand side $f \in X^*$ and there holds

$$\|u\|_X \leq \frac{1}{c_1}\|f\|_{X^*}.$$

A proof can be found in e.g. [37, Theorem 2.1]. For a general introduction to variational inequalities see [31].

2.3 Sobolev spaces

In this section we introduce some of the well known Sobolev spaces. More about this topic can be found in e.g. [1, 39, 69]. $\Omega \subset \mathbb{R}^3$ is assumed to be a bounded Lipschitz domain. The boundary of Ω is denoted by Γ, i.e.

$$\Gamma := \bar{\Omega} \cap \left(\mathbb{R}^3 \setminus \Omega\right).$$

The outer normal vector is denoted by $\boldsymbol{n}$. The support of a function $u\colon \Omega \to \mathbb{C}$ is defined by

$$\operatorname{supp} u := \overline{\{\boldsymbol{x} \in \Omega\colon u(\boldsymbol{x}) \neq 0\}}.$$

For compact sets $K \subset \Omega$ we can define the space

$$\mathcal{C}_K^r(\Omega) := \{u \in \mathcal{C}^r(\Omega) : \operatorname{supp} u \subset K\}$$

and put

$$\mathcal{C}_K^\infty(\Omega) := \bigcap_{r \geq 0} \mathcal{C}_K^r(\Omega).$$

Further important spaces are given by

$$\mathcal{D}(\Omega) := \{u \in \mathcal{C}_K^\infty(\Omega) \text{ for some } K \Subset \Omega\}$$

and

$$\mathcal{S}\left(\mathbb{R}^3\right) := \left\{\phi \in \mathcal{C}^\infty\left(\mathbb{R}^3\right) : \sup_{\boldsymbol{x} \in \mathbb{R}^3} \left|\boldsymbol{x}^\alpha \partial^\beta \phi(\boldsymbol{x})\right| < \infty \text{ for all multi-indices } \alpha, \beta\right\}.$$

For these two spaces we can define the spaces of linear and continuous functionals $\mathcal{D}^*(\Omega)$ and $\mathcal{S}^*(\mathbb{R}^3)$ respectively. The elements of $\mathcal{D}^*(\Omega)$ are called Schwartz distributions and the elements of $\mathcal{S}^*(\mathbb{R}^3)$ temperate distributions. The concept of continuity for these two function spaces is explained in more details in [39]. For a Schwartz distribution $l \in \mathcal{D}^*(\Omega)$ we introduce

$$\langle l, \varphi \rangle_{\mathcal{D}^*(\Omega) \times \mathcal{D}(\Omega)} := l(\varphi) \quad \text{and} \quad (l, \varphi)_{\mathcal{D}^*(\Omega) \times \mathcal{D}(\Omega)} := \langle \bar{l}, \varphi \rangle_{\mathcal{D}^*(\Omega) \times \mathcal{D}(\Omega)},$$

for all $\varphi \in \mathcal{D}(\Omega)$ and for a temperate distribution $l \in \mathcal{S}^*(\mathbb{R}^3)$ we introduce

$$\langle l, \varphi \rangle_{\mathcal{S}^*(\mathbb{R}^3)\times\mathcal{S}(\mathbb{R}^3)} := l(\varphi) \quad \text{and} \quad (l, \varphi)_{\mathcal{S}^*(\mathbb{R}^3)\times\mathcal{S}(\mathbb{R}^3)} := \langle \bar{l}, \varphi \rangle_{\mathcal{S}^*(\mathbb{R}^3)\times\mathcal{S}(\mathbb{R}^3)},$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$.

For $s \in \mathbb{R}$ we use the Sobolev space $\mathrm{H}^s(\mathbb{R}^3)$ and the corresponding norm $\|\cdot\|_{\mathrm{H}^s(\mathbb{R}^3)}$ as defined in [39, Chapter 3]. For $s \in \mathbb{R}$ the Sobolev space, defined on Ω, is then given by

$$\mathrm{H}^s(\Omega) := \left\{ u \in \mathcal{D}(\Omega)^* : u = U|_\Omega, \text{ for some } U \in \mathrm{H}^s\left(\mathbb{R}^3\right) \right\}.$$

The corresponding norm can be expressed by the norm of $\mathrm{H}^s(\mathbb{R}^3)$:

$$\|u\|_{\mathrm{H}^s(\Omega)} := \min_{U \in \mathrm{H}^s(\mathbb{R}^3):\, U|_\Omega = u} \|U\|_{\mathrm{H}^s(\mathbb{R}^3)}.$$

Two further Sobolev spaces are defined by

$$\tilde{\mathrm{H}}^s(\Omega) := \overline{\mathcal{D}(\Omega)}^{\|\cdot\|_{\mathrm{H}^s(\mathbb{R}^3)}} \quad \text{and} \quad \mathrm{H}_0^s(\Omega) := \overline{\mathcal{D}(\Omega)}^{\|\cdot\|_{\mathrm{H}^s(\Omega)}}.$$

In Theorem [39, Theorem 3.30] it is shown that there holds

$$\mathrm{H}^s(\Omega)^* = \tilde{\mathrm{H}}^{-s}(\Omega) \text{ and } \tilde{\mathrm{H}}^s(\Omega)^* = \mathrm{H}^{-s}(\Omega), \text{ for all } s \in \mathbb{R}.$$

As we are interested in boundary integral equations, the main focus is on Sobolev spaces defined on the boundary, see [25]. For $s \in [0, 1)$, the space $\mathrm{H}^s(\Gamma)$ is defined by

$$\mathrm{H}^s(\Gamma) := \overline{\mathcal{C}^0(\Gamma)}^{\|\cdot\|_{\mathrm{H}^s(\Gamma)}}.$$

The norm $\|\cdot\|_{\mathrm{H}^s(\Gamma)}$ is defined by

$$\|u\|^2_{\mathrm{H}^s(\Gamma)} := \int_\Gamma |u|^2 \,\mathrm{d}\mu + \int_\Gamma \int_\Gamma \frac{|u(\boldsymbol{x}) - u(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|^{2+2s}} \,\mathrm{d}\mu_{\boldsymbol{x}} \,\mathrm{d}\mu_{\boldsymbol{y}},$$

if $s \neq 0$ and

$$\|u\|^2_{\mathrm{H}^s(\Gamma)} := \int_\Gamma |u|^2 \,\mathrm{d}\mu$$

otherwise. For $s \in (0,1)$ we also define the seminorm $|\cdot|_{\mathrm{H}^s(\Gamma)}$ by

$$|u|^2_{\mathrm{H}^s(\Gamma)} := \int_\Gamma \int_\Gamma \frac{|u(\boldsymbol{x}) - u(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|^{2+2s}} \,\mathrm{d}\mu_{\boldsymbol{x}} \,\mathrm{d}\mu_{\boldsymbol{y}}.$$

For $s \in [0,1)$, the Sobolev space $\mathrm{H}^{-s}(\Gamma)$ is defined as the dual space of $\mathrm{H}^s(\Gamma)$.

If Ω is more regular, we are able to define Sobolev spaces of higher order. The space $\mathrm{H}^s(\Gamma)$ is well defined for $|s| \leq k$, if Ω is $\mathcal{C}^{k-1,1}$, for $k \geq 1$.

Let $\Gamma_O \subset \Gamma$ be a given non-empty, open and sufficiently smooth part of the boundary. For $s \in \mathbb{R}$ we define

$$\mathrm{H}^s(\Gamma_O) := \left\{ \tilde{u}|_{\Gamma_O} \colon \tilde{u} \in \mathrm{H}^s(\Gamma) \right\}.$$

The corresponding norm is defined by

$$\|u\|_{\mathrm{H}^s(\Gamma_O)} := \inf_{\tilde{u} \in \mathrm{H}^s(\Gamma) \colon \tilde{u}|_{\Gamma_O} = u} \|\tilde{u}\|_{\mathrm{H}^s(\Gamma)}.$$

If Γ is piecewise smooth, i.e. if Γ can be decomposed into $J \in \mathbb{N}$ smooth parts Γ_j, $j \in \{1, \cdots, J\}$ such that

$$\Gamma = \bigcup_{j=1}^{J} \bar{\Gamma}_j, \quad \Gamma_i \cap \Gamma_j = \emptyset \quad \text{for } i \neq j,$$

we define the spaces $\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma)$ and $\mathrm{H}^{-\mathrm{s}}_{\mathrm{pw}}(\Gamma)$, for $s > 0$, by

$$\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma) := \left\{ u \in \mathrm{L}^2(\Gamma) : u|_{\Gamma_j} \in \mathrm{H}^s(\Gamma_j),\, j \in \{1, \cdots, J\} \right\},$$
$$\mathrm{H}^{-\mathrm{s}}_{\mathrm{pw}}(\Gamma) := \prod_{j=1}^{J} \mathrm{H}^s(\Gamma_j)^*.$$

The corresponding norms are defined by

$$\|u\|^2_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma)} := \sum_{j=1}^{J} \left\| u|_{\Gamma_j} \right\|^2_{\mathrm{H}^s(\Gamma_j)},$$
$$\|u\|_{\mathrm{H}^{-\mathrm{s}}_{\mathrm{pw}}(\Gamma)} := \sum_{j=1}^{J} \left\| u|_{\Gamma_j} \right\|_{\mathrm{H}^s(\Gamma_j)^*}.$$

One important statement about Sobolev spaces is the following theorem, see [39, Theorem 3.37].

Theorem 2.9. *Let $k \geq 1$ and let Ω be a $\mathrm{C}^{k-1,1}$ domain. For $\frac{1}{2} < s \leq k$ the trace operator $\gamma_0 \colon \mathrm{H}^s(\Omega) \to \mathrm{H}^{s-1/2}(\Gamma)$ is a bounded and linear operator.*

In case of a Lipschitz domain, i.e. Ω is $\mathrm{C}^{0,1}$, this result can be improved to the following theorem.

Theorem 2.10. *Let Ω be a Lipschitz domain, then the trace operator γ_0 is linear and bounded for $\frac{1}{2} < s < \frac{3}{2}$.*

For a proof see [15].

As we are dealing with exterior domains, we define for a bounded Lipschitz domain Ω the corresponding exterior domain by $\Omega^c := \mathbb{R}^3 \setminus \bar{\Omega}$. In general the space $\mathrm{H}^s(\Omega^c)$ is too small, when dealing with partial differential equations like the Laplace equation or the Helmholtz equation. Instead of $\mathrm{H}^1(\Omega^c)$ we will use the space $\mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$, which is defined by

$$\mathrm{H}^1_{\mathrm{loc}}(\Omega^c) := \left\{ u \in \mathcal{D}(\Omega)^* : u|_{\Omega^c_\varrho} \in \mathrm{H}^1\left(\Omega^c_\varrho\right), \forall \varrho > 0 \text{ such that } \bar{\Omega} \subset B_\varrho \right\}.$$

In the above definition B_ϱ is the open ball with radius ϱ centered at zero and $\Omega^c_\varrho := \Omega^c \cap B_\varrho$. This space is not a Hilbert space as we cannot define a norm on this space.

Concerning the trace γ_0 we will use the following notation: The one sided trace operator for Ω is denoted by γ_0^{int} and the one sided trace operator for Ω^c is denoted by γ_0^{ext}, respectively. The traces $\gamma_0, \gamma_0^{\mathrm{int}}, \gamma_0^{\mathrm{ext}}$ are called Dirichlet traces.

Another trace is denoted by γ_1. Again, when dealing with the one-sided traces, we will use the notation γ_1^{int} and γ_1^{ext}. These traces are called Neumann traces and defined via

$$\gamma_1^{\mathrm{int}} u := \boldsymbol{n} \cdot \gamma_0^{\mathrm{int}} \nabla u,$$
$$\gamma_1^{\mathrm{ext}} u := \boldsymbol{n} \cdot \gamma_0^{\mathrm{ext}} \nabla u.$$

The γ_0 operator applied to a vector valued function has to be understood as the component-wise application of the γ_0 operator and the occurring derivatives have to be understood as weak derivatives. The Neumann trace is well defined

for functions $u \in \mathrm{H}^2(\Omega)$. We can extend this definition also to special $\mathrm{H}^1(\Omega)$ functions. In this thesis it is enough to consider $\mathrm{H}^1(\Omega)$ functions, which satisfy

$$-\Delta u - \kappa^2 u = 0 \quad \text{in } \Omega$$

in the distributional sense, where $\kappa \geq 0$ is a given real number. The $\mathrm{H}^1(\Omega)$ functions which satisfy the above criteria define the space $\mathrm{H}^1_*(\Omega)$. In this case, we use Greens first formula to define γ_1^{int}, i.e.

$$\left(\gamma_1^{\mathrm{int}} u, \gamma_0^{\mathrm{int}} v\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} := \int_\Omega \overline{\nabla u} \cdot \nabla v \,\mathrm{d}x - \kappa^2 \int_\Omega \bar{u} v \,\mathrm{d}x,$$

for all $v \in \mathrm{H}^1(\Omega)$. Therefore, γ_1^{int} is a mapping from $\mathrm{H}^1_*(\Omega)$ to $\mathrm{H}^{-1/2}(\Gamma)$.

For unbounded domains a similar approach leads to the same result. The only difference is that u belongs to $\mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ and therefore we have to choose $v \in \mathcal{D}(\Omega^c)$. For more details see e.g. [44, Section 1.2.7].

2.4 Boundary integral equations

The aim of this section is to find a boundary integral formulation for the Helmholtz equation. The main references for this section are [25, 44, 57].

Therefore, $\Omega \subset \mathbb{R}^3$ is assumed to be a bounded Lipschitz domain. By Γ we denote the boundary of Ω and by Ω^c we denote the corresponding exterior domain, i.e. $\Omega^c = \mathbb{R}^3 \setminus \bar{\Omega}$.

Of course one motivation in using boundary integral equations is that we have to solve the Helmholtz equation in an unbounded domain Ω^c. We are mainly interested in the following two types of problems.

Exterior Dirichlet boundary value problem: Let $g \in \mathrm{H}^{1/2}(\Gamma)$ be a given Dirichlet datum and $\kappa \in \mathbb{R}^+$ a given wave number. We are interested in finding $u \in \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ which satisfies

$$-\Delta u - \kappa^2 u = 0 \quad \text{in } \Omega^c, \tag{2.2}$$

$$u = g \quad \text{on } \Gamma. \tag{2.3}$$

Additionally, u has to satisfy the radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \, \mathrm{d}\mu = 0. \tag{2.4}$$

Exterior Neumann boundary value problem: Let $t \in \mathrm{H}^{-1/2}(\Gamma)$ be a given Neumann datum and $\kappa \in \mathbb{R}^+$ a given wave number. We are interested in finding $u \in \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ which satisfies

$$-\Delta u - \kappa^2 u = 0 \quad \text{in } \Omega^c, \tag{2.5}$$

$$\frac{\partial}{\partial \boldsymbol{n}} u = t \quad \text{on } \Gamma. \tag{2.6}$$

Again u has to satisfy the radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \, \mathrm{d}\mu = 0. \tag{2.7}$$

In both cases the partial differential equation has to be understood in the distributional sense.

Theorem 2.11. *Let Ω be a bounded Lipschitz domain with boundary Γ and Ω^c the corresponding exterior domain and let $g \in \mathrm{H}^{1/2}(\Gamma_C)$ be a given Dirichlet datum, or in case of the Neumann problem let $t \in \mathrm{H}^{-1/2}(\Gamma)$ be a given Neumann datum. There exists a unique $u \in \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ which satisfies the Dirichlet problem* (2.2)-(2.4)*, or* (2.5)-(2.7) *in case of the Neumann problem.*

The proof can be found in e.g. [39, Theorem 9.11] for the Dirichlet problem. For the idea of the proof in case of the Neumann problem, see [39, Page 294]. See also [40, Theorem 2.6.5 and Theorem 2.6.6].

Fundamental solution: A basic ingredient for boundary integral equations is the fundamental solution. For the Helmholtz equation the fundamental solution G_κ is defined via

$$G_\kappa(\boldsymbol{x}, \boldsymbol{y}) := \frac{1}{4\pi} \frac{e^{i\kappa|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{2.8}$$

One can derive easily that for $\boldsymbol{x} \neq \mathbf{0}$, the fundamental solution $G_\kappa(\boldsymbol{x}, \mathbf{0})$ is a solution of the Helmholtz equation. Furthermore, $G_\kappa(\boldsymbol{x}, \mathbf{0})$ interpreted as an element of $\mathcal{D}^*(\mathbb{R}^3)$ is a distributional solution of

$$(-\Delta - \kappa^2) G_\kappa = \delta,$$

where δ is the Dirac delta function. **Volume potential, Newton potential:** For any given function $f \in \mathcal{S}(\mathbb{R}^3)$ the volume potential or Newton potential $\mathcal{G}_\kappa f$ is defined via

$$(\mathcal{G}_\kappa f)(\boldsymbol{x}) := \int_{\mathbb{R}^3} G_\kappa(\boldsymbol{x}, \boldsymbol{y}) f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y},$$

for $\boldsymbol{x} \in \mathbb{R}^3$. This potential has the mapping property

$$\mathcal{G}_\kappa \colon \mathcal{S}\big(\mathbb{R}^3\big) \to \mathcal{S}\big(\mathbb{R}^3\big).$$

By defining

$$(\mathcal{G}_\kappa f, \phi)_{\mathcal{S}^*(\mathbb{R}^3) \times \mathcal{S}(\mathbb{R}^3)} := (f, \mathcal{G}_{-\kappa} \phi)_{\mathcal{S}^*(\mathbb{R}^3) \times \mathcal{S}(\mathbb{R}^3)},$$

for $f \in \mathcal{S}^*(\mathbb{R}^3)$ and $\phi \in \mathcal{S}(\mathbb{R}^3)$, the Newton potential can be extended to

$$\mathcal{G}_\kappa \colon \mathcal{S}^*\big(\mathbb{R}^3\big) \to \mathcal{S}^*\big(\mathbb{R}^3\big).$$

Using the property of the fundamental solution, we obtain that $\mathcal{G}_\kappa f$ is a distributional solution of

$$(-\Delta - \kappa^2) \mathcal{G}_\kappa f = f,$$

for all $f \in \mathcal{S}^*(\mathbb{R}^3)$. In [57, Theorem 6.1] it is shown that for the Laplace equation, i.e. $\kappa = 0$, the Newton potential

$$\mathcal{G}_0 \colon \tilde{\mathrm{H}}^{-1}(\Omega) \to \mathrm{H}^1(\Omega)$$

is a bounded and linear operator. This remains true for the Helmholtz equation.

Single layer potential: We can define the trace operator γ_0 for functions $\varphi \in \mathcal{S}(\mathbb{R}^3)$ by

$$\begin{aligned} \gamma_0 \colon \mathcal{S}\big(\mathbb{R}^3\big) &\to \mathrm{H}^{1/2}(\Gamma) \\ \varphi &\mapsto \varphi|_\Gamma. \end{aligned}$$

Therefore the adjoint operator γ_0^* has the mapping property

$$\gamma_0^* \colon \mathrm{H}^{-1/2}(\Gamma) \to \mathcal{S}^*\big(\mathbb{R}^3\big)$$

and is defined via

$$(\gamma_0^* w, \varphi)_{\mathcal{S}^*(\mathbb{R}^3)\times\mathcal{S}(\mathbb{R}^3)} = (w, \gamma_0\varphi)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)},$$

for all $w \in \mathrm{H}^{-1/2}(\Gamma)$ and $\varphi \in \mathcal{S}(\mathbb{R}^3)$. Using the Newton potential and the adjoint trace operator γ_0^*, we can define the single layer potential

$$\begin{aligned} SL_\kappa &\colon \mathrm{H}^{-1/2}(\Gamma) \to \mathcal{S}^*\big(\mathbb{R}^3\big), \\ SL_\kappa &:= \mathcal{G}_\kappa \gamma_0^*. \end{aligned}$$

The following result can be found in e.g. [39, Chapter 6].

Lemma 2.12. *If $w \in \mathrm{L}^\infty(\Gamma)$ it follows that*

$$(SL_\kappa w)(\boldsymbol{x}) = \int_\Gamma G_\kappa(\boldsymbol{x}, \boldsymbol{y}) w(\boldsymbol{y}) \, \mathrm{d}\mu_{\boldsymbol{y}},$$

for $\boldsymbol{x} \in \Omega \cup \Omega^c$.

Double layer potential: A similar approach leads to the double layer potential. Therefore, we define the trace operator γ_1 for functions $\varphi \in \mathcal{S}(\mathbb{R}^3)$ by

$$\begin{aligned} \gamma_1 &\colon \mathcal{S}\big(\mathbb{R}^3\big) \to \mathrm{H}^{-1/2}(\Gamma), \\ &\qquad \varphi \mapsto \boldsymbol{n} \cdot (\nabla\varphi|_\Gamma). \end{aligned}$$

The adjoint operator γ_1^* has the mapping property

$$\gamma_1^* \colon \mathrm{H}^{1/2}(\Gamma) \to \mathcal{S}^*\big(\mathbb{R}^3\big)$$

and is defined via

$$(\gamma_1^* v, \varphi)_{\mathcal{S}^*(\mathbb{R}^3)\times\mathcal{S}(\mathbb{R}^3)} = (\gamma_1\varphi, v)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)},$$

for all $v \in \mathrm{H}^{1/2}(\Gamma)$ and $\varphi \in \mathcal{S}(\mathbb{R}^3)$. Next, we introduce the double layer potential by

$$\begin{aligned} DL_\kappa &\colon \mathrm{H}^{1/2}(\Gamma) \to \mathcal{S}^*\big(\mathbb{R}^3\big), \\ DL_\kappa &:= \mathcal{G}_\kappa \gamma_1^*. \end{aligned}$$

Again, the following result can be found in [39, Chapter 6].

Lemma 2.13. *If $v \in \mathrm{L}^\infty(\Gamma)$ it follows that*

$$(DL_\kappa w)(\boldsymbol{x}) = \int_\Gamma [\boldsymbol{n}(\boldsymbol{y}) \cdot \nabla_{\boldsymbol{y}} G_\kappa(\boldsymbol{x}, \boldsymbol{y})]\, v(\boldsymbol{y})\, \mathrm{d}\mu_{\boldsymbol{y}},$$

for $\boldsymbol{x} \in \Omega \cup \Omega^c$.

Representation formula: A very important formula is given by the next theorem, see [39, Theorem 7.15].

Theorem 2.14. *Let u be the unique solution of the Dirichlet or Neumann problem. For a point $\boldsymbol{x} \in \Omega^c$, u has the representation*

$$u(\boldsymbol{x}) = -\left(SL_\kappa \gamma_1^{\mathrm{ext}} u\right)(\boldsymbol{x}) + \left(DL_\kappa \gamma_0^{\mathrm{ext}} u\right)(\boldsymbol{x}). \tag{2.9}$$

If the complete Cauchy data are known, the solution u can be constructed via the representation formula (2.9). Hence, we are interested in finding the unknown Neumann datum in case of the Dirichlet problem. Vice versa, we are interested in finding the unknown Dirichlet datum in case of the Neumann problem. In both cases we want to get an equation defined on the boundary Γ, which allows us to compute the missing datum.

To obtain boundary integral equations, the Dirichlet trace γ_0^{ext} and the Neumann trace γ_1^{ext} are applied to the representation formula (2.9). Therefore, we get four operators, which are discussed in the following.

Single layer boundary integral operator: First, we apply the Dirichlet trace to the single layer potential SL_κ. The result V_κ is called single layer boundary integral operator and has the following properties

$$V_\kappa t := \gamma_0^{\mathrm{int}}(SL_\kappa t) = \gamma_0^{\mathrm{ext}}(SL_\kappa t) : \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma),$$

for $t \in \mathrm{H}^{-1/2}(\Gamma)$. It follows that $V_\kappa^* = V_{-\kappa}$, i.e.

$$(V_{-\kappa} s, t)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} = (V_\kappa^* s, t)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} = (s, V_\kappa t)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)},$$

for all $s, t \in \mathrm{H}^{-1/2}(\Gamma)$.

Theorem 2.15. *The operator* $V_\kappa \colon \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma)$ *is bounded and linear. Additionally, for* $\kappa = 0$ *the single layer boundary integral operator is* $\mathrm{H}^{-1/2}(\Gamma)$*-elliptic, i.e. there exists a constant* $c > 0$ *such that*

$$\Re\left(V_0 t, t\right)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} \geq c \left\|t\right\|^2_{\mathrm{H}^{-1/2}(\Gamma)},$$

for all $t \in \mathrm{H}^{-1/2}(\Gamma)$.

Another important theorem can be found in [50, Lemma 3.9.8].

Theorem 2.16. *The operator* $V_\kappa - V_0$ *is compact.*

With the help of the last two theorems, we can prove the following corollary.

Corollary 2.17. *The single layer boundary integral operator* V_κ *is* $\mathrm{H}^{-1/2}(\Gamma)$*-coercive, i.e. there exists a compact operator* $C \colon \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma)$ *and a constant* $c > 0$ *such that the inequality*

$$\Re\left(\left(V_\kappa + C\right) t, t\right)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} \geq c \left\|t\right\|^2_{\mathrm{H}^{-1/2}(\Gamma)}$$

is satisfied, for all $t \in \mathrm{H}^{-1/2}(\Gamma)$.

When dealing with the discretization, the following lemma is important.

Lemma 2.18. *Let* $t \in \mathrm{L}^\infty(\Gamma)$*, then the single layer boundary integral operator can be interpreted as a weakly singular integral, i.e.*

$$\left(V_\kappa t\right)(\boldsymbol{x}) = \int_\Gamma G_\kappa(\boldsymbol{x}, \boldsymbol{y}) t(\boldsymbol{y}) \,\mathrm{d}\mu_{\boldsymbol{y}},$$

for $\boldsymbol{x} \in \Gamma$.

Double layer boundary integral operator: Next we want to apply the Dirichlet trace to the double layer potential DL_κ. We get two bounded, linear operators

$$\gamma_0^{\mathrm{int}} DL_\kappa \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma),$$
$$\gamma_0^{\mathrm{ext}} DL_\kappa \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma).$$

The double layer boundary integral operator is defined by

$$K_\kappa := \frac{1}{2}\left(\gamma_0^{\text{ext}} DL_\kappa + \gamma_0^{\text{int}} DL_\kappa\right) : \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{1/2}(\Gamma)$$

and satisfies

$$\gamma_0^{\text{int}}(DL_\kappa g) = \left(-\frac{1}{2} + K_\kappa\right) g,$$
$$\gamma_0^{\text{ext}}(DL_\kappa g) = \left(\frac{1}{2} + K_\kappa\right) g,$$

for almost all $\boldsymbol{x} \in \Gamma$ and for all $g \in \mathrm{H}^{1/2}(\Gamma)$, provided that Γ is piecewise smooth. For $g \in \mathrm{H}^{1/2}(\Gamma)$, the double layer boundary integral operator admits the representation

$$(K_\kappa g)(\boldsymbol{x}) = \int_\Gamma [\boldsymbol{n}(\boldsymbol{y}) \cdot \nabla_{\boldsymbol{y}} G_\kappa(\boldsymbol{x}, \boldsymbol{y})]\, g(\boldsymbol{y})\, \mathrm{d}\mu_{\boldsymbol{y}},$$

for $\boldsymbol{x} \in \Gamma$. This integral has to be interpreted as a Cauchy singular integral. For a detailed description see [39, Theorem 7.3, Theorem 7.4].

Adjoint double layer boundary integral operator: Next we want to apply the Neumann trace to the single layer potential. We get two bounded, linear operators

$$\gamma_1^{\text{int}} SL_\kappa \colon \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma),$$
$$\gamma_1^{\text{ext}} SL_\kappa \colon \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma).$$

The adjoint double layer boundary integral operator K'_κ is defined by

$$K'_\kappa := \frac{1}{2}\left(\gamma_1^{\text{ext}} SL_\kappa + \gamma_1^{\text{int}} SL_\kappa\right) : \mathrm{H}^{-1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma)$$

and satisfies

$$\gamma_1^{\text{int}}(SL_\kappa t) = \left(\frac{1}{2} + K'_\kappa\right) t,$$
$$\gamma_1^{\text{ext}}(SL_\kappa t) = \left(-\frac{1}{2} + K'_\kappa\right) t$$

in the sense of $\mathrm{H}^{-1/2}(\Gamma)$, for all $t \in \mathrm{H}^{-1/2}(\Gamma)$. For details see [39, Chapter 7]. If t has more regularity, i.e. $t \in \mathrm{H}^{-1/2}(\Gamma) \cap \mathrm{L}^{\infty}(\Gamma)$, the adjoint double layer boundary integral operator K'_{κ} has the representation

$$(K'_{\kappa} t)(\boldsymbol{x}) := \int_{\Gamma} [\boldsymbol{n}(\boldsymbol{y}) \cdot \nabla_{\boldsymbol{x}} G_{\kappa}(\boldsymbol{x}, \boldsymbol{y})]\, t(\boldsymbol{y})\, \mathrm{d}\mu_{\boldsymbol{y}}.$$

This integral has to be interpreted as a Cauchy singular integral, see [45, Theorem 3.26].

Remark 2.19. *K'_{κ} is not the adjoint operator of K_{κ}, i.e. $K'_{\kappa} \neq K^*_{\kappa}$. But $K'_{-\kappa} = K^*_{\kappa}$ holds, i.e.*

$$\left(K'_{-\kappa} t, g\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = (K^*_{\kappa} t, g)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = (t, K_{\kappa} g)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)},$$

for all $t \in \mathrm{H}^{-1/2}(\Gamma)$ and $g \in \mathrm{H}^{1/2}(\Gamma)$.

Hypersingular boundary integral operator: This operator is defined by

$$D_{\kappa} g := -\gamma_1^{\mathrm{int}}(D L_{\kappa} g) = -\gamma_1^{\mathrm{ext}}(D L_{\kappa} g) : \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma).$$

It follows that $D^*_{\kappa} = D_{-\kappa}$, i.e.

$$(D_{-\kappa} g, w)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = (D^*_{\kappa} g, w)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = (g, D_{\kappa} w)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)},$$

for all $g, w \in \mathrm{H}^{1/2}(\Gamma)$. In [57, Chapter 6] the following properties are shown.

Theorem 2.20. *The operator $D_{\kappa} \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma)$ is bounded and linear. For $\kappa = 0$ the hypersingular boundary integral operator is $\mathrm{H}^{1/2}(\Gamma)$-semi-elliptic, i.e. a constant $c > 0$ exists, such that*

$$\Re\,(D_0 g, g)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} \geq c\,|g|^2_{\mathrm{H}^{1/2}(\Gamma)},$$

for all $g \in \mathrm{H}^{1/2}(\Gamma)$.

Corollary 2.21. *The operator $\tilde{D}_0 \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma)$, which is defined by*

$$\left(\tilde{D}_0 g, w\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} := (D_0 g, w)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} + \int_{\Gamma} g(\boldsymbol{x})\,\mathrm{d}\mu \int_{\Gamma} w(\boldsymbol{x})\,\mathrm{d}\mu,$$

for $g, w \in \mathrm{H}^{1/2}(\Gamma)$, as well as the operator $\hat{D}_0 \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma)$, which is defined by

$$\left(\hat{D}_0 g, w\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} := (D_0 g, w)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} + \int_\Gamma g(\boldsymbol{x}) w(\boldsymbol{x}) \,\mathrm{d}\mu,$$

for $g, w \in \mathrm{H}^{1/2}(\Gamma)$, are $\mathrm{H}^{1/2}(\Gamma)$-elliptic, i.e. there exists a constant $c > 0$, such that

$$\Re\left(\tilde{D}_0 g, g\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} \geq c \left\|g\right\|^2_{\mathrm{H}^{1/2}(\Gamma)}$$

and

$$\Re\left(\hat{D}_0 g, g\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} \geq c \left\|g\right\|^2_{\mathrm{H}^{1/2}(\Gamma)}$$

for all $g \in \mathrm{H}^{1/2}(\Gamma)$.

As for the single layer boundary integral operator, the following statement holds, see [50, Lemma 3.9.8].

Theorem 2.22. *The operator $D_\kappa - D_0$ is compact.*

Corollary 2.23. *The hypersingular boundary integral operator D_κ is $\mathrm{H}^{1/2}(\Gamma)$-coercive, i.e. there exists a compact operator $C \colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^{-1/2}(\Gamma)$ and a constant $c > 0$, such that the inequality*

$$\Re\left((D_\kappa + C)\, g, g\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} \geq c \left\|g\right\|^2_{\mathrm{H}^{1/2}(\Gamma)}$$

is satisfied, for all $g \in \mathrm{H}^{1/2}(\Gamma)$.

Theorem 2.24. *Let Γ be a piecewise smooth closed surface and let $g, w \in \mathrm{H}^{1/2}(\Gamma)$ be globally continuous and piecewise differentiable. It follows that*

$$\begin{aligned}(D_\kappa g, w)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = \\ \int_\Gamma \int_\Gamma \overline{G_\kappa(\boldsymbol{x}, \boldsymbol{y})} \left(\overline{\mathbf{curl}_\Gamma g(\boldsymbol{x})} \cdot \mathbf{curl}_\Gamma w(\boldsymbol{y})\right) \,\mathrm{d}\mu_{\boldsymbol{x}} \,\mathrm{d}\mu_{\boldsymbol{y}} - \\ \kappa^2 \int_\Gamma \int_\Gamma \overline{G_\kappa(\boldsymbol{x}, \boldsymbol{y}) g(\boldsymbol{x})} w(\boldsymbol{y}) \left(\boldsymbol{n}_{\boldsymbol{x}} \cdot \boldsymbol{n}_{\boldsymbol{y}}\right) \,\mathrm{d}\mu_{\boldsymbol{x}} \,\mathrm{d}\mu_{\boldsymbol{y}}.\end{aligned}$$

In the previous theorem the tangential rotational $\mathbf{curl}_{\boldsymbol{\Gamma}}$ was used, which is defined by

$$\mathbf{curl}_{\boldsymbol{\Gamma}} g(\boldsymbol{x}) := \mathbf{curl}\left(\tilde{g}(\boldsymbol{x})\boldsymbol{n}\right),$$

where $\tilde{g}$ is an extension of g into a neighborhood of Γ. For details and for a proof see e.g. [40, Theorem 3.4.2], or in case of the Laplace equation [57, Theorem 6.17]. When considering the discretization, Theorem 2.24 turns out to be very useful.

Boundary integral equations: Using all four boundary integral operators, we are in the position to state the first and the second boundary integral equation. We obtain the first boundary integral equation

$$V_\kappa t = \left(-\frac{1}{2} + K_\kappa\right) g, \tag{2.10}$$

by applying the trace operator γ_0^{ext} to the representation formula (2.9). In case of a Dirichlet boundary value problem we prefer this boundary integral equation to find the unknown Neumann datum t. Therefore, we have to ensure that the operator V_κ is invertible to get the unknown Neumann datum. If this is not the case, we will use a different formulation, which will be introduced later.

By applying the Neumann trace to the representation formula (2.9), we obtain the second boundary integral equation

$$t = \left(\frac{1}{2} - K_{-\kappa}^*\right) t - D_\kappa g. \tag{2.11}$$

In case of a Neumann boundary value problem this boundary integral equation is preferred to find the unknown Dirichlet datum g. Hence, we have to ensure that the hypersingular boundary integral operator D_κ is invertible to get the unknown Dirichlet datum. If this is not the case, we will again introduce a modified boundary integral equation to overcome this difficulty.

The system of the first boundary integral equation (2.10) and the second boundary integral equation (2.11) is called the Caldéron projection,

$$\begin{pmatrix} g \\ t \end{pmatrix} = C_{ext} \begin{pmatrix} g \\ t \end{pmatrix} := \begin{pmatrix} \frac{1}{2} + K_\kappa & -V_\kappa \\ -D_\kappa & \frac{1}{2} - K_{-\kappa}^* \end{pmatrix} \begin{pmatrix} g \\ t \end{pmatrix}.$$

One can show that $C_{ext} = C_{ext}^2$ is fulfilled. From this result we get the following lemma.

Lemma 2.25. *The following relations hold:*

$$V_\kappa D_\kappa = \left(\frac{1}{2} + K_\kappa\right)\left(\frac{1}{2} - K_\kappa\right),$$
$$D_\kappa V_\kappa = \left(\frac{1}{2} + K_{-\kappa}^*\right)\left(\frac{1}{2} - K_{-\kappa}^*\right),$$

as well as $K_\kappa V_\kappa = V_\kappa K_{-\kappa}^*$ *and* $D_\kappa K_\kappa = K_{-\kappa}^* D_\kappa$.

The proof for the Laplace equation (i.e. $\kappa = 0$) can be found in e.g. [57, Corollary 6.19]. For the Helmholtz equation the proof is similar.

Although the exterior Dirichlet and Neumann problems in case of the Helmholtz equation have a unique solution for all $\kappa \in \mathbb{R}^+$, the first and second boundary integral equation can suffer from eigenvalues of the corresponding interior Dirichlet or Neumann problems.

Interior Dirichlet boundary value problem: Let $g \in \mathrm{H}^{1/2}(\Gamma)$ be a given Dirichlet datum and $\kappa \in \mathbb{R}^+$ a given wave number. We are interested in finding $u \in \mathrm{H}^1(\Omega)$ which satisfies

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega, \\ u &= g \quad \text{on } \Gamma \end{aligned}$$

in the distributional sense.

Interior Neumann boundary value problem: Let $t \in \mathrm{H}^{-1/2}(\Gamma)$ be a given Neumann datum and $\kappa \in \mathbb{R}^+$ a given wave number. We are interested in finding $u \in \mathrm{H}^1(\Omega)$ which satisfies

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 \quad \text{in } \Omega, \\ \frac{\partial}{\partial \boldsymbol{n}} u &= t \quad \text{on } \Gamma \end{aligned}$$

in the distributional sense. In [39, Page 286] it is shown that the interior Dirichlet boundary value problem has a unique solution, if and only if κ^2 is

not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem. Vice versa, the interior Neumann boundary value problem has a unique solution, if and only if κ^2 is not an eigenvalue of the interior Neumann Laplace eigenvalue problem. For both eigenvalue problems countable many eigenvalues exist.

The relation between the interior Dirichlet Laplace eigenvalue problem and the single layer boundary integral operator V_κ is characterized in the following theorem, see e.g. [65, Theorem 2.4.3].

Theorem 2.26 (Characterization of the Dirichlet Laplace eigenvalue problem)**.** *Let $(\kappa, u) \in \mathbb{R}^+ \times \mathrm{H}^1(\Omega)$ be an eigenpair of*

$$-\Delta u = \kappa^2 u \text{ in } \Omega, \quad u = 0 \text{ on } \Gamma, \tag{2.12}$$

where the partial differential equation has to be understood in the distributional sense. Then $\gamma_1^{\mathrm{int}} u \neq 0$ holds and

$$V_\kappa \gamma_1^{\mathrm{int}} u = 0$$

follows. Vice versa, if $(\kappa, t) \in \mathbb{R}^+ \times \mathrm{H}^{-1/2}(\Gamma)$ satisfies $V_\kappa t = 0$, then u, which is defined by $u := SL_\kappa t$, is a distributional solution of (2.12)*.*

For the interior Neumann Laplace eigenvalue problem and the hypersingular boundary integral operator D_κ a similar result exists, see e.g. [65, Theorem 2.4.4].

Theorem 2.27 (Characterization of the Neumann Laplace eigenvalue problem)**.** *Let $(\kappa, u) \in \mathbb{R}^+ \times \mathrm{H}^1(\Omega)$ be an eigenpair of*

$$-\Delta u = \kappa^2 u \text{ in } \Omega, \quad \frac{\partial}{\partial \boldsymbol{n}} u = 0 \text{ on } \Gamma, \tag{2.13}$$

where the partial differential equation has to be understood in the distributional sense. Then $\gamma_0^{\mathrm{int}} u \neq 0$ holds and

$$D_\kappa \gamma_0^{\mathrm{int}} u = 0$$

follows. Vice versa, if $(\kappa, g) \in \mathbb{R}^+ \times \mathrm{H}^{1/2}(\Gamma)$ satisfies $D_\kappa g = 0$, then u, which is defined by $u := DL_\kappa g$, is a distributional solution of (2.13)*.*

Summing up, we have seen that we can use standard boundary integral equations in the case where κ^2 is not an eigenvalue. A priori we do not known, if κ corresponds to an eigenvalue.

Modified boundary integral equations: There are many different approaches to get modified boundary integral equations which are unique solvable for all $\kappa \in \mathbb{R}^+$. A very famous indirect approach was introduced by Brakhage and Werner [6]. In this approach the complex linear combination of the single layer and the double layer potential is used to describe the solution

$$u(\boldsymbol{x}) = (DL_\kappa w)(\boldsymbol{x}) - i(SL_\kappa w)(\boldsymbol{x}),$$

for $\boldsymbol{x} \in \Omega^c$. w is the unknown density function, which can be found by using the corresponding boundary integral equation. Burton and Miller introduced a direct approach, see [10]. The disadvantage of these two approaches is that unique solvability can be ensured only in case of smooth domains. In [9] and [23] regularized versions were suggested. In the following we use an approach which was introduced by Windisch, see [68] or [56, 60, 61]. The advantage of this approach is that it can be applied in the general case of Lipschitz domains. For the Dirichlet problem the following system is solved instead of the first boundary integral equation:

$$\begin{pmatrix} D_\kappa + i\eta\tilde{D}_0 & \frac{1}{2} + K^*_{-\kappa} \\ -\frac{1}{2} - K_\kappa & V_\kappa \end{pmatrix} \begin{pmatrix} \tilde{g} \\ t \end{pmatrix} = \begin{pmatrix} i\eta\tilde{D}_0 g \\ -g \end{pmatrix}. \tag{2.14}$$

In the previous formula the hypersingular boundary integral operator D_0 was stabilized by the rank one term which was introduced in Corollary 2.21. Another possibility is to use $\hat{D}_0$ instead of $\tilde{D}_0$. $\eta \in \mathbb{R} \setminus \{0\}$ is an arbitrary but fixed constant. In this formulation we use the auxiliary variable $\tilde{g} \in \mathrm{H}^{1/2}(\Gamma)$. Due to this new variable, we have to solve a bigger system, but on the other hand we can guarantee that this system has a unique solution for all $\kappa \in \mathbb{R}^+$. This is due to the $\mathrm{H}^{1/2}(\Gamma) \times \mathrm{H}^{-1/2}(\Gamma)$-coercivity and surjectivity, hence injectivity, of the system (2.14), which is shown in [68, Theorem 5.25] and [68, Theorem 5.26]. It can be shown that the auxiliary variable $\tilde{g}$ is nothing else than the Dirichlet datum g.

When dealing with the Neumann problem, the following system is used

$$\begin{pmatrix} D_\kappa & -\frac{1}{2} + K^*_{-\kappa} \\ \frac{1}{2} - K_\kappa & V_\kappa + i\eta V_0 \end{pmatrix} \begin{pmatrix} g \\ \tilde{t} \end{pmatrix} = \begin{pmatrix} -t \\ i\eta V_0 t \end{pmatrix}. \tag{2.15}$$

As for the Dirichlet problem, we introduce an auxiliary variable $\tilde{t}$, which is equal to t, and fix an arbitrary but fixed $\eta \in \mathbb{R} \setminus \{0\}$. Again this system has a unique solution for every $\kappa \in \mathbb{R}^+$, due to the $\mathrm{H}^{1/2}(\Gamma) \times \mathrm{H}^{-1/2}(\Gamma)$-coercivity and surjectivity, see [68, Section 5.7].

2.5 Approximation methods

In the following, we want to solve operator equations of the form

$$Au = f \tag{2.16}$$

numerically, where X is a Hilbert space, $u \in X$ is the unknown function and $f \in X^*$ is a given right-hand side. The operator $A\colon X \to X^*$ is either a bounded and X-elliptic operator or a bounded and X-coercive operator.

Before we have a look at the discretization, we introduce the equivalent variational equation: Find $u \in X$ such that

$$(Au, v)_{X^* \times X} = (f, v)_{X^* \times X},$$

for all $v \in X$.

The Galerkin-Bubnov method is used to obtain an approximation method. For more details see [57]. Therefore, finite dimensional spaces $X_M \subset X$, $M \in \mathcal{M} \subset \mathbb{N}$, with $\dim X_M = M$, are used. We assume that $X_{M_1} \subset X_{M_2}$ holds, if $M_1 < M_2$ and that $\bigcup_{M \in \mathcal{M}} X_M$ is dense in X. We denote a basis of X_M by $\{\varphi_k\}_{k=1}^M$, i.e.

$$X_M = \operatorname{span}\{\varphi_k\}_{k=1}^M$$

and all elements $v_M \in X_M$ have the unique representation

$$v_M = \sum_{k=1}^{M} \boldsymbol{v}[k]\varphi_k.$$

Therefore, an element v_M is characterized by the vector

$$\boldsymbol{v} = (\boldsymbol{v}[1], \cdots, \boldsymbol{v}[M])^\top.$$

The idea is to solve the following discrete problem: Find $u_M \in X_M$ such that

$$(Au_M, v_M)_{X^* \times X} = (f, v_M)_{X^* \times X}\,, \tag{2.17}$$

for all $v_M \in X_M$. This is equivalent to the following system of linear equations

$$A_M \boldsymbol{u} = \boldsymbol{f},$$

where $A_M \in \mathbb{C}^{M \times M}$ is the matrix which is defined by

$$A_M[i,j] = (A\varphi_j, \varphi_i)_{X^* \times X}\,, \quad i,j \in \{1, \cdots, M\}$$

and the vector $\boldsymbol{f}$ is defined by

$$\boldsymbol{f}[i] = (f, \varphi_i)_{X^* \times X}\,, \quad i \in \{1, \cdots, M\}.$$

In the elliptic case the resulting matrix turns out to be positive definite, i.e. the system of linear equations has a unique solution and the well known Lemma of Cea can be used to get an a priori error estimate, see [12].

Theorem 2.28 (Cea's Lemma)**.** *Let X be a Hilbert space and $A\colon X \to X^*$ be bounded and X-elliptic. The ellipticity constant is denoted by c_1 and the boundedness constant by c_2. The unique solution u_M of the discrete variational equation* (2.17) *satisfies the stability estimate*

$$\|u_M\|_X \leq \frac{1}{c_1}\|f\|_{X^*}$$

and there holds the error estimate

$$\|u - u_M\|_X \leq \frac{c_2}{c_1} \inf_{v_M \in X_M} \|u - v_M\|_X,$$

where u is the unique solution of (2.16)*.*

In the X-coercive case we have to ensure the inf-sup condition

$$\sup_{v_M \in X_M} \frac{|\,(Au_M, v_M)_{X^* \times X}\,|}{\|v_M\|_X} \geq c\|u_M\|_X,$$

for all $u_M \in X_M$. It turns out that this condition is satisfied, if the finite dimensional subset X_M is large enough, see the following lemma.

Lemma 2.29. *Let X be a Hilbert space and $A\colon X \to X^*$ be a bounded and X-coercive operator, which is assumed to be injective. Then a constant $c > 0$ exists, such that the inf-sup condition*

$$\sup_{v_M \in X_M} \frac{|\,(Au_M, v_M)_{X^* \times X}\,|}{\|v_M\|_X} \geq c\|u_M\|_X$$

is satisfied for all $u_M \in X_M$, provided M is large enough.

A proof can be found in [23] or [51]. Now it is possible to state the Lemma of Cea also for the X-coercive case.

Theorem 2.30 (Cea's Lemma)**.** *Let the assumptions of Lemma 2.29 be satisfied and assume that M is sufficiently large such that the inf-sup condition is valid. Then a unique discrete solution $u_M \in X_M$ exists, which satisfies equation* (2.17)*. Furthermore, a constant $c > 0$ exists, such that the following error estimate is true*

$$\|u - u_M\|_X \leq c \inf_{v_M \in X_M} \|u - v_M\|_X,$$

where u is the unique solution of equation (2.16)*.*

Again, the proof can be found in [23].

Finally, we want to discretize the variational inequality: Find $u \in X_{ad}$, which satisfies

$$\Re\,(Au, v - u)_{X^* \times X} \geq \Re\,(f, v - u)_{X^* \times X}\,,$$

for all $v \in X_{ad}$. As in Theorem 2.8, it is assumed that the operator $A\colon X \to X^*$ is a bounded and X-elliptic operator and that X_{ad} is a non-empty, bounded, closed and convex subset of X. For the discretization a sequence of finite dimensional spaces $X_{ad,M} \subset X$ is used.

The discrete variational inequality is given by: Find $u_M \in X_{ad,M}$ such that

$$\Re\,(Au_M, v_M - u_M) \geq \Re\,(f, v_M - u_M)\,, \tag{2.18}$$

for all $v_M \in X_{ad,M}$.

Remark 2.31. *In general the set $X_{ad,M}$ is not a subset of X_{ad}. In the following we state a theorem which does not use more assumptions. As a corollary we get a statement for the special case $X_{ad,M} \subset X_{ad}$.*

The following theorem is based on [21, Lemma 7.16].

Theorem 2.32. *Let X be a Hilbert space and $A\colon X \to X^*$ be a bounded and X-elliptic operator. The ellipticity constant is denoted by c_1 and the boundedness constant by c_2. Furthermore, let $f \in X^*$ be given. The discrete variational inequality* (2.18) *has a unique solution u_M, which satisfies the stability estimate*

$$\|u_M\|_X \leq \frac{1}{c_1}\|f\|_{X^*}$$

and the error estimate

$$\begin{aligned}\frac{c_1}{2}\|u-u_M\|_X^2 \leq \inf_{v\in X_{ad}} \Re\left(Au-f, v-u_M\right)_{X^*\times X} + \\ \inf_{v_M\in X_{ad,M}} \left(\Re\left(Au-f, v_M-u\right)_{X^*\times X} + \frac{c_2^2}{2c_1}\|u-v_M\|_X^2\right),\end{aligned}$$

where u is the unique solution of the variational inequality (2.1).

Proof. Using Theorem 2.8, we get unique solvability of the discrete variational inequality and the stability estimate. To show the error estimate, we start with the X-ellipticity:

$$\begin{aligned}c_1\|u-u_M\|_X^2 \leq& \Re\left(A(u-u_M), u-u_M\right)_{X^*\times X} = \\ & \Re\left(Au-f, u-u_M\right)_{X^*\times X} - \Re\left(Au_M-f, u-u_M\right)_{X^*\times X} = \\ & \Re\left(Au-f, u-v\right)_{X^*\times X} + \Re\left(Au-f, v-u_M\right)_{X^*\times X} - \\ & \Re\left(Au_M-f, u-v_M\right)_{X^*\times X} - \Re\left(Au_M-f, v_M-u_M\right)_{X^*\times X},\end{aligned}$$

where $v \in X_{ad}$ and $v_M \in X_{ad,M}$ are arbitrary. Next, we use the fact that

$$\Re\left(Au-f, u-v\right)_{X^*\times X} \leq 0 \quad \text{and} \quad \Re\left(Au_M-f, v_M-u_M\right)_{X^*\times X} \geq 0.$$

Hence, we obtain

$$\begin{aligned}c_1\|u-u_M\|_X^2 &\leq \Re\left(Au-f, v-u_M\right)_{X^*\times X} - \Re\left(Au_M-f, u-v_M\right)_{X^*\times X} \\ &= \Re\left(Au-f, v-u_M\right)_{X^*\times X} + \Re\left(Au-f, v_M-u\right)_{X^*\times X} \\ &\quad + \Re\left(Au-Au_M, u-v_M\right)_{X^*\times X}.\end{aligned}$$

Using the Cauchy-Schwarz inequality, the boundedness of A and the simple fact that $a^2 + b^2 \geq 2ab$ with

$$a = \|u - u_M\|_X \sqrt{\frac{c_1}{2c_2}} \quad \text{and} \quad b = \|u - v_M\|_X \sqrt{\frac{c_2}{2c_1}},$$

we can estimate $c_1\|u - u_M\|_X^2$ by

$$\begin{aligned}
&\Re\left(Au - f, v - u_M\right)_{X^* \times X} + \Re\left(Au - f, v_M - u\right)_{X^* \times X} + \\
&\qquad\qquad c_2\|u - u_M\|_X \|u - v_M\|_X \leq \\
&\Re\left(Au - f, v - u_M\right)_{X^* \times X} + \Re\left(Au - f, v_M - u\right)_{X^* \times X} + \\
&\qquad\qquad \frac{c_1}{2}\|u - u_M\|_X^2 + \frac{c_2^2}{2c_1}\|u - v_M\|_X^2.
\end{aligned}$$

Summing up, we obtain

$$\begin{aligned}
&\frac{c_1}{2}\|u - u_M\|_X^2 \leq \\
&\qquad \Re\left(Au - f, v - u_M\right)_{X^* \times X} + \Re\left(Au - f, v_M - u\right)_{X^* \times X} + \frac{c_2^2}{2c_1}\|u - v_M\|_X^2,
\end{aligned}$$

which proves the theorem. □

As a simple consequence, we obtain the following corollary.

Corollary 2.33. *Let the assumptions of Theorem 2.32 be satisfied and let $X_{ad,M}$ be a subset of X_{ad}, then the improved error estimate*

$$\frac{c_1}{2}\|u - u_M\|_X^2 \leq \inf_{v_M \in X_{ad,M}} \left(\Re\left(Au - f, v_M - u\right)_{X^* \times X} + \frac{c_2^2}{2c_1}\|u - v_M\|_X^2 \right)$$

holds.

Finally, we want to analyze what happens, if the operator A is approximated by an operator $\tilde{A}\colon X \to X^*$, which is assumed to be $X_{ad,M}$-elliptic. In addition to variational inequality (2.1) and to discrete variational inequality (2.18) we introduce the discrete variational inequality: Find $\tilde{u}_M \in X_{ad,M}$, which satisfies

$$\Re\left(\tilde{A}\tilde{u}_M - f, v_M - \tilde{u}_M\right)_{X^* \times X} \geq 0, \tag{2.19}$$

for all $v_M \in X_{ad,M}$.

Theorem 2.34. *Let the assumptions of Theorem 2.32 be satisfied. u and u_M are defined as in Theorem 2.32. Furthermore, let $\tilde{u}_M$ be the unique solution of the discrete variational inequality* (2.19)*. The operator $\tilde{A}\colon X \to X^*$ is assumed to be $X_{ad,M}$-elliptic. Then the error estimate*

$$\|u - \tilde{u}_M\|_X \leq c \left(\|u - u_M\|_X + \left\| \left(\tilde{A} - A \right) u \right\|_{X^*} \right)$$

holds.

Proof. We can use the triangle inequality to obtain

$$\|u - \tilde{u}_M\|_X \leq \|u - u_M\|_X + \|u_M - \tilde{u}_M\|_X.$$

Therefore, we have to estimate the second term on the right hand side. Using the $X_{ad,M}$-ellipticity, we obtain

$$\begin{aligned} \tilde{c}\|u_M - \tilde{u}_M\|_X^2 &\leq \Re \left(\tilde{A}\left(u_M - \tilde{u}_M\right), u_M - \tilde{u}_M \right)_{X^* \times X} \\ &= \Re \left(\tilde{A} u_M, u_M - \tilde{u}_M \right)_{X^* \times X} - \Re \left(\tilde{A}\tilde{u}_M, u_M - \tilde{u}_M \right)_{X^* \times X}. \end{aligned}$$

Due to (2.18) and (2.19), it follows that

$$\begin{aligned} &-\Re \left(\tilde{A}\tilde{u}_M, u_M - \tilde{u}_M \right)_{X^* \times X} \\ &\qquad = -\Re \left(\tilde{A}\tilde{u}_M - f, u_M - \tilde{u}_M \right)_{X^* \times X} - \Re \left(f - A u_M, u_M - \tilde{u}_M \right)_{X^* \times X} \\ &\qquad - \Re \left(A u_M, u_M - \tilde{u}_M \right)_{X^* \times X} \leq -\Re \left(A u_M, u_M - \tilde{u}_M \right)_{X^* \times X}. \end{aligned}$$

Therefore, we conclude

$$\begin{aligned} \tilde{c}\|u_M - \tilde{u}_M\|_X^2 \leq \Re \left(\left(\tilde{A} - A \right) u_M, u_M - \tilde{u}_M \right)_{X^* \times X} \leq \\ \left\| \left(\tilde{A} - A \right) u_M \right\|_{X^*} \|u_M - \tilde{u}_M\|_X. \end{aligned}$$

Hence, we have proved that

$$\|u_M - \tilde{u}_M\|_X \leq \frac{1}{\tilde{c}} \left\| \left(\tilde{A} - A \right) u_M \right\|_{X^*} \leq \frac{1}{\tilde{c}} \left(\left\| \left(\tilde{A} - A \right) u \right\|_{X^*} + \tilde{\tilde{c}} \|u - u_M\|_X \right).$$

Summing up, we obtain

$$\|u - \tilde{u}_M\|_X \leq c \left(\left\| \left(\tilde{A} - A \right) u \right\|_{X^*} + \|u - u_M\|_X \right),$$

where c is a suitable constant. □

2.6 Boundary element method

In this section we want to solve boundary integral equations, which were introduced in Section 2.4, numerically. As boundary integral equations are defined on the boundary Γ, we will introduce sequences of finite dimensional subsets of $\mathrm{H}^{1/2}(\Gamma)$ and $\mathrm{H}^{-1/2}(\Gamma)$, respectively. In the following we claim that the boundary Γ is a polyhedral surface. More about boundary element methods can be found in e.g. [50, 57].

In this thesis we use a sequence of triangular meshes $(\mathcal{T}_n)_{n=1}^{\infty}$ to decompose the boundary Γ. Due to the above assumption, we do not get an approximation error of the geometry. A more general case is discussed in [13]. Each mesh $\mathcal{T}_n$, $n \in \mathbb{N}$, has a finite number of (open) triangles called $\tau_{n,i}$, $i \in \{1, \cdots, N_n\}$, where N_n is the number of triangles of mesh number n, such that

$$\Gamma = \bigcup_{i=1}^{N_n} \bar{\tau}_{n,i}.$$

The nodes of the mesh are denoted by $x_{n,i}, i \in \{1, \cdots, M_n\}$, where M_n is the number of nodes of mesh number n. A characteristic value of an element $\tau_{n,i}$ is the mesh size $h_{n,i}$, which is defined via

$$h_{n,i} := \left(\int_{\tau_{n,i}} 1 \, \mathrm{d}\mu \right)^{\frac{1}{2}}$$

and the diameter $d_{n,i}$ of $\tau_{n,i}$, which is defined via

$$d_{n,i} := \sup_{\boldsymbol{x},\boldsymbol{y} \in \tau_{n,i}} |\boldsymbol{x} - \boldsymbol{y}|.$$

Assumption 2.35. *The sequence of meshes $(\mathcal{T}_n)_{n=1}^{\infty}$ is admissible, i.e. the intersection of the closure of two elements (triangles) $\tau_{n,i}$ and $\tau_{n,j}$, $i, j \in \{1, \cdots, N_n\}, n \in \mathbb{N}$, is empty, a node, an edge or the closure of the whole element. In particular, this excludes hanging nodes.*

Another property we want to assume is shape regularity. The sequence $(\mathcal{T}_n)_{n=1}^{\infty}$ is called shape regular, if a constant c_f exists, such that

$$h_{n,i} \leq d_{n,i} \leq c_f h_{n,i},$$

for all $n \in \mathbb{N}$ and for all $i \in \{1, \cdots, N_n\}$. It is important to mention that the constant c_f does not depend on the indices n and i.

Finally, we assume that the mesh is globally quasi-uniform, i.e. a constant c_g independent of n exists, such that

$$\frac{\max_{i\in\{1,\cdots,N_n\}} h_{n,i}}{\min_{i\in\{1,\cdots,N_n\}} h_{n,i}} \leq c_g.$$

For $n \in \mathbb{N}$ we use the definition

$$h_n := \max_{i\in\{1,\cdots,N_n\}} h_{n,i}.$$

To make the notation easier, we avoid the index n if there are no ambiguities. E.g., we use h instead of h_n.

Now we are in the position to introduce for each $n \in \mathbb{N}$ the space of piecewise constant ansatz functions. This space is denoted by $\mathrm{S}_{\mathrm{h}}^0(\Gamma)$ and defined via

$$\mathrm{S}_{\mathrm{h}}^0(\Gamma) := \operatorname{span}\{\psi_i\}_{i=1}^N,$$

where ψ_i are defined by

$$\psi_i(\boldsymbol{x}) := \begin{cases} 1 & \text{for } \boldsymbol{x} \in \tau_i, \\ 0 & \text{else.} \end{cases}$$

There holds $\mathrm{S}_{\mathrm{h}}^0(\Gamma) \subset \mathrm{H}^{-1/2}(\Gamma)$. The approximation property of this space is the content of the next theorem.

Theorem 2.36. *Let Γ be a Lipschitz boundary with polyhedral surface. Furthermore, let us assume that Assumption 2.35 is satisfied. For $t \in \mathrm{H}_{\mathrm{pw}}^{\mathrm{s}}(\Gamma)$ with $s \in [-\frac{1}{2}, 1]$ we get*

$$\inf_{v_h\in\mathrm{S}_{\mathrm{h}}^0(\Gamma)} \|t - v_h\|_{\mathrm{H}^{-1/2}(\Gamma)} \leq c h^{s+1/2} \|t\|_{\mathrm{H}_{\mathrm{pw}}^{\mathrm{s}}(\Gamma)}.$$

A proof of this theorem can be found in e.g. [57, Chapter 10.2].

Another discrete space is given by the piecewise linear and globally continuous ansatz functions. This space is denoted by $\mathrm{S}_{\mathrm{h}}^{1}(\Gamma)$. The functions φ_i, which are defined by

$$\varphi_i(\boldsymbol{x}) := \begin{cases} 1 & \text{for } \boldsymbol{x} = \boldsymbol{x_i}, \\ 0 & \text{for } \boldsymbol{x} = \boldsymbol{x_j} \neq \boldsymbol{x_i}, \\ \text{linear} & \text{else}, \end{cases}$$

define a basis of $\mathrm{S}_{\mathrm{h}}^{1}(\Gamma)$, i.e.

$$\mathrm{S}_{\mathrm{h}}^{1}(\Gamma) := \operatorname{span}\{\varphi_i\}_{i=1}^{M}.$$

The space $\mathrm{S}_{\mathrm{h}}^{1}(\Gamma)$ is a subset of $\mathrm{H}^{1/2}(\Gamma)$ and as for the piecewise constant ansatz space we get an approximation property, which is the content of the following theorem.

Theorem 2.37. *Let Γ be a Lipschitz boundary with a polyhedral surface. Let Assumption 2.35 be satisfied. For $u \in \mathrm{H}^{s}(\Gamma)$ with $s \in [\frac{1}{2}, 2]$ it follows that*

$$\inf_{v_h \in \mathrm{S}_{\mathrm{h}}^{1}(\Gamma)} \|u - v_h\|_{\mathrm{H}^{1/2}(\Gamma)} \leq c h^{s-1/2} |u|_{\mathrm{H}^{s}(\Gamma)}.$$

A proof of this theorem can be found in e.g. [57, Chapter 10.2].

Next we want to consider the **Dirichlet boundary value problem**. Let us assume for a moment that κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem. As a consequence, we get that the first boundary integral equation (2.10) is uniquely solvable. Therefore, the following variational problem is also uniquely solvable: Find $t \in \mathrm{H}^{-1/2}(\Gamma)$ such that

$$(V_\kappa t, w)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} = \left(\left(-\frac{1}{2} + K_\kappa\right) g, w\right)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}$$

is satisfied for all $w \in \mathrm{H}^{-1/2}(\Gamma)$. The corresponding discrete variational problem is given by: Find $t_h \in \mathrm{S}_{\mathrm{h}}^{0}(\Gamma)$ such that

$$(V_\kappa t_h, w_h)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)} = \left(\left(-\frac{1}{2} + K_\kappa\right) g, w_h\right)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}$$

is satisfied, for all $w_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma)$. The equivalent system of linear equations is given by

$$V_{\kappa,h}\boldsymbol{t} = \boldsymbol{f},$$

where the matrix $V_{\kappa,h}$ is defined via

$$V_{\kappa,h} \in \mathbb{C}^{N\times N}, \quad V_{\kappa,h}[i,j] := (V_\kappa \psi_j, \psi_i)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}$$

and the vector $\boldsymbol{f}$ is defined by

$$\boldsymbol{f} \in \mathbb{C}^N, \quad \boldsymbol{f}[i] := \left(\left(-\frac{1}{2} + K_\kappa\right) g, \psi_i\right)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}.$$

Of course, from a practical point of view, we need to think about additional approximation errors due to the inexact calculation of the entries of the matrix $V_{\kappa,h}$ and the entries of the vector $\boldsymbol{f}$. For simplicity this is neglected here. In [57, Chapter 8] this topic is discussed in detail.

Using the abstract results of Section 2.5 and the approximation property of the space $\mathrm{S}^0_{\mathrm{h}}(\Gamma)$, we get unique solvability, if h is fine enough. In this case we end up with the error estimate

$$\|t - t_h\|_{\mathrm{H}^{-1/2}(\Gamma)} \leq c h^{s+1/2} \|t\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma)},$$

if $t \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma)$ for some $s \in [-\frac{1}{2}, 1]$.

If we cannot guarantee that κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem, we prefer to use the modified system (2.14). This system has always a unique solution. The discrete system of linear equations is then given by

$$\begin{pmatrix} D_{\kappa,h} + i\eta\tilde{D}_{0,h} & \frac{1}{2}M_h^* + K^*_{-\kappa,h} \\ -\frac{1}{2}M_h - K_{\kappa,h} & V_{\kappa,h} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{g}} \\ \boldsymbol{t} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f_1} \\ \boldsymbol{f_2} \end{pmatrix}.$$

The used matrices are defined by

$$\begin{aligned}
D_{\kappa,h} &\in \mathbb{C}^{M\times M}, & D_{\kappa,h}[i,j] &:= (D_\kappa \varphi_j, \varphi_i)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \\
\tilde{D}_{0,h} &\in \mathbb{C}^{M\times M}, & \tilde{D}_{0,h}[i,j] &:= \left(\tilde{D}_0 \varphi_j, \varphi_i\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \\
K_{\kappa,h} &\in \mathbb{C}^{N\times M}, & K_{\kappa,h}[i,j] &:= (K_{\kappa,h} \varphi_j, \psi_i)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}, \\
K^*_{-\kappa,h} &\in \mathbb{C}^{M\times N}, & K^*_{-\kappa,h}[i,j] &:= \left(K^*_{-\kappa,h} \psi_j, \varphi_i\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \\
M_h &\in \mathbb{C}^{N\times M}, & M_h[i,j] &:= (\varphi_j, \psi_i)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)},
\end{aligned}$$

and the right hand side is defined by

$$\begin{aligned} \boldsymbol{f_1} &\in \mathbb{C}^M, & \boldsymbol{f_1}[i] &:= \left(i\eta \tilde{D}_0 g, \varphi_i\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \\ \boldsymbol{f_2} &\in \mathbb{C}^N, & \boldsymbol{f_2}[i] &:= (-g, \psi_i)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}. \end{aligned}$$

We can use the same arguments as in the case where κ^2 is no eigenvalue of the interior Dirichlet Laplace eigenvalue problem to get the same convergence rates.

Finally, we discuss the **Neumann boundary value problem**. Let us assume for a moment that κ^2 is not an eigenvalue of the interior Neumann Laplace eigenvalue problem. As a consequence, we get that the hypersingular boundary integral operator is invertible. For this kind of problem we prefer to use the second boundary integral equation (2.10). The equivalent variational problem is given by: Find $g \in \mathrm{H}^{1/2}(\Gamma)$ such that

$$(D_\kappa g, v)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = -\left(\left(\frac{1}{2} + K^*_{-\kappa}\right) t, v\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}$$

is satisfied for all $v \in \mathrm{H}^{1/2}(\Gamma)$. The corresponding discrete variational inequality is given by: Find $g_h \in \mathrm{S}^1_{\mathrm{h}}(\Gamma)$ such that

$$(D_\kappa g_h, v_h)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)} = -\left(\left(\frac{1}{2} + K^*_{-\kappa}\right) t, v_h\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}$$

is satisfied for all $v_h \in \mathrm{S}^1_{\mathrm{h}}(\Gamma)$. The equivalent system of linear equations is given by

$$D_{\kappa,h}\boldsymbol{g} = \boldsymbol{f},$$

where the right hand side is defined by

$$\boldsymbol{f} \in \mathbb{C}^M, \quad \boldsymbol{f}[i] := -\left(\left(\frac{1}{2} + K^*_{-\kappa}\right) t, \varphi_i\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}.$$

Again, using the abstract results of the previous section and the approximation property of the discrete space $\mathrm{S}^1_{\mathrm{h}}(\Gamma)$, we get unique solvability if h is fine enough. In that case we end up with the error estimate

$$\|g - g_h\|_{\mathrm{H}^{1/2}(\Gamma)} \leq c h^{s-1/2} |g|_{\mathrm{H}^s(\Gamma)},$$

if $g \in \mathrm{H}^s(\Gamma)$ for some $s \in [\frac{1}{2}, 2]$.

As for the Dirichlet problem, we discuss the case of κ^2 being an eigenvalue of the interior Neumann Laplace eigenvalue problem. In that case we use the modified system (2.15), which is uniquely solvable for all $\kappa \in \mathbb{R}^+$. The discrete system of linear equations is given by

$$\begin{pmatrix} D_{\kappa,h} & -\frac{1}{2}M_h^* + K_{-\kappa,h}^* \\ \frac{1}{2}M_h - K_{\kappa,h} & V_{\kappa,h} + iV_{0,h} \end{pmatrix} \begin{pmatrix} \boldsymbol{g} \\ \tilde{\boldsymbol{t}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f_1} \\ \boldsymbol{f_2} \end{pmatrix}.$$

The right hand side is defined by

$$\begin{aligned} &\boldsymbol{f_1} \in \mathbb{C}^M, && \boldsymbol{f_1}[i] := -(t, \varphi_i)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \\ &\boldsymbol{f_2} \in \mathbb{C}^N, && \boldsymbol{f_2}[i] := (iV_0 t, \psi_i)_{\mathrm{H}^{1/2}(\Gamma)\times\mathrm{H}^{-1/2}(\Gamma)}. \end{aligned}$$

For this approach we end up with the same error estimate as for the standard approach, if we claim the same assumptions.

In the following, we generate meshes by using the software GMSH, see [20]. The assembling of all matrices and right hand sides is done via the software package BEM++, see [53]. Adaptive cross-approximation (ACA) is used for assembling the matrices. Therefore, the AHMED software library is used, see [3]. For further details see [4].

3 Exterior Dirichlet boundary control problems

In this chapter we will introduce an optimal control problem. The Helmholtz equation with given wave number κ will occur as PDE constraint. One important property of this problem will be that the Helmholtz equation has to be solved in an unbounded exterior domain Ω^c. The control will act on the boundary Γ_C of this unbounded domain and we will observe on a subset Γ_O of Ω^c. The set Γ_O can be a three dimensional object, a two dimensional manifold, a curve or a set of finitely many points.

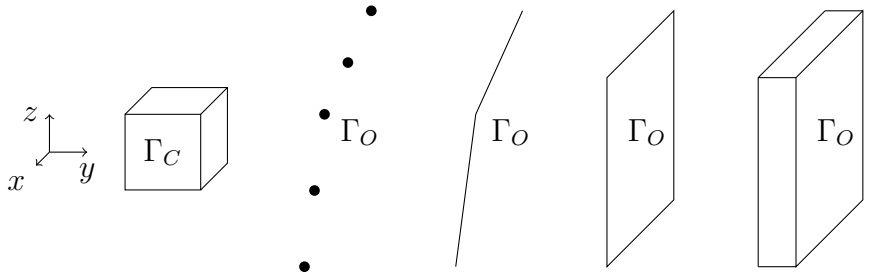
Boundary control problems are also discussed in e.g. [11, 16, 32, 35, 38, 66]. As it is suggested in [42, 43], an energy regularization is used for the Dirichlet boundary control problem. This is a main difference to standard literature, where the $\mathrm{L}^2(\Gamma_C)$-regularization is more common.

In Section 2.4 it was shown that if κ^2 corresponds to an interior Dirichlet Laplace eigenvalue problem, spurious modes can appear. In the first three sections of this chapter we will assume that this is not the case. I.e. the wave number κ is chosen in a way, such that the single layer boundary integral operator and its adjoint are invertible.

Using boundary integral equations, the analysis of the boundary control problem will be tackled in the first section of this chapter.

In the second part we will discuss the discretization. A Galerkin approach will be used. The main results of this section are error estimates for the control in the energy norm.

Due to control constraints, a variational inequality will be derived in the first section and a discrete variational inequality in the second section, respectively.



Control boundary. Different observation domains.

Figure 3.1: Geometric setting.

A semi-smooth Newton method will be introduced and analyzed in the third section to solve discrete variational inequalities.

In the fourth section we will analyze the case, if κ^2 is an eigenvalue of the interior Dirichlet Laplace eigenvalue problem. Modified boundary integral equations will be used to overcome this difficulty.

Finally, numerical examples will be presented in the fifth section. We will compare the numerical results with the theoretical results of the previous sections.

3.1 The optimal control problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. The corresponding exterior domain is denoted by Ω^c, i.e. $\Omega^c = \mathbb{R}^3 \setminus \bar{\Omega}$. The boundary of Ω is denoted by Γ_C and is called the control boundary. To be able to state the minimization problem, we additionally introduce the subset $\Gamma_O \subset \Omega^c$. On this subset the observation takes place. There are four settings we are interested in:

- Γ_O is a three dimensional domain,
- Γ_O is a two dimensional manifold,
- Γ_O is a one dimensional curve,
- Γ_O is a set of finitely many points,

see Figure 3.1. If Γ_O is the set of finitely many points $\boldsymbol{x_i}$, the given desired state $\tilde{u}_o$ is defined by finitely many complex values $\tilde{u}_o(\boldsymbol{x_i})$. Otherwise, $\tilde{u}_o$ is a given function in $\mathrm{L}^2(\Gamma_O)$. Furthermore, let $\varrho \in \mathbb{R}^+$ be a given cost coefficient and let $\kappa \in \mathbb{R}^+$ be a given wave number.

We are interested in the following minimization problem: Find $(z,u) \in Z_{ad} \times \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$, which is a minimizer of the cost functional

$$J(z,u) := \frac{1}{2} \|u|_{\Gamma_O} - \tilde{u}_o\|^2_{\mathrm{L}^2(\Gamma_O)} + \frac{\varrho}{2} \left(\hat{D}_0^{cc} z, z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)}, \tag{3.1}$$

or in case of Γ_O is the set of finitely many points a minimizer of

$$J(z,u) := \frac{1}{2} \sum_{\boldsymbol{x_i} \in \Gamma_O} \left(u_o(\boldsymbol{x_i}) - \tilde{u}_o(\boldsymbol{x_i}) \right)^2 + \frac{\varrho}{2} \left(\hat{D}_0^{cc} z, z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)}, \tag{3.2}$$

subject to

$$-\Delta u - \kappa^2 u = 0 \quad \text{in } \Omega^c, \tag{3.3}$$

$$\gamma_0^{\mathrm{ext}} u = z \quad \text{on } \Gamma_C \tag{3.4}$$

in the distributional sense. Additionally, u has to satisfy the radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R \to \infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \mathrm{d}\mu = 0. \tag{3.5}$$

The set of admissible controls is given by

$$Z_{ad} = \left\{ z \in \mathrm{H}^{1/2}(\Gamma_C) : |z(\boldsymbol{x})| \leq c \text{ a.e.} \right\},$$

where $c \in \mathbb{R}^+$ is a given upper bound for the absolute value of the control.

The regularization is realized by using the regularized hypersingular boundary integral $\hat{D}_0^{cc}$. Of course it would be also possible to use $\tilde{D}_0^{cc}$ instead. Another possibility would be to use the Steklov-Poincaré operator for the exterior Laplace problem S_0^{cc}, i.e.

$$S_0^{ccc} := \left(\frac{1}{2} - K_0^{cc*} \right) (V_0^{cc})^{-1} \left(\frac{1}{2} - K_0^{cc} \right) + D_0^{cc}.$$

Therefore, $S_0^{cc} z = -\gamma_1^{\text{ext}} w$, where w solves

$$\begin{aligned} -\Delta w &= 0 \quad \text{in } \Omega^c, \\ \gamma_0^{\text{ext}} w &= z \quad \text{on } \Gamma_C \end{aligned}$$

in the distributional sense and $w(\boldsymbol{x})$ behaves like $\frac{1}{|\boldsymbol{x}|}$, if $|\boldsymbol{x}|$ tends to infinity. For the Helmholtz equation the Steklov-Poincaré operator has no advantage. To the contrary, the realization of the operator S_0^{cc} is more expensive. However, if the Helmholtz equation is replaced by the Laplace equation, the regularization with the Steklov-Poincaré operator has a natural relation to the state variable. For further details see e.g. [42, 46].

Often the term $\|z\|^2_{\mathrm{L}^2(\Gamma_C)}$ is used for regularization. When dealing with boundary integral equations, it turns out that this choice is not practicable, as the control is a priori only an element of $\mathrm{L}^2(\Gamma_C)$ instead of $\mathrm{H}^{1/2}(\Gamma_C)$.

In our case, the constraint $z \in Z_{ad}$ is not called box constraint, as it claims

$$(\Re z)^2 + (\Im z)^2 \leq c^2.$$

This will cause some difficulties in the error analysis and in the algorithmic part, which will be discussed later.

To make the notation easier, we use in the following the abbreviation $u_o := u|_{\Gamma_O}$.

Remark 3.1. *The restriction of u to the observation boundary and the interpretation as an element of $\mathrm{L}^2(\Gamma_O)$ is well defined. In the three dimensional case this is clear. In all the other cases the restriction is well defined because of the regularity of u. As the right hand side of the Helmholtz equation is zero, we immediately get that u is locally arbitrary regular due to the local maximal regularity theorem, see [17, Section 6.3.1].*

Now we can define the control to state operator $H\colon \mathrm{H}^{1/2}(\Gamma_C) \to \mathrm{L}^2(\Gamma_O)$, which is defined by

$$Hz := u_o \quad \text{on } \Gamma_O,$$

where u_o has to be seen as an $\mathrm{L}^2(\Gamma_O)$ function. Using the representation formula (2.9), we get

$$Hz = \left(-SL_\kappa^c t + DL_\kappa^c z\right)|_{\Gamma_O},$$

where SL_κ^c is the single layer potential and DL_κ^c the double layer potential, respectively. Next, we define the operators

$$\begin{aligned} V_\kappa^{oc} \colon \mathrm{H}^{-1/2}(\Gamma_C) &\to \mathrm{L}^2(\Gamma_O), \\ t &\mapsto SL_\kappa^c t|_{\Gamma_O} \end{aligned}$$

and

$$\begin{aligned} K_\kappa^{oc} \colon \mathrm{H}^{1/2}(\Gamma_C) &\to \mathrm{L}^2(\Gamma_O), \\ z &\mapsto DL_\kappa^c z|_{\Gamma_O}, \end{aligned}$$

hence the point evaluation can be rewritten as

$$u_o = -V_\kappa^{oc} t + K_\kappa^{oc} z \quad \text{on } \Gamma_O. \tag{3.6}$$

The two defined operators V_κ^{oc} and K_κ^{oc} are well defined, because no singularity of the fundamental solution occurs in the definition of these operators. This is due to the fact that the points $\boldsymbol{x} \in \Gamma_O$ and $\boldsymbol{y} \in \Gamma_C$ are separated. Using the first boundary integral equation (2.10), i.e.

$$V_\kappa^{cc} t = -\left(\frac{1}{2} - K_\kappa^{cc}\right) z \quad \text{on } \Gamma_C, \tag{3.7}$$

we get

$$Hz = V_\kappa^{oc} \left(V_\kappa^{cc}\right)^{-1} \left(\frac{1}{2} - K_\kappa^{cc}\right) z + K_\kappa^{oc} z \quad \text{on } \Gamma_O.$$

Of course this makes only sense, if the inverse of V_κ^{cc} exists. Therefore, we claim the assumption:

Assumption 3.2. *In this section we assume that the wave number $\kappa \in \mathbb{R}^+$ is chosen, so that the single layer boundary integral operator is invertible. This is equivalent to: κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem, see Theorem 2.26. In Section 3.4 the situation in which the assumption is not satisfied will be discussed.*

As a result we get that the operator H has the representation

$$H = V_\kappa^{oc} \left(V_\kappa^{cc}\right)^{-1} \left(\frac{1}{2} - K_\kappa^{cc}\right) + K_\kappa^{oc}$$

and therefore H is a bounded and linear operator. With the help of this operator, we can define the reduced cost functional $\hat{J}$ as

$$\hat{J}(z) = J(z, Hz).$$

In the next theorem the existence and uniqueness of a minimizer is discussed.

Theorem 3.3. *There is a unique solution* $(z, u) \in Z_{ad} \times \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ *to the exterior Dirichlet boundary control problem* (3.1)-(3.5).

Proof. The theorem can be proven by using [64, Theorem 2.14]. This can be done, because the stabilized hypersingular boundary integral defines an equivalent norm in $\mathrm{H}^{1/2}(\Gamma_C)$. Additionally, the set of admissible controls Z_{ad} is a bounded, closed and convex non-empty set and the control to state operator H is bounded and linear and therefore continuous. □

If the constant of the control constraint is ∞, we get $Z_{ad} = \mathrm{H}^{1/2}(\Gamma_C)$. Hence, the set Z_{ad} is not bounded anymore and we cannot apply the above theorem directly. However, this problem can be circumvent. In this case we choose an arbitrary admissible control $\tilde{z} \in Z_{ad}$. For elements $z \in Z_{ad}$, such that

$$\left(\hat{D}_0^{cc} z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} > 2\varrho^{-1} \hat{J}(\tilde{z}),$$

we get

$$\begin{aligned} \hat{J}(z) &= \frac{1}{2} \left\| Hz - \tilde{u}_o \right\|^2_{\mathrm{L}^2(\Gamma_O)} + \frac{\varrho}{2} \left(\hat{D}_0^{cc} z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} \\ &\geq \frac{\varrho}{2} \left(\hat{D}_0^{cc} z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} > \hat{J}(\tilde{z}) \end{aligned}$$

and hence it is enough to use the bounded set

$$\left\{ z \in \mathrm{H}^{1/2}(\Gamma_C) : \left(\hat{D}_0^{cc} z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} \leq 2\varrho^{-1} \hat{J}(\tilde{z}) \right\}.$$

As we have shown that a unique minimizer exists, we are now interested in first order optimality conditions.

Theorem 3.4. *$z \in Z_{ad}$ is a minimizer of (3.1)-(3.5), if and only if $z \in Z_{ad}$ is a solution of the variational inequality*

$$\Re\left(H^*(Hz - \tilde{u}_o) + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq 0, \tag{3.8}$$

for all $v \in Z_{ad}$.

Proof. We can use the idea of [64, Lemma 2.21]. The only difference is that we have to deal with complex problems here. For an arbitrary $h \in Z_{ad}$ we therefore have a look at

$$\lim_{t\to 0^+} \frac{1}{t}\left[\frac{1}{2}\left\|H(z+th) - \tilde{u}_o\right\|^2_{\mathrm{L}^2(\Gamma_O)} - \frac{1}{2}\left\|Hz - \tilde{u}_o\right\|^2_{\mathrm{L}^2(\Gamma_O)}\right] =$$
$$\frac{1}{2}\left[(Hz - \tilde{u}_o, Hh)_{\mathrm{L}^2(\Gamma_O)} + \overline{(Hz - \tilde{u}_o, Hh)_{\mathrm{L}^2(\Gamma_O)}}\right] = \Re\left(Hz - \tilde{u}_o, Hh\right)_{\mathrm{L}^2(\Gamma_O)}$$

and analogously

$$\lim_{t\to 0^+} \frac{\varrho}{2t}\left[\left(\hat{D}_0^{cc}(z+th), z+th\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}\right.$$
$$\left. - \left(\hat{D}_0^{cc} z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}\right] = \Re\left(\varrho \hat{D}_0^{cc} z, h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}.$$

Therefore, we get a formula for the directional derivative in z in direction h

$$\hat{J}(z)'(h) = \Re\left(H^*(Hz - \tilde{u}_o) + \varrho \hat{D}_0^{cc} z, h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}. \tag{3.9}$$

The first implication: If z is the minimizer and $v \in Z_{ad}$ is arbitrary, then $z + t(v - z) \in Z_{ad}$ for $t \in (0, 1)$ due to the convexity of Z_{ad}. We get

$$\hat{J}(z + t(v - z)) - \hat{J}(z) \geq 0.$$

We can multiply this inequality by the factor $\frac{1}{t}$. Passing to the limit $t \to 0$, we obtain

$$\hat{J}(z)'(v - z) \geq 0,$$

for all $v \in Z_{ad}$. By using (3.9), we obtain the desired variational inequality.

The second direction uses the convexity of the reduced cost functional $\hat{J}$. Due to the convexity and the assumption $0 \leq \hat{J}(z)'(v-z)$ we get

$$0 \leq \hat{J}(z)'(v-z) \leq \hat{J}(v) - \hat{J}(z),$$

for all $v \in Z_{ad}$. Hence, z is a minimizer, because $\hat{J}(z) \leq \hat{J}(v)$ for all $v \in Z_{ad}$. □

As we know a representation of the control to state operator H, we get a representation for the adjoint operator H^*

$$H^* = \left(\frac{1}{2} - K_\kappa^{cc*}\right) \left(V_\kappa^{cc*}\right)^{-1} V_\kappa^{oc*} + K_\kappa^{oc*}.$$

Next, we introduce the dual variable $q \in \mathrm{H}^{-1/2}(\Gamma_C)$,

$$q = \left(V_\kappa^{cc*}\right)^{-1} V_\kappa^{oc*} u_o$$

and the function $f \in \mathrm{H}^{-1/2}(\Gamma_C)$,

$$f = \left(\frac{1}{2} - K_\kappa^{cc*}\right) \left(V_\kappa^{cc*}\right)^{-1} V_\kappa^{oc*} \tilde{u}_o + K_\kappa^{oc*} \tilde{u}_o.$$

Therefore, the dual problem is defined via the equation

$$V_\kappa^{cc*} q = V_\kappa^{oc*} u_o \quad \text{on } \Gamma_C. \tag{3.10}$$

Corollary 3.5. *Using the dual variable q, the variational inequality* (3.8) *turns into*

$$\Re\left(\left(\frac{1}{2} - K_\kappa^{cc*}\right) q + K_\kappa^{oc*} u_o + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v-z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}, \tag{3.11}$$

for all $v \in Z_{ad}$.

Next, we want to know, where this dual variable q comes from. Therefore, we have a look at the so called dual problem: Find the distributional solution of

$$\begin{aligned} -\Delta p - \kappa^2 p &= u_o \delta_{\Gamma_O} && \text{in } \Omega^c, \\ \gamma_0^{\mathrm{ext}} p &= 0 && \text{on } \Gamma_C. \end{aligned}$$

Furthermore, p has to satisfy the following radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla p + i\kappa p \right|^2 \mathrm{d}\mu = 0,$$

where the sign has changed in the second term compared to the radiation condition (3.5).

In the case, where Γ_O is three dimensional, the solution has the following representation

$$p(\boldsymbol{x}) = -\left(SL^c_{-\kappa} q\right)(\boldsymbol{x}) + \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y}) u_o(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y},$$

for $\boldsymbol{x} \in \Omega^c$. In all the other cases, the representation of p is almost similar, i.e.

$$\begin{aligned}
p(\boldsymbol{x}) &= -\left(SL^c_{-\kappa} q\right)(\boldsymbol{x}) + \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y})\, u_o(\boldsymbol{y}) \,\mathrm{d}\mu_{\boldsymbol{y}}, \\
p(\boldsymbol{x}) &= -\left(SL^c_{-\kappa} q\right)(\boldsymbol{x}) + \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y})\, u_o(\boldsymbol{y}) \,\mathrm{d}\tau_{\boldsymbol{y}}, \\
p(\boldsymbol{x}) &= -\left(SL^c_{-\kappa} q\right)(\boldsymbol{x}) + \sum_{\boldsymbol{y_i} \in \Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y_i})\, u_o(\boldsymbol{y_i}),
\end{aligned}$$

for $\boldsymbol{x} \in \Omega^c \setminus \bar{\Gamma}_O$. In all cases q is given by $\gamma_1^{\mathrm{ext}} p$.

The first boundary integral equation is therefore given by

$$V^{cc}_{-\kappa} q - V^{co}_{-\kappa} u_o = 0 \quad \text{on } \Gamma_C,$$

where $V^{co}_{-\kappa} u_o$ is defined by the restriction of the integral over Γ_O to Γ_C. Hence, $V^{co}_{-\kappa}$ is an operator, mapping from $\mathrm{L}^2(\Gamma_O) \to \mathrm{H}^{1/2}(\Gamma_C)$. For example in three dimensions this yields

$$\left(V^{co}_{-\kappa} u_o\right)(\boldsymbol{x}) := \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y}) u_o(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y} \Big|_{\Gamma_C}.$$

The adjoint operator of V^{oc}_{κ} is given by $V^{co}_{-\kappa}$ i.e.

$$\left(V^{co}_{-\kappa} u_o, t\right)_{\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)} = \left(V^{oc*}_{\kappa} u_o, t\right)_{\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)} = \left(u_o, V^{oc}_{\kappa} t\right)_{\mathrm{L}^2(\Gamma_O)},$$

for $t \in \mathrm{H}^{-1/2}(\Gamma_C)$ and $u_o \in \mathrm{L}^2(\Gamma_O)$. In the case, where Γ_O is a three dimensional domain this is true, because for an element t in the dense subspace $\mathrm{L}^\infty(\Gamma_C) \cap \mathrm{H}^{-1/2}(\Gamma_C)$ we get

$$\begin{aligned}(V_\kappa^{oc*} u_o, t)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)} &= (u_o, V_\kappa^{oc} t)_{\mathrm{L}^2(\Gamma_O)} = \\ \left(u_o, \int_{\Gamma_C} G_\kappa(\cdot, \boldsymbol{y}) t(\boldsymbol{y}) \,\mathrm{d}\mu_{\boldsymbol{y}}\right)_{\mathrm{L}^2(\Gamma_O)} &= \left(\int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \cdot) u_o(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}, t\right)_{\mathrm{L}^2(\Gamma_C)} = \\ &\left(V_{-\kappa}^{co} u_o, t\right)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)}.\end{aligned}$$

Therefore, this is true for all $t \in \mathrm{H}^{-1/2}(\Gamma_C)$, too. If Γ_O is of lower dimension, the arguments are the same.

Hence, the first boundary integral equation can be rewritten in the form

$$V_\kappa^{cc*} q - V_\kappa^{oc*} u_o = 0 \quad \text{on } \Gamma_C.$$

The second boundary integral equation is given by

$$q = \left(\frac{1}{2} - K_{-\kappa}^{cc\,\prime}\right) q + K_{-\kappa}^{oc\,\prime} u_o \quad \text{on } \Gamma_C.$$

E.g. in the case, where Γ_O is a three dimensional object, the operator $K_{-\kappa}^{oc\,\prime}$ is defined by

$$\left(K_{-\kappa}^{oc\,\prime} u_o\right)(\boldsymbol{x}) := \gamma_1^{\mathrm{ext}} \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y}) u_o(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}.$$

In all other cases the definition is similar and therefore $K_{-\kappa}^{oc\,\prime}$ is an operator, mapping from $\mathrm{L}^2(\Gamma_O)$ to $\mathrm{H}^{-1/2}(\Gamma_C)$. The adjoint operator of K_κ^{oc} is given by $K_{-\kappa}^{oc\,\prime}$, i.e.

$$\left(K_{-\kappa}^{oc\,\prime} u_o, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} = (K_\kappa^{oc*} u_o, z)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} = (u_o, K_\kappa^{oc} z)_{\mathrm{L}^2(\Gamma_O)},$$

for $z \in \mathrm{H}^{1/2}(\Gamma_C)$ and $u_o \in \mathrm{L}^2(\Gamma_O)$. Again we can prove this for the case, where Γ_O is a three dimensional object, by proving this property for elements z of

the dense subspace $\mathrm{L}^\infty(\Gamma_C) \cap \mathrm{H}^{1/2}(\Gamma_C)$ of $\mathrm{H}^{1/2}(\Gamma_C)$:

$$\begin{aligned}
(K_\kappa^{oc*} u_o, z)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} &= (u_o, K_\kappa^{oc} z)_{\mathrm{L}^2(\Gamma_O)} \\
&= \left(u_o, \int_{\Gamma_C} [\boldsymbol{n}(\boldsymbol{y}) \cdot \nabla_{\boldsymbol{y}} G_\kappa(\cdot, \boldsymbol{y})]\, z(\boldsymbol{y})\, \mathrm{d}\mu_{\boldsymbol{y}} \right)_{\mathrm{L}^2(\Gamma_O)} \\
&= \left(\boldsymbol{n}(\cdot) \cdot \nabla_{\boldsymbol{y}} \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \cdot) u_o(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}, z \right)_{\mathrm{L}^2(\Gamma_C)} \\
&= \left(K_{-\kappa}^{oc\,\prime} u_o, z \right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \mathrm{L}^2(\Gamma_C).
\end{aligned}$$

Hence, this property holds also for $z \in \mathrm{H}^{1/2}(\Gamma_C)$. In the case, where Γ_O is of lower dimension, the arguments are the same.

Therefore, we get the equation

$$q = \left(\frac{1}{2} - K_\kappa^{cc*} \right) q + K_\kappa^{oc*} u_o \quad \text{on } \Gamma_C.$$

In the special, where case Γ_O is a three dimensional domain, the dual problem has the form

$$-\Delta p - \kappa^2 p = \begin{cases} u_o & \text{in } \Gamma_O, \\ 0 & \text{in } \Omega^c \setminus \Gamma_O. \end{cases}$$

The boundary condition and the radiation condition keep unchanged. In the case, where Γ_O is a two dimensional manifold, we obtain

$$\begin{aligned}
-\Delta p - \kappa^2 p = 0 \qquad & \text{in } \Omega^c \setminus \bar{\Gamma}_O, \\
\gamma_0^{\mathrm{ext}} p = 0 \qquad & \text{on } \Gamma_C, \\
[\gamma_{0,O} p] = 0 \qquad & \text{on } \Gamma_O, \\
[\gamma_{1,O} p] = u_o \qquad & \text{on } \Gamma_O.
\end{aligned}$$

Again the radiation condition is the same as in the general case. The two used expressions are defined by the jumps

$$\begin{aligned}
[\gamma_{0,O} p] &:= \gamma_{0,O}^- p - \gamma_{0,O}^+ p, \\
[\gamma_{1,O} p] &:= \gamma_{1,O}^- p - \gamma_{1,O}^+ p,
\end{aligned}$$

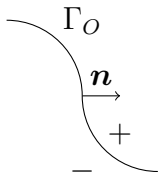


Figure 3.2: Observation boundary.

see Figure 3.2. The two conditions on the observation boundaries can be derived by using the representation of p and the jump conditions of the boundary integral operators. It turns out that it does not matter how we define the normal vector of Γ_O. This is true because if we change the normal vector, we have to switch the region + and − in Figure 3.2 too.

Due to the second boundary integral equation, it would be possible to transfer the variational inequality to

$$\Re\left(q + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}, \quad (3.12)$$

for all $v \in Z_{ad}$. This variational inequality looks simpler and is of course equivalent to (3.11). However, when doing the discretization, it turns out that the variational inequality (3.11) has a better structure than the variational inequality (3.12). This is due to the fact that we get a symmetric representation of the symmetric operator $H^*H + \varrho \hat{D}_0^{cc}$, when using the variational inequality (3.11). For an explanation we look at a similar problem. For the Steklov-Poincaré operator of the Laplace equation we have two boundary integral representations. The symmetric representation is given by

$$S_0^{cc} = \left(\frac{1}{2} - K_0^{cc*}\right)(V_0^{cc})^{-1}\left(\frac{1}{2} - K_0^{cc}\right) + D_0^{cc}$$

and the non-symmetric representation is given by

$$S_0^{cc} = (V_0^{cc})^{-1}\left(\frac{1}{2} - K_0^{cc}\right).$$

In the symmetric case, standard arguments can be used to get convergence results. However, in the non-symmetric case, a discrete inf-sup condition has

to be guaranteed, which leads to some difficulties. For more details, see [58, Section 3.4] or [59].

Summing up, we have to solve the optimality system, i.e. the primal problem (3.7), the point evaluation (3.6), the dual problem (3.10) and the optimality condition (3.11).

In case of "$c = \infty$", i.e. $Z_{ad} = \mathrm{H}^{1/2}(\Gamma_C)$, we get the following optimality system: For given $\tilde{u}_o \in \mathrm{L}^2(\Gamma_O)$ find $q, t \in \mathrm{H}^{-1/2}(\Gamma_C)$, $u_o \in \mathrm{L}^2(\Gamma_O)$ and $z \in Z_{ad}$, such that

$$\begin{pmatrix} 0 & V_\kappa^{cc} & 0 & \frac{1}{2} - K_\kappa^{cc} \\ V_\kappa^{cc*} & 0 & -V_\kappa^{oc*} & 0 \\ 0 & -V_\kappa^{oc} & -1 & K_\kappa^{oc} \\ \frac{1}{2} - K_\kappa^{cc*} & 0 & K_\kappa^{oc*} & \varrho \hat{D}_0^{cc} \end{pmatrix} \begin{pmatrix} q \\ t \\ u_o \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ f \end{pmatrix}. \tag{3.13}$$

In the more general case the last equation in (3.13) has to be exchanged by the variational inequality:

$$\Re\left(\left(\frac{1}{2} - K_\kappa^{cc*}\right) q + K_\kappa^{oc*} u_o + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)},$$

for all $v \in Z_{ad}$. From Theorem 3.3 we know that the minimization problem (3.1)-(3.5) has a unique solution. Hence, the optimality system has a unique solution too. This is due to the equivalence of the optimality system and the minimization problem. However, for the discretization we want to understand the structure of the optimality system in more detail.

Theorem 3.6. *Assume that Assumption 3.2 is satisfied. Then the operator* $H^*H + \varrho \hat{D}_0^{cc}$ *is* $\mathrm{H}^{1/2}(\Gamma_C)$*-elliptic, i.e.*

$$\Re\left(\left(H^*H + \varrho \hat{D}_0^{cc}\right) z, z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \varrho c_1 \left\|z\right\|^2_{\mathrm{H}^{1/2}(\Gamma_C)}$$

holds, for all $z \in \mathrm{H}^{1/2}(\Gamma_C)$*. The constant* c_1 *is the ellipticity constant of the stabilized hypersingular boundary integral* $\hat{D}_0^{cc}$*.*

This statement is true because the term $(H^*Hz, z)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}$ is non-negative and the regularization operator is $\mathrm{H}^{1/2}(\Gamma_C)$-elliptic.

Next, we introduce the notation

$$S := H^* H + \varrho \hat{D}_0^{cc}$$

and using the (boundary integral operator) representation of H and H^* respectively, we obtain the representation

$$S = \left(\left(\frac{1}{2} - K_\kappa^{cc*} \right) (V_\kappa^{cc*})^{-1} V_\kappa^{oc*} + K_\kappa^{oc*} \right) \left(V_\kappa^{oc} (V_\kappa^{cc})^{-1} \left(\frac{1}{2} - K_\kappa^{cc} \right) + K_\kappa^{oc} \right) + \varrho \hat{D}_0^{cc}.$$

As a consequence, we can apply Theorem 2.8 to obtain unique solvability of the variational inequality (3.8), which is equivalent to: Find $z \in Z_{ad}$ such that

$$\Re \left(Sz, v - z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} \geq \left(f, v - z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)}$$

is satisfied for all $v \in Z_{ad}$.

As we have assumed that κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem, we conclude that the optimality system has a unique solution.

Corollary 3.7. *Let Assumption 3.2 be satisfied. Then the optimality system, which is given by* (3.7), (3.10), (3.6) *and* (3.11), *i.e.*

$$V_\kappa^{cc} t = \left(\frac{1}{2} - K_\kappa^{cc} \right) z, \qquad V_\kappa^{cc*} q = V_\kappa^{oc*} u_o, \qquad u_o = -V_\kappa^{oc} t + K_\kappa^{oc} z,$$

and

$$\Re \left(\left(\frac{1}{2} - K_\kappa^{cc*} \right) q + K_\kappa^{oc*} u_o + \varrho \hat{D}_0^{cc} z, v - z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} \geq \Re \left(f, v - z \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)},$$

for all $v \in Z_{ad}$, has a unique solution $q, t \in \mathrm{H}^{-1/2}(\Gamma_C)$, $u_o \in \mathrm{L}^2(\Gamma_O)$ and $z \in Z_{ad}$.

From a structural point of view it would have been more elegant, if we had analyzed the block system instead of the operator $H^*H + \varrho \hat{D}_0^{cc}$. But it turns out that the block system has not the correct structure to apply for example the well known Theorem of Brezzi, see e.g. [8] or textbooks like [5] and [7].

This has a consequence for the discretization. As the inverse operators of V_κ^{cc} and $V_{-\kappa}^{cc}$ appear in the operator H and H^* respectively, we have to apply some kind of Strang lemmata, see [57]. This is due to the fact that the inverse operators cannot be applied exactly and therefore an additional perturbation occurs.

In the next section the main focus is on the discretization of the optimality system.

3.2 Discretization

In this section we assume that κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem. Under this assumption we have seen in the previous section that the optimality system of Corollary 3.7 has a unique solution

$$(q, t, u_o, z) \in \mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{L}^2(\Gamma_O) \times Z_{ad}.$$

Section 3.4 discusses the case, when this assumption is not satisfied. In this section we want to apply a standard Galerkin approach. A more detailed explanation can be found in e.g. [50, 57].

In Section 2.6 we have already introduced the discrete spaces $\mathrm{S}_{\mathrm{h}}^0(\Gamma_C)$ and $\mathrm{S}_{\mathrm{h}}^1(\Gamma_C)$.

In the following we claim the same assumptions, which were used in Section 2.6. I.e. Γ_C is assumed to be a polyhedral surface and the corresponding meshes satisfy Assumption 2.35.

For Γ_O we will need the space of piecewise constant functions, which will be denoted by $\mathrm{S}_{\mathrm{h}}^0(\Gamma_O)$. Therefore, we apply the same procedure as for Γ_C. So we assume that Γ_O is a polyhedron, if the dimension of Γ_O is three. In case of dimension two we assume that Γ_O is a polyhedral manifold and in case of dimension one we assume that Γ_O is a polygonal curve. If Γ_O is a set of finitely

many points, we do not need further assumptions. The corresponding mesh is assumed to be admissible, shape regular and globally quasi uniform.

We additionally need a discrete space $Z_{ad,h} \subset Z_{ad}$, which is defined by

$$Z_{ad,h} := Z_{ad} \cap \mathrm{S}_{\mathrm{h}}^{1}(\Gamma_C).$$

An element $v_h \in Z_{ad,h}$ is characterized by $v_h \in \mathrm{S}_{\mathrm{h}}^{1}(\Gamma_C)$ which satisfies $|v_h(\boldsymbol{x_i})| \leq c$ for all $i \in \{1, \cdots, M^c\}$.

In the following we will introduce the discrete optimality system. Starting point is the discretization of the control, i.e. we introduce the discrete variable z_h,

$$Z_{ad} \ni z \approx z_h \in Z_{ad,h}.$$

Right now we do not discretize the other variables. For a given $z \in Z_{ad}$ and therefore also for $z_h \in Z_{ad,h}$ we compute the primal variable $t = t(z) \in \mathrm{H}^{-1/2}(\Gamma_C)$, by using the primal problem (3.7). Therefore, $t(z)$ is the unique solution of the problem: Find $t \in \mathrm{H}^{-1/2}(\Gamma_C)$, such that

$$V_{\kappa}^{cc} t = \left(-\frac{1}{2} + K_{\kappa}^{cc}\right) z \quad \text{on } \Gamma_C. \tag{3.14}$$

By using the point evaluation (3.6), we can construct $u_o = u_o(t(z), z) \in \mathrm{L}^2(\Gamma_O)$ via

$$u_o = -V_{\kappa}^{oc} t + K_{\kappa}^{oc} z \quad \text{on } \Gamma_O \tag{3.15}$$

and finally $q = q(u_o(t(z), z)) \in \mathrm{H}^{-1/2}(\Gamma_C)$, by using the dual problem (3.10), i.e.

$$V_{\kappa}^{cc*} q = V_{\kappa}^{oc*} u_o \quad \text{on } \Gamma_C. \tag{3.16}$$

It is important to mention that if z is an element of the respective discrete space $Z_{ad,h}$, the variables t, u_o and q are not elements of the discrete spaces. Therefore, this approach is only an auxiliary result, which cannot be used in practice.

Using this semi discrete approach, we end up with the variational inequality: Find $\tilde{z}_h \in Z_{ad,h}$, such that

$$\Re\Bigg(\left(\frac{1}{2} - K_\kappa^{cc*}\right) q(u_o(t(\tilde{z}_h), \tilde{z}_h)) + K_\kappa^{oc*} u_o(t(\tilde{z}_h), \tilde{z}_h) + \varrho \hat{D}_0^{cc} \tilde{z}_h, v_h - \tilde{z}_h \Bigg)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v_h - \tilde{z}_h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}$$

is satisfied for all $v_h \in Z_{ad,h}$. This is equivalent to: Find $\tilde{z}_h \in Z_{ad,h}$, such that

$$\Re\left(S\tilde{z}_h, v_h - \tilde{z}_h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v_h - \tilde{z}_h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}$$

is satisfied for all $v_h \in Z_{ad,h}$. As the operator S is $\mathrm{H}^{1/2}(\Gamma_C)$-elliptic and therefore also $Z_{ad,h}$-elliptic, we immediately obtain unique solvability, by using Theorem 2.8. To get an a priori error estimate, we use Corollary 2.33. We obtain

$$\|z - \tilde{z}_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c \inf_{v_h \in Z_{ad,h}} \left(\Re\left(\mu, v_h - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} + \|z - v_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \right),$$

where μ is defined by

$$\mu := \left(\frac{1}{2} - K_\kappa^{cc*}\right) q(u_o(t(z), z)) + K_\kappa^{oc*} u_o(t(z), z) + \varrho \hat{D}_0^{cc} z - f.$$

If we assume that $\mu \in \mathrm{L}^2(\Gamma_C)$, we can extend this to

$$\|z - \tilde{z}_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c \inf_{v_h \in Z_{ad,h}} \left(\|\mu\|_{\mathrm{L}^2(\Gamma_C)} \|z - v_h\|_{\mathrm{L}^2(\Gamma_C)} + \|z - v_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \right).$$

If we assume further that $z \in \mathrm{H}^s(\Gamma_C)$, for $s \in (1, 2]$, we can define the piecewise linear interpolation of z, which is denoted by $I_h z$. $I_h z \in Z_{ad,h}$ holds, due to $z \in Z_{ad}$. Using the piecewise linear interpolation, we end up with the estimate

$$\|z - \tilde{z}_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c \left(\|\mu\|_{\mathrm{L}^2(\Gamma_C)} \|z - I_h z\|_{\mathrm{L}^2(\Gamma_C)} + \|z - I_h z\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \right).$$

Standard estimates for the interpolation, see e.g. [57, Section 10.2] yield

$$\|z - \tilde{z}_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c \left(h^s + h^{2s-1}\right) \leq c h^s,$$

where the constant c depends now on $|z|_{\mathrm{H}^s(\Gamma_C)}$ and $\|\mu\|_{\mathrm{L}^2(\Gamma_C)}$. Summing up, we have proven the a priori error estimate:

Lemma 3.8. *For the semi discrete approximation we end up with the error estimate*

$$\|z - \tilde{z}_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} \leq ch^{s/2} \, |z|_{\mathrm{H}^s(\Gamma_C)} \,,$$

if $\mu \in \mathrm{L}^2(\Gamma_C)$ *and* $z \in \mathrm{H}^s(\Gamma_C)$, $s \in (1,2]$.

This error estimate is not optimal. However, if we neglect the control constraints, i.e. $Z_{ad} = \mathrm{H}^{1/2}(\Gamma_C)$, we immediately obtain the following error estimate:

Lemma 3.9. *If the set of admissible controls is given by* $Z_{ad} = \mathrm{H}^{1/2}(\Gamma_C)$, *we get the error estimate*

$$\|z - \tilde{z}_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} \leq ch^{s-1/2}$$

for the semi discrete approximation, provided $z \in \mathrm{H}^s(\Gamma_C)$ *for* $s \in [\frac{1}{2}, 2]$.

Next we want to consider and analyze a more practical approach, where the variables t, u_o and q are discretized by q_h, t_h and $u_{o,h}$. The used discrete functions belong to the following spaces

$$\mathrm{H}^{-1/2}(\Gamma_C) \ni q \approx q_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C) \,, \quad \mathrm{H}^{-1/2}(\Gamma_C) \ni t \approx t_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$$

and

$$\mathrm{L}^2(\Gamma_O) \ni u_o \approx u_{o,h} \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O) \,.$$

For a given element $z \in Z_{ad}$, and therefore also for $z_h \in Z_{ad,h}$, we define $t_h(z)$ as the unique solution of the discrete variational problem: Find $t_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$, such that

$$(V^{cc}_\kappa t_h, w_h)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} = \left(\left(-\frac{1}{2} + K^{cc}_\kappa\right) z, w_h\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \tag{3.17}$$

is satisfied for all $w_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$. Using Theorem 2.30 and Theorem 2.36, we get the error estimate

$$\|t - t_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq ch^{s+1/2} \, \|t\|_{\mathrm{H}^s_{\mathrm{pw}}(\Gamma_C)} \,, \tag{3.18}$$

provided $t \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)$, $s \in [-\frac{1}{2}, 1]$ and h small enough, such that the inf-sup condition of Lemma 2.29 is satisfied.

With the help of $t_h(z)$ we can define the (non discrete) auxiliary function $\hat{u}_o$ by

$$\hat{u}_o := u_o(t_h(z), z) = -V_\kappa^{oc} t_h(z) + K_\kappa^{oc} z \quad \text{on } \Gamma_O.$$

Using the error estimate for t_h, we immediately get the estimate

$$\begin{aligned} \|u_o - \hat{u}_o\|_{\mathrm{H}^{-1/2}(\Gamma_O)} &= \|-V_\kappa^{oc} t + K_\kappa^{oc} z + V_\kappa^{oc} t_h - K_\kappa^{oc} z\|_{\mathrm{H}^{-1/2}(\Gamma_O)} \\ &\leq c \|t - t_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq c h^{s+1/2} \|t\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}, \end{aligned}$$

if $t \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)$, $s \in [-\frac{1}{2}, 1]$. The discrete variable $u_{o,h}$ is defined as the unique solution of: Find $u_{o,h} \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O)$ which satisfies

$$(u_{o,h}, w_h)_{\mathrm{L}^2(\Gamma_O)} = (\hat{u}_o, w_h)_{\mathrm{L}^2(\Gamma_O)} = (-V_\kappa^{oc} t_h(z) + K_\kappa^{oc} z, w_h)_{\mathrm{L}^2(\Gamma_O)}, \tag{3.19}$$

for all $w_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O)$. Using the error estimate for the piecewise constant projection to Γ_O, we obtain

$$\|\hat{u}_o - u_{o,h}\|_{\mathrm{H}^{-1/2}(\Gamma_O)} \leq c h^{s+1/2} \|\hat{u}_o\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_O)},$$

for $s \in [-\frac{1}{2}, 1]$. As the function $\hat{u}_o$ is arbitrary regular, this yields to no further assumptions. By using the above error estimates and the triangle inequality, we obtain the error estimate

$$\|u_o - u_{o,h}\|_{\mathrm{H}^{-1/2}(\Gamma_O)} \leq c h^{s+1/2} \|t\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}, \tag{3.20}$$

provided t is regular enough.

To handle the dual variable, we first define the (non discrete) auxiliary variable $\hat{q} := q(u_{o,h}(t_h(z), z))$, which is the unique solution of

$$V_\kappa^{cc*} \hat{q} = V_\kappa^{oc*} u_{o,h} \quad \text{on } \Gamma_C.$$

We immediately get the error estimate

$$\begin{aligned} \|q - \hat{q}\|_{\mathrm{H}^{-1/2}(\Gamma_C)} &= \left\| (V_\kappa^{cc*})^{-1} V_\kappa^{oc*} u_o - (V_\kappa^{cc*})^{-1} V_\kappa^{oc*} u_{o,h} \right\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \\ &\leq c \|u_o - u_{o,h}\|_{\mathrm{H}^{-1/2}(\Gamma_O)} \leq c h^{s+1/2} \|t\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}, \end{aligned}$$

if t is regular enough. Finally, we introduce the discrete variable q_h, which is the discrete solution of: Find $q_h \in \mathrm{S}_{\mathrm{h}}^0(\Gamma_C)$ which satisfies

$$(V_\kappa^{cc*} q_h, w_h)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} = (V_\kappa^{oc*} u_{o,h}, w_h)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}, \tag{3.21}$$

for all $w_h \in \mathrm{S}_{\mathrm{h}}^0(\Gamma_C)$. As for the primal problem, we get the error estimate

$$\|\hat{q} - q_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq c h^{s+1/2} \|q\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)},$$

if q is regular enough. Using the derived error estimates for $\hat{q}$ and for q_h and using the triangle inequality, we end up with

$$\|q - q_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq c h^{s+1/2} \|q\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}, \tag{3.22}$$

provided that t and q are regular enough.

Next we want to find the discrete solution $z_h \in Z_{ad,h}$ of the variational inequality

$$\begin{aligned}\Re\Bigg(\left(\frac{1}{2} - K_\kappa^{cc*}\right) q_h(u_{o,h}(t_h(z_h), z_h)) + K_\kappa^{oc*} u_{o,h}(t_h(z_h), z_h) + \\ \varrho \hat{D}_0^{cc} z_h, v_h - z_h \Bigg)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\,(f, v_h - z_h)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)},\end{aligned} \tag{3.23}$$

for all $v_h \in Z_{ad,h}$.

In the following we want to discuss unique solvability and error estimates for this variational inequality. As usually, we introduce the notation $\boldsymbol{q}, \boldsymbol{t} \in \mathbb{C}^{N^c}$, $\boldsymbol{u_o} \in \mathbb{C}^{N^o}$ and $\boldsymbol{z} \in \mathbb{C}^{M^c}$ for the coefficient vectors of the variables $q_h, t_h, u_{o,h}$ and z_h. From (3.17) we obtain the equivalent system of linear equations

$$V_{\kappa,h}^{cc} \boldsymbol{t} + \left(\frac{1}{2} M_h^{cc} - K_{\kappa,h}^{cc}\right) \boldsymbol{z} = \boldsymbol{0}.$$

The discrete point evaluation (3.19) can be characterized by

$$-V_{\kappa,h}^{oc} \boldsymbol{t} - M_h^{oo} \boldsymbol{u_o} + K_{\kappa,h}^{oc} \boldsymbol{z} = \boldsymbol{0}.$$

The remaining matrices are defined via

$$\begin{aligned} V_{\kappa,h}^{oc} &\in \mathbb{C}^{N^o \times N^c}, & V_{\kappa,h}^{oc}[i,j] &:= \left(V_\kappa^{oc}\psi_j^c, \psi_i^o\right)_{\mathrm{L}^2(\Gamma_O)}, \\ K_{\kappa,h}^{oc} &\in \mathbb{C}^{N^o \times M^c}, & K_{\kappa,h}^{oc}[i,j] &:= \left(K_\kappa^{oc}\varphi_j^c, \psi_i^o\right)_{\mathrm{L}^2(\Gamma_O)}, \\ M_h^{oo} &\in \mathbb{C}^{M^o \times M^o}, & M_h^{oo}[i,j] &:= \left(\psi_j^o, \psi_i^o\right)_{\mathrm{L}^2(\Gamma_O)}. \end{aligned}$$

For the dual problem we obtain the linear system

$$V_{\kappa,h}^{cc\,*}\boldsymbol{q} - V_{\kappa,h}^{oc\,*}\boldsymbol{u_o} = \boldsymbol{0}.$$

The variational inequality (3.23) turns into

$$\Re\left(\left(\frac{1}{2}M_h^{cc*} - K_{\kappa,h}^{cc\,*}\right)\boldsymbol{q} + K_{\kappa,h}^{oc\,*}\boldsymbol{u_o} + \varrho\tilde{D}_{0,h}^{cc}\boldsymbol{z}, \boldsymbol{v}-\boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq (\boldsymbol{f}, \boldsymbol{v}-\boldsymbol{z})_{\mathbb{C}^{M^c}},$$

where the vector $\boldsymbol{f} \in \mathbb{C}^{M^c}$ is defined by

$$\boldsymbol{f}[i] := (f, \varphi_i)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}.$$

Due to $v_h, z_h \in Z_{ad,h}$, $|\boldsymbol{v}[i]| \leq c$ and $|\boldsymbol{z}[i]| \leq c$ follow. Summing up, we have to solve the system: Find $\boldsymbol{q}, \boldsymbol{t} \in \mathbb{C}^{N^c}$, $\boldsymbol{u_o} \in \mathbb{C}^{N^o}$ and

$$\boldsymbol{z} \in \{\boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c\},$$

such that

$$\begin{pmatrix} 0 & V_{\kappa,h}^{cc} & 0 & \frac{1}{2}M_h^{cc} - K_{\kappa,h}^{cc} \\ V_{\kappa,h}^{cc\,*} & 0 & -V_{\kappa,h}^{oc\,*} & 0 \\ 0 & -V_{\kappa,h}^{oc} & -M_h^{oo} & K_{\kappa,h}^{oc} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{t} \\ \boldsymbol{u_o} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \end{pmatrix} \tag{3.24}$$

and

$$\Re\left(\left(\frac{1}{2}M_h^{cc*} - K_{\kappa,h}^{cc\,*}\right)\boldsymbol{q} + K_{\kappa,h}^{oc\,*}\boldsymbol{u_o} + \varrho\tilde{D}_{0,h}^{cc}\boldsymbol{z}, \boldsymbol{v}-\boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq (\boldsymbol{f}, \boldsymbol{v}-\boldsymbol{z})_{\mathbb{C}^{M^c}} \tag{3.25}$$

is satisfied for all $\boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c$. If we do not use constraints for the control, we end up with: Find $\boldsymbol{q}, \boldsymbol{t} \in \mathbb{C}^{N^c}$, $\boldsymbol{u_o} \in \mathbb{C}^{N^o}$ and $\boldsymbol{z} \in \mathbb{C}^{M^c}$, such that

$$\begin{pmatrix} 0 & V_{\kappa,h}^{cc} & 0 & \frac{1}{2}M_h^{cc} - K_{\kappa,h}^{cc} \\ V_{\kappa,h}^{cc\,*} & 0 & -V_{\kappa,h}^{oc\,*} & 0 \\ 0 & -V_{\kappa,h}^{oc} & -M_h^{oo} & K_{\kappa,h}^{oc} \\ \frac{1}{2}M_h^{cc*} - K_{\kappa,h}^{cc\,*} & 0 & K_{\kappa,h}^{oc\,*} & \varrho\tilde{D}_{0,h}^{cc} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{t} \\ \boldsymbol{u_o} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{f} \end{pmatrix}. \tag{3.26}$$

The symmetric structure of system (3.25) yields to an important advantage in proving unique solvability. This topic was already discussed in Section 3.1. As we have assumed that κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem and furthermore that the mesh is fine enough, such that the inf-sup condition of Lemma 2.29 is satisfied, the matrices $V_{\kappa,h}^{cc}$ and $V_{\kappa,h}^{cc\,*}$ are invertible. Of course the matrix M_h^{oo} is invertible too and therefore we can build the Schur complement matrix S_h, which is defined by

$$S_h := \left(\left(\frac{1}{2}M_h^{cc*} - K_{\kappa,h}^{cc\,*}\right)\left(V_{\kappa,h}^{cc\,*}\right)^{-1} V_{\kappa,h}^{oc\,*} + K_{\kappa,h}^{oc\,*}\right)(M_h^{oo})^{-1} \left(V_{\kappa,h}^{oc}\left(V_{\kappa,h}^{cc}\right)^{-1}\left(\frac{1}{2}M_h^{cc} - K_{\kappa,h}^{cc}\right) + K_{\kappa,h}^{oc}\right) + \varrho\tilde{D}_{0,h}^{cc}.$$

Using the Schur complement matrix S_h, we can formulate an equivalent discrete system to (3.24)-(3.25) by: Find

$$\boldsymbol{z} \in \left\{\boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c\right\},$$

such that

$$\Re\left(S_h\boldsymbol{z}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq \left(\boldsymbol{f}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \tag{3.27}$$

is satisfied, for all $\boldsymbol{v} \in \mathbb{C}^{M^c}$, such that $|\boldsymbol{v}[i]| \leq c$.

Now we benefit from the symmetric structure, since we can easily prove unique solvability of the Schur complement system. This is due to the fact that

$$\left(S_h\boldsymbol{z}, \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq \varrho\left(\tilde{D}_{0,h}^{cc}\boldsymbol{z}, \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq c(\varrho)\|\boldsymbol{z}\|_{\mathbb{C}^{M^c}}^2,$$

i.e. the matrix S_h is positive definite.

If we use the non-symmetric version, as mentioned in the previous section, the proof for unique solvability is much more involved. In that case we have to use different meshes to guarantee an additional inf-sup condition for the non-symmetric Schur complement matrix. Therefore, the mesh for the matrices $V_{\kappa,h}^{cc}$ and $V_{\kappa,h}^{cc\,*}$ has to be chosen fine enough. One advantage of the non symmetric approach is that less matrices have to be assembled. However, due to the mentioned disadvantages, we prefer the symmetric approach.

Now we are in the position to estimate the error of the perturbed approach. For any $z \in Z_{ad}$ we have already defined the operator $S(z)$. It follows that

$$S(z) = \left(\frac{1}{2} - K_\kappa^{cc*}\right) q(u_o(t(z), z)) + K_\kappa^{oc*} u_o(t(z), z) + \varrho \hat{D}_0^{cc} z.$$

The perturbation $\tilde{S}$ is defined by

$$\tilde{S}(z) := \left(\frac{1}{2} - K_\kappa^{cc*}\right) q_h(u_{o,h}(t_h(z), z)) + K_\kappa^{oc*} u_{o,h}(t_h(z), z) + \varrho \hat{D}_0^{cc} z.$$

Lemma 3.10. *Let z be a given function in the space Z_{ad}. Furthermore, let $q, t \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)$, $s \in [-\frac{1}{2}, 1]$, be satisfied. Then a constant c independently of h exists, which depends on $\|q\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}$ and $\|t\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}$ such that the difference between $S(z_h)$ and $\tilde{S}(z_h)$ can be estimated by*

$$\left\| S(z_h) - \tilde{S}(z_h) \right\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq c h^{s+1/2}.$$

Moreover $\tilde{S}$ is $Z_{ad,h}$-elliptic, i.e. a constant c exists, such that

$$\Re \left(\tilde{S} z_h, z_h \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} \geq c \, \|z_h\|^2_{\mathrm{H}^{1/2}(\Gamma_C)}$$

is satisfied for all $z_h \in Z_{ad,h}$.

Proof. Using the error estimates (3.20) and (3.22), we obtain the stated error estimate. The $Z_{ad,h}$-ellipticity is a simple consequence of the positive definiteness of the matrix S_h, due to

$$\left(\tilde{S} z_h, z_h \right)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)} = (S_h \boldsymbol{z}, \boldsymbol{z})_{\mathbb{C}^{M^c}},$$

for all $z_h \in Z_{ad,h}$ and corresponding coefficient vectors $\boldsymbol{z}$. □

Using Theorem 2.34, we can state the main theorem of this section.

Theorem 3.11. *Let $\mu \in \mathrm{L}^2(\Gamma_C)$ and $z \in \mathrm{H}^s(\Gamma_C)$ for $s \in (1,2]$. Furthermore, let us assume that $q,t \in \mathrm{H}^{\tilde{s}}_{\mathrm{pw}}(\Gamma_C), \tilde{s} = \frac{s-1}{2}$. The unique solution $z_h \in Z_{ad,h}$ to the discrete variational inequality (3.23) satisfies the a priori error estimate*

$$\|z - z_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c \left(\|z - \tilde{z}_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} + \left\| \left(S - \tilde{S} \right) z \right\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \right)$$

and therefore it follows that

$$\|z - z_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c h^{s/2}.$$

In case of no control constraints, i.e. $Z_{ad} = \mathrm{H}^{1/2}(\Gamma_C)$ and $Z_{ad,h} = \mathrm{S}^1_{\mathrm{h}}(\Gamma_C)$, we gain

$$\|z - z_h\|_{\mathrm{H}^{1/2}(\Gamma_C)} \leq c h^{s-1/2},$$

if we replace the assumptions on z and q,t by $z \in \mathrm{H}^s(\Gamma_C), s \in [\frac{1}{2}, 2]$ and $q,t \in \mathrm{H}^{\tilde{s}}(\Gamma_C), \tilde{s} = s - 1$.

In case of no control constraints we can guarantee the optimal convergence rate. However, this is not true in the case of control constraints.

Remark 3.12. *In the special case of $\kappa = 0$ we obtain the (real valued) Laplace equation instead of the Helmholtz equation. In this case the theory gets easier because X-coercivity can be replaced by X-ellipticity and so on. But most results are similar. However, when dealing with control constraints, the results get better. This is due to the simpler set of admissible controls:*

$$Z_{ad} := \{ z \in \mathrm{H}^{1/2}(\Gamma_C) : \ -c \leq z \leq c \}.$$

Using these box constraints, it is shown in e.g. [55] that the convergence rate can be improved.

Until now we have always assumed that we are able to construct the right hand side vector exactly. As this vector is given by

$$\boldsymbol{f}[i] := (f, \varphi_i)_{\mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C)}$$

and the function f is defined by

$$\left(\frac{1}{2} - K_{\kappa}^{cc*}\right) \left(V_{\kappa}^{cc*}\right)^{-1} V_{\kappa}^{oc*} \tilde{u}_o + K_{\kappa}^{oc*} \tilde{u}_o,$$

this is in general not possible. In practice, the used right hand side vector, which is denoted by $\tilde{\boldsymbol{f}}$, uses an approximation of $\tilde{u}_o$. This approximation is denoted by $\tilde{u}_{o,h}$ and is an element of $\mathrm{S}_{\mathrm{h}}^{0}(\Gamma_O)$. It is defined by the unique solution of the problem: Find $\tilde{u}_{o,h} \in \mathrm{S}_{\mathrm{h}}^{0}(\Gamma_O)$ which satisfies

$$\left(\tilde{u}_{o,h}, w_h\right)_{\mathrm{L}^2(\Gamma_O)} = \left(\tilde{u}_o, w_h\right)_{\mathrm{L}^2(\Gamma_O)},$$

for all $w_h \in \mathrm{S}_{\mathrm{h}}^{0}(\Gamma_O)$. The used right hand side vector is then defined by

$$\tilde{\boldsymbol{f}} := \left(\frac{1}{2} M_h^{cc*} - K_{\kappa,h}^{cc\,*}\right) \left(V_{\kappa,h}^{cc\,*}\right)^{-1} V_{\kappa,h}^{oc\,*} \tilde{\boldsymbol{u}}_{\boldsymbol{o}} + K_{\kappa,h}^{oc\,*} \tilde{\boldsymbol{u}}_{\boldsymbol{o}},$$

where $\tilde{\boldsymbol{u}}_{\boldsymbol{o}}$ is the coefficient vector of $\tilde{u}_{o,h}$. Using standard results of the $\mathrm{L}^2(\Gamma_O)$-projection, it is possible to show that the approximation is good enough such that the convergence rate is not destroyed by the approximation.

3.3 Semi-smooth Newton method

In the previous section we have introduced the discrete variational inequality (3.27):

Find $\boldsymbol{z} \in \boldsymbol{Z_{ad}} := \left\{\boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c \text{ for all } i \in \{1, \cdots, M^c\}\right\}$, *such that*

$$\Re\left(S_h \boldsymbol{z}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq \left(\boldsymbol{f}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}}$$

is satisfied for all $\boldsymbol{v} \in \boldsymbol{Z_{ad}}$.

Problem 3.1: Discrete variational inequality.

We are interested in Hermitian, positive definite matrices $S_h \in \mathbb{C}^{M^c \times M^c}$ and $\boldsymbol{f}$ is therefore a complex vector of dimension M^c.

Furthermore, we have proven an error estimate for the solution of this discrete variational inequality. In this section we want to focus on the algorithmic part. In particular we want to find an algorithm to solve the discrete variational problem (3.27).

In the following we use the notation $\boldsymbol{\mu} := S_h \boldsymbol{z} - \boldsymbol{f}$ for the Lagrange parameter and $\boldsymbol{\lambda} \in \mathbb{R}^{M^c}$: $\boldsymbol{\lambda}[i] = |\boldsymbol{\mu}[i]|, i \in \{1, \cdots, M^c\}$. The following problem is equivalent to Problem 3.1.

Find $\boldsymbol{z} \in \boldsymbol{Z_{ad}} := \left\{ \boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c \text{ for all } i \in \{1, \cdots, M^c\} \right\}$ *such that*

$$\Re \left(\boldsymbol{\mu}[i], v - \boldsymbol{z}[i] \right)_{\mathbb{C}} \geq 0$$

is satisfied for all $i \in \{1, \cdots, M^c\}$ *and for all* $v \in \mathbb{C}$: $|v| \leq c$. *The vector* $\boldsymbol{\mu} \in \mathbb{C}^{M^c}$ *is defined by* $\boldsymbol{\mu} := S_h \boldsymbol{z} - \boldsymbol{f}$.

Problem 3.2: Equivalent discrete variational inequality.

Let i be in the set $\{1, \cdots, M^c\}$. We distinguish between two cases

$$\boldsymbol{\mu}[i] = 0 \quad \text{and} \quad \boldsymbol{\mu}[i] \neq 0.$$

In the second case we will show that $|\boldsymbol{z}[i]| = c$. We want to prove this by contradiction, i.e. we assume that $|\boldsymbol{z}[i]| < c$. Therefore, an $\varepsilon > 0$ exists, such that $|\boldsymbol{z}[i] \pm \varepsilon| \leq c$ and $|\boldsymbol{z}[i] \pm i\varepsilon| \leq c$. The vectors which are defined by

$$\begin{aligned}
\boldsymbol{v_1}[j] &= \boldsymbol{z}[j], \text{ for } j \in \{1, \cdots, M^c\}, j \neq i, & \boldsymbol{v_1}[i] &= \boldsymbol{z}[i] + \varepsilon, \\
\boldsymbol{v_2}[j] &= \boldsymbol{z}[j], \text{ for } j \in \{1, \cdots, M^c\}, j \neq i, & \boldsymbol{v_2}[i] &= \boldsymbol{z}[i] - \varepsilon, \\
\boldsymbol{v_3}[j] &= \boldsymbol{z}[j], \text{ for } j \in \{1, \cdots, M^c\}, j \neq i, & \boldsymbol{v_3}[i] &= \boldsymbol{z}[i] + i\varepsilon, \\
\boldsymbol{v_4}[j] &= \boldsymbol{z}[j], \text{ for } j \in \{1, \cdots, M^c\}, j \neq i, & \boldsymbol{v_4}[i] &= \boldsymbol{z}[i] - i\varepsilon
\end{aligned}$$

are elements of $\boldsymbol{Z_{ad}}$ and hence it follows that

$$\Re(\overline{\boldsymbol{\mu}[i]} \cdot (\pm\varepsilon)) \geq 0 \quad \text{and} \quad \Re(\overline{\boldsymbol{\mu}[i]} \cdot i(\pm\varepsilon)) \geq 0.$$

The first inequality yields $\Re\boldsymbol{\mu}[i] = 0$ and the second $\Im\boldsymbol{\mu}[i] = 0$, which is a contradiction to $\boldsymbol{\mu}[i] \neq 0$, i.e. $|\boldsymbol{z}[i]| = c$. Summing up both cases, we have proven that

$$(|\boldsymbol{z}[i]| - c)\,\boldsymbol{\lambda}[i] = 0$$

holds, for all $i \in \{1, \cdots, M^c\}$.

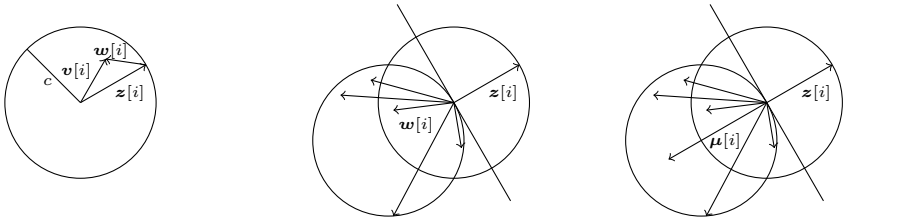
In the case of $i \in \{1, \cdots, M^c\}$ and $\boldsymbol{\mu}[i] \neq 0$, and therefore $|\boldsymbol{z}[i]| = c$, we get

$$\boldsymbol{z}[i] = -c\frac{\boldsymbol{\mu}[i]}{|\boldsymbol{\mu}[i]|} = -c\frac{\boldsymbol{\mu}[i]}{\boldsymbol{\lambda}[i]}. \tag{3.28}$$

Figure 3.3 gives an explanation for this formula: The angles between $\boldsymbol{\mu}[i]$ and all $\boldsymbol{w}[i]$ have to be in $[-\frac{\pi}{2}, \frac{\pi}{2}]$ due to

$$\cos(\sphericalangle(\boldsymbol{\mu}[i], \boldsymbol{w}[i]))\,|\boldsymbol{\mu}[i]|\,|\boldsymbol{w}[i]| = \Re\left(\overline{\boldsymbol{\mu}[i]} \cdot \boldsymbol{w}[i]\right) \geq 0.$$

Therefore, the only possible situation is the one which is given in (3.28).



$\boldsymbol{w}[i] := \boldsymbol{v}[i] - \boldsymbol{z}[i]$. Different $\boldsymbol{w}[i]$. Lagrange parameter $\boldsymbol{\mu}[i]$.

Figure 3.3: Relation between $\boldsymbol{\mu}[i]$ and $\boldsymbol{z}[i]$.

Summing up, we have to solve:

Find $\boldsymbol{z} \in \mathbb{C}^{M^c}$ *such that*

$$|\boldsymbol{z}[i]| \leq c \quad \textit{and} \quad \boldsymbol{z}[i]\boldsymbol{\lambda}[i] = -c\boldsymbol{\mu}[i],$$

for all $i \in \{1, \cdots, M^c\}$. *The vectors* $\boldsymbol{\mu} \in \mathbb{C}^{M^c}$ *and* $\boldsymbol{\lambda} \in \mathbb{R}^{M^c}$ *are defined by*

$$\boldsymbol{\mu} := S_h\boldsymbol{z} - \boldsymbol{f} \quad \textit{and} \quad \boldsymbol{\lambda}[i] := |\boldsymbol{\mu}[i]|, i \in \{1, \cdots, M^c\}.$$

Problem 3.3: Discrete complementary conditions.

We have already proven that Problem 3.1 implies Problem 3.3. The other way around is also true. To prove this we show the equivalence of Problem 3.3 to Problem 3.2. In the case of $i \in \{1, \cdots, M^c\}$ with $\boldsymbol{\lambda}[i] = 0$ we trivially obtain

$$\Re\left(\boldsymbol{\mu}[i], v - \boldsymbol{z}[i]\right)_{\mathbb{C}} \geq 0,$$

for all $v \in \mathbb{C}$: $|v| \leq c$. For $\boldsymbol{\lambda}[i] \neq 0$ we obtain $\boldsymbol{z}[i] = -c\frac{\boldsymbol{\mu}[i]}{\boldsymbol{\lambda}[i]}$. We have to show that the variational inequality

$$\Re\left(\boldsymbol{\mu}[i], v - \boldsymbol{z}[i]\right)_{\mathbb{C}} \geq 0$$

is true, for all $v \in \mathbb{C}$: $|v| \leq c$. Due to the special structure of $\boldsymbol{z}[i]$, this is equivalent to

$$\frac{1}{\boldsymbol{\lambda}[i]c}\Re\left(\boldsymbol{\mu}[i], v + c\frac{\boldsymbol{\mu}[i]}{\boldsymbol{\lambda}[i]}\right)_{\mathbb{C}} \geq 0, \quad \text{for all } v \in \mathbb{C}\text{: } |v| \leq c.$$

Furthermore, this is equivalent to

$$\frac{1}{\boldsymbol{\lambda}[i]c}\Re\left(\boldsymbol{\mu}[i], v\right)_{\mathbb{C}} + 1 \geq 0, \quad \text{for all } v \in \mathbb{C}\text{: } |v| \leq c,$$

and therefore equivalent to

$$\frac{|v|}{c}\cos(\sphericalangle(\boldsymbol{\mu}[i], v)) \geq -1, \quad \text{for all } v \in \mathbb{C}\text{: } |v| \leq c,$$

which is a true statement.

Finally, we want to introduce another equivalent formulation, by using a complementarity function.

Let $\gamma \in \mathbb{R}^+$ be given. Find $\boldsymbol{z} \in \mathbb{C}^{M^c}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{M^c}$ such that

$$\left(S_h \boldsymbol{z} - \boldsymbol{f}\right)[i] + \frac{1}{c}\boldsymbol{\lambda}[i]\boldsymbol{z}[i] = 0$$

and

$$\boldsymbol{\lambda}[i] = \max\left\{0, \boldsymbol{\lambda}[i] + \gamma\left(|\boldsymbol{z}[i]| - c\right)\right\},$$

for all $i \in \{1, \cdots, M^c\}$.

Problem 3.4: Equivalent problem using complementarity function.

First we show that, if $\boldsymbol{z} \in \mathbb{C}^{M^c}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{M^c}$ solve Problem 3.4, $\boldsymbol{z}$ is also a solution of Problem 3.3. As usual we define the vector $\boldsymbol{\mu} \in \mathbb{C}^{M^c}$ by $\boldsymbol{\mu} := S_h \boldsymbol{z} - \boldsymbol{f}$. Therefore, it follows that $\boldsymbol{z}[i]\boldsymbol{\lambda}[i] = -c\boldsymbol{\mu}[i]$. In the case of $\boldsymbol{\lambda}[i] = 0$ we get $|\boldsymbol{z}[i]| \leq c$ due to the complementarity function. If on the other hand $\boldsymbol{\lambda}[i] \neq 0$, we can conclude that $|\boldsymbol{z}[i]| = c$. Again the complementarity function was used. Hence, we get $|\boldsymbol{z}[i]| \leq c$. By using the formula $|\boldsymbol{\mu}[i]| = \frac{1}{c}\boldsymbol{\lambda}[i]|\boldsymbol{z}[i]|$, we can finally conclude that $|\boldsymbol{\mu}[i]| = \boldsymbol{\lambda}[i]$.

The other way around is straight forward.

In the following we will use the non-linear equations in Problem 3.4 to solve the discrete variational inequality. For the implementation it is easier to solve a pure real valued problem instead of a mixture (due to $\boldsymbol{z} \in \mathbb{C}^{M^c}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{M^c}$). Therefore, we split the complex valued vectors $\boldsymbol{z}$ and $\boldsymbol{f}$ and the complex valued matrix S_h into its real and imaginary part, i.e. $\boldsymbol{z} = \boldsymbol{z_1} + i\boldsymbol{z_2}$, $\boldsymbol{f} = \boldsymbol{f_1} + i\boldsymbol{f_2}$ and $S_h = S_{h,1} + iS_{h,2}$.

For all $i \in \{1, \cdots, M^c\}$ we therefore have to solve the three nonlinear equations

$$\boldsymbol{F_1}(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda})[i] := \left(S_{h,1}\boldsymbol{z_1} - S_{h,2}\boldsymbol{z_2} - \boldsymbol{f_1}\right)[i] + \frac{1}{c}\boldsymbol{\lambda}[i]\boldsymbol{z_1}[i] = 0, \tag{3.29}$$

$$\boldsymbol{F_2}(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda})[i] := \left(S_{h,1}\boldsymbol{z_2} + S_{h,2}\boldsymbol{z_1} - \boldsymbol{f_2}\right)[i] + \frac{1}{c}\boldsymbol{\lambda}[i]\boldsymbol{z_2}[i] = 0 \tag{3.30}$$

and

$$\boldsymbol{F_3}(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda})[i] := \boldsymbol{\lambda}[i] - \max\left\{0, \boldsymbol{\lambda}[i] + \gamma\left(\left(\boldsymbol{z_1}[i]^2 + \boldsymbol{z_2}[i]^2\right)^{1/2} - c\right)\right\} = 0. \quad (3.31)$$

Due to the complementarity function, which is not smooth, we are not able to apply Newton's method. Therefore, we apply the semi-smooth Newton method, see [22, 26]. Hence, we have to introduce the concept of slant derivatives.

Definition 3.13 (Slant derivative)**.** *Let $\boldsymbol{F}\colon \mathbb{R}^n \to \mathbb{R}^n$ be a given mapping. $\boldsymbol{F}$ is said to be slantly differentiable, if a family of mappings*

$$G\colon \mathbb{R}^n \to \mathbb{R}^{n\times n}$$

exists, such that for an arbitrary $\boldsymbol{h} \in \mathbb{R}^n$

$$\lim_{\boldsymbol{h}\to\boldsymbol{0}} \frac{1}{\|\boldsymbol{h}\|_{\mathbb{R}^n}} \|\boldsymbol{F}(\boldsymbol{x}+\boldsymbol{h}) - \boldsymbol{F}(\boldsymbol{x}) - G(\boldsymbol{x}+\boldsymbol{h})\boldsymbol{h}\|_{\mathbb{R}^n} = 0,$$

for every $\boldsymbol{x} \in \mathbb{R}^n$. G is called slanting function and does not have to be unique as described in [22].

Before we state the slanting function of $(\boldsymbol{F_1}, \boldsymbol{F_2}, \boldsymbol{F_3})^\top$, we introduce the matrix valued function

$$G_m\colon \mathbb{R}^{M^c} \to \mathbb{R}^{M^c\times M^c} \quad \boldsymbol{v} \mapsto G_m(\boldsymbol{v}),$$

which is defined by

$$G_m(\boldsymbol{v})[i,j] = 0, \quad i \neq j$$

and

$$G_m(\boldsymbol{v})[i,i] := \begin{cases} 1, & \boldsymbol{v}[i] > 0, \\ 0, & \boldsymbol{v}[i] \leq 0. \end{cases}$$

G_m is one possible choice of a slanting function for the "max"-function. One slanting function of $(\boldsymbol{F_1}, \boldsymbol{F_2}, \boldsymbol{F_3})^\top$ at $(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda})^\top$ is therefore defined by the

matrix $G \in \mathbb{R}^{3Mc \times 3Mc}$,

$$G(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda}) := \begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\{\boldsymbol{\lambda}[i]\} & -S_{h,2} & \frac{1}{c}\mathrm{diag}\{\boldsymbol{z_1}[i]\} \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\{\boldsymbol{\lambda}[i]\} & \frac{1}{c}\mathrm{diag}\{\boldsymbol{z_2}[i]\} \\ -\mathrm{diag}\left\{\frac{\gamma G_m(\boldsymbol{v})[i,i]\boldsymbol{z_1}[i]}{(\boldsymbol{z_1}[i]^2+\boldsymbol{z_2}[i]^2)^{1/2}}\right\} & -\mathrm{diag}\left\{\frac{\gamma G_m(\boldsymbol{v})[i,i]\boldsymbol{z_2}[i]}{(\boldsymbol{z_1}[i]^2+\boldsymbol{z_2}[i]^2)^{1/2}}\right\} & I - G_m(\boldsymbol{v}) \end{pmatrix}.$$

In the second block row we used the relation $S_{h,2} = -S_{h,2}^\top$, which is valid due to $S_h = S_h^*$. The vector $\boldsymbol{v} \in \mathbb{R}^{Mc}$ is defined by

$$\boldsymbol{v}[i] := \boldsymbol{\lambda}[i] + \gamma\left(\left(\boldsymbol{z_1}[i]^2 + \boldsymbol{z_2}[i]^2\right)^{1/2} - c\right)$$

and the matrix $I \in \mathbb{R}^{Mc \times Mc}$ is the identity matrix. We use the Newton algorithm, which is described in [22], i.e.

$$\begin{pmatrix} \boldsymbol{z_{1,k+1}} \\ \boldsymbol{z_{2,k+1}} \\ \boldsymbol{\lambda_{k+1}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{z_{1,k}} \\ \boldsymbol{z_{2,k}} \\ \boldsymbol{\lambda_k} \end{pmatrix} - G(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k})^{-1} \begin{pmatrix} \boldsymbol{F_1}(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k}) \\ \boldsymbol{F_2}(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k}) \\ \boldsymbol{F_3}(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k}) \end{pmatrix}.$$

Therefore, we end up with the system

$$\begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\{\boldsymbol{\lambda_k}[i]\} & -S_{h,2} & \frac{1}{c}\mathrm{diag}\{\boldsymbol{z_{1,k}}[i]\} \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\{\boldsymbol{\lambda_k}[i]\} & \frac{1}{c}\mathrm{diag}\{\boldsymbol{z_{2,k}}[i]\} \\ -\mathrm{diag}\left\{\frac{\gamma G_m(\boldsymbol{v_k})[i,i]\boldsymbol{z_{1,k}}[i]}{(\boldsymbol{z_{1,k}}[i]^2+\boldsymbol{z_{2,k}}[i]^2)^{1/2}}\right\} & -\mathrm{diag}\left\{\frac{\gamma G_m(\boldsymbol{v_k})[i,i]\boldsymbol{z_{2,k}}[i]}{(\boldsymbol{z_{1,k}}[i]^2+\boldsymbol{z_{2,k}}[i]^2)^{1/2}}\right\} & I - G_m(\boldsymbol{v_k}) \end{pmatrix} \begin{pmatrix} \boldsymbol{z_{1,k+1}} \\ \boldsymbol{z_{2,k+1}} \\ \boldsymbol{\lambda_{k+1}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{g_{1,k}} \\ \boldsymbol{g_{2,k}} \\ \boldsymbol{g_{3,k}} \end{pmatrix},$$

for each iteration, $k = 0, 1, 2, \ldots$. The vector $\boldsymbol{v_k} \in \mathbb{R}^{Mc}$ is defined by

$$\boldsymbol{v_k}[i] := \boldsymbol{\lambda_k}[i] + \gamma\left(\left(\boldsymbol{z_{1,k}}[i]^2 + \boldsymbol{z_{2,k}}[i]^2\right)^{1/2} - c\right)$$

and the right hand side vectors $\boldsymbol{g_{1,k}}, \boldsymbol{g_{2,k}}$ and $\boldsymbol{g_{3,k}}$ are vectors in $\mathbb{R}^{Mc}$ and are defined by

$$\begin{aligned} \boldsymbol{g_{1,k}}[i] &:= \boldsymbol{f_1}[i] + \frac{1}{c}\boldsymbol{z_{1,k}}[i]\boldsymbol{\lambda_k}[i], \\ \boldsymbol{g_{2,k}}[i] &:= \boldsymbol{f_2}[i] + \frac{1}{c}\boldsymbol{z_{2,k}}[i]\boldsymbol{\lambda_k}[i], \\ \boldsymbol{g_{3,k}}[i] &:= -G_m(\boldsymbol{v_k})[i,i]c, \end{aligned}$$

for $i \in \{1, \cdots, M^c\}$.

Due to the third equation, we get

$$(I - G_m(\boldsymbol{v_k}))\, \boldsymbol{\lambda_{k+1}} = 0$$

and hence $\boldsymbol{\lambda_{k+1}} = G_m(\boldsymbol{v_k})\boldsymbol{\lambda_{k+1}}$. Therefore, we get

$$\boldsymbol{\lambda_{k+1}}[i] = 0, \quad \text{if } G(\boldsymbol{v_k})[i,i] = 0.$$

Using this property, we want to modify the system of linear equations to get a better structure. Therefore, we introduce the new matrix

$$\tilde{G}_m(\boldsymbol{v_k}) \in \mathbb{R}^{M^c \times \tilde{M}^c},$$

where $\tilde{M}^c$ is defined by

$$\tilde{M}^c := \left|\{i \in \{1, \cdots, M^c\} \colon G_m(\boldsymbol{v_k})[i,i] \neq 0\}\right|.$$

The matrix $\tilde{G}_m(\boldsymbol{v_k})$ is defined by the matrix $G_m(\boldsymbol{v_k})$, where the zero columns are deleted. For example, if we use the matrix

$$G_m(\boldsymbol{v_k}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

i.e. $M^c = 4$, we obtain

$$\tilde{G}_m(\boldsymbol{v_k}) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix},$$

i.e. $\tilde{M}^c = 2$. We introduce the new vector

$$\tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}} := \tilde{G}_m^\top(\boldsymbol{v_k})\boldsymbol{\lambda_{k+1}} \in \mathbb{R}^{\tilde{M}^c}$$

and therefore we get

$$\tilde{G}_m(\boldsymbol{v_k})\tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}} = \tilde{G}_m(\boldsymbol{v_k})\tilde{G}_m^\top(\boldsymbol{v_k})\boldsymbol{\lambda_{k+1}} = G_m(\boldsymbol{v_k})\boldsymbol{\lambda_{k+1}} = \boldsymbol{\lambda_{k+1}}.$$

Of course, if $\tilde{M}^c$ is zero, the matrix $\tilde{G}_m(\boldsymbol{v_k})$ and therefore also the vector $\tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}}$ are not well defined. In this case we simply get $\boldsymbol{\lambda_{k+1}} = \mathbf{0}$, i.e. we do not need the matrix $\tilde{G}_m(\boldsymbol{v_k})$ and the vector $\tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}}$.

Using the new defined matrix and vector, we can modify the system above to

$$\begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{\lambda_k}[i]\right\} & -S_{h,2} & \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{z_{1,k}}[i]\right\}\tilde{G}_m(\boldsymbol{v_k}) \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{\lambda_k}[i]\right\} & \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{z_{2,k}}[i]\right\}\tilde{G}_m(\boldsymbol{v_k}) \\ -\tilde{G}_m^\top(\boldsymbol{v_k})\mathrm{diag}\left\{\frac{\gamma \boldsymbol{z_{1,k}}[i]}{\left(\boldsymbol{z_{1,k}}[i]^2+\boldsymbol{z_{2,k}}[i]^2\right)^{1/2}}\right\} & -\tilde{G}_m^\top(\boldsymbol{v_k})\mathrm{diag}\left\{\frac{\gamma \boldsymbol{z_{2,k}}[i]}{\left(\boldsymbol{z_{1,k}}[i]^2+\boldsymbol{z_{2,k}}[i]^2\right)^{1/2}}\right\} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{z_{1,k+1}} \\ \boldsymbol{z_{2,k+1}} \\ \tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{g_{1,k}} \\ \boldsymbol{g_{2,k}} \\ \tilde{\boldsymbol{g}}_{\boldsymbol{3,k}} \end{pmatrix}.$$

The vector $\tilde{\boldsymbol{g}}_{\boldsymbol{3,k}} \in \mathbb{R}^{\tilde{M}^c}$ is defined by $\tilde{\boldsymbol{g}}_{\boldsymbol{3,k}}[i] := -c$. Finally, this can be transformed into the system

$$\begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{\lambda_k}[i]\right\} & -S_{h,2} & \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{z_{1,k}}[i]\right\}\tilde{G}_m(\boldsymbol{v_k}) \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{\lambda_k}[i]\right\} & \frac{1}{c}\mathrm{diag}\left\{\boldsymbol{z_{2,k}}[i]\right\}\tilde{G}_m(\boldsymbol{v_k}) \\ \frac{1}{c}\tilde{G}_m^\top(\boldsymbol{v_k})\mathrm{diag}\left\{\boldsymbol{z_{1,k}}[i]\right\} & \frac{1}{c}\tilde{G}_m^\top(\boldsymbol{v_k})\mathrm{diag}\left\{\boldsymbol{z_{2,k}}[i]\right\} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{z_{1,k+1}} \\ \boldsymbol{z_{2,k+1}} \\ \tilde{\boldsymbol{\lambda}}_{\boldsymbol{k+1}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{g_{1,k}} \\ \boldsymbol{g_{2,k}} \\ \hat{\boldsymbol{g}}_{\boldsymbol{3,k}} \end{pmatrix}, \quad (3.32)$$

which has a better structure than the system above, i.e. the matrix is symmetric. The used matrix is denoted by $\tilde{G}(\boldsymbol{z_1}, \boldsymbol{z_2}, \boldsymbol{\lambda})$. The vector $\hat{\boldsymbol{g}}_{\boldsymbol{3,k}} \in \mathbb{R}^{\tilde{M}^c}$ is defined by

$$\hat{\boldsymbol{g}}_{\boldsymbol{3,k}} = \frac{1}{\gamma}\tilde{G}_m^\top(\boldsymbol{v_k}) \begin{pmatrix} \vdots \\ \left(\boldsymbol{z_{1,k}}[i]^2 + \boldsymbol{z_{2,k}}[i]^2\right)^{1/2} \\ \vdots \end{pmatrix}.$$

This system can be solved by e.g. the GMRES method, see [49]. For the matrix-vector-multiplication the matrix S_h can be used instead of $S_{h,1}$ and $S_{h,2}$ to construct a temporary vector. This can be important, since the splitting of S_h is not provided in most implementations. However, then the resulting temporary

vector has to be split into the real and imaginary part to get the correct matrix-vector-multiplication.

Concerning the initial guess, we claim that, if $\boldsymbol{z_{1,0}}[i] = \boldsymbol{z_{2,0}}[i] = 0$, then $\boldsymbol{\lambda_0}[i] = 0$ too. As initial guess we choose e.g.

$$\boldsymbol{z}_0 = S_h^{-1}\boldsymbol{f} \quad \text{and} \quad \boldsymbol{\lambda}_0 = \mathbf{0},$$

which satisfies the mentioned condition of the initial guess. Of course this means that the algorithm terminates immediately, if the control constraints are not active, i.e. if $|\boldsymbol{z}_0[i]| \leq c$ for all $i \in \{1, \cdots, M^c\}$.

Alternatively, we can choose the discrete solution of a coarser mesh, prolongated to the current mesh as initial guess. Dependent on the control constraint this can lead to a better convergence of the semi-smooth Newton method.

To get superlinear convergence in the Newton algorithm, we have to ensure that $\tilde{G}(\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})$ is non-singular in a neighborhood U of the exact solution. Furthermore, the set

$$\left\{ \left\| \tilde{G}(\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})^{-1} \right\|_2 : (\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})^\top \in U \right\}$$

has to be bounded and of course the initial guess $(\boldsymbol{z_{1,0}}, \boldsymbol{z_{2,0}}, \boldsymbol{\lambda_0})^\top$ has to be sufficiently close to the exact solution.

Concerning the invertibility of the matrix $\tilde{G}(\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})$, we prove the following lemma.

Lemma 3.14. *If the initial solution $(\boldsymbol{z_{1,0}}, \boldsymbol{z_{2,0}}, \boldsymbol{\lambda_0})$ is sufficiently close to the exact solution, we can choose the neighborhood U such that the matrix $\tilde{G}(\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})$ is regular for all $(\tilde{\boldsymbol{z}}_{\mathbf{1}}, \tilde{\boldsymbol{z}}_{\mathbf{2}}, \tilde{\boldsymbol{\lambda}})^\top \in U$.*

Proof. Let U be a neighborhood of $(\boldsymbol{z}_{\mathbf{1}}, \boldsymbol{z}_{\mathbf{2}}, \boldsymbol{\lambda})$ with radius ε. Therefore, it follows that

$$\sum_{i=1}^{M^c} \left((\tilde{\boldsymbol{z}}_{\mathbf{1}}[i] - \boldsymbol{z}_{\mathbf{1}}[i])^2 + (\tilde{\boldsymbol{z}}_{\mathbf{2}}[i] - \boldsymbol{z}_{\mathbf{2}}[i])^2 + \left(\tilde{\boldsymbol{\lambda}}[i] - \boldsymbol{\lambda}[i] \right)^2 \right) \leq \varepsilon^2. \tag{3.33}$$

To prove that the matrix $\tilde{G}(\tilde{\boldsymbol{z}}_{\boldsymbol{1}}, \tilde{\boldsymbol{z}}_{\boldsymbol{2}}, \tilde{\boldsymbol{\lambda}})$ is regular, we use the positive definiteness of the matrix S_h. In the following we denote the constant for positive definiteness by d. We immediately obtain that the perturbed matrix

$$S_h + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\}$$

stays positive definite, if $\tilde{\boldsymbol{\lambda}}[i] \geq 0$ for all $i \in \{1, \cdots, M^c\}$. If at least one index i exists such that $\tilde{\boldsymbol{\lambda}}[i] < 0$, we choose the index i^* such that

$$\tilde{\boldsymbol{\lambda}}[i^*] = \min\left\{\tilde{\boldsymbol{\lambda}}[1], \cdots, \tilde{\boldsymbol{\lambda}}[M^c]\right\}.$$

Due to $\boldsymbol{\lambda}[i] \geq 0$ for all indices $i \in \{1, \cdots, M^c\}$ and

$$\left(\tilde{\boldsymbol{\lambda}}[i^*] - \boldsymbol{\lambda}[i^*]\right)^2 \leq \varepsilon^2,$$

we get $\tilde{\boldsymbol{\lambda}}[i^*]^2 \leq \varepsilon^2$ and therefore

$$\Re\left(\left(S_h + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\}\right)\boldsymbol{z}, \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq \left(d - \frac{\varepsilon}{c}\right)\|\boldsymbol{z}\|^2_{\mathbb{C}^{M^c}}.$$

Therefore, we have to choose $\varepsilon < cd$ to obtain that

$$\begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\} & -S_{h,2} \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\} \end{pmatrix}$$

is invertible.

Next we prove that the third block row of (3.32) has full rank. The only problematic situation occurs, if an index $i \in \{1, \cdots, M^c\}$ exists such that

$$G_m(\tilde{\boldsymbol{v}})[i,i] = 1 \quad \text{and} \quad \tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i] = \tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i] = 0.$$

Let us assume that this is the case for index i. Due to the assumption of the lemma, we know that

$$(\tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i] + \boldsymbol{z}_{\boldsymbol{1}}[i])^2 + (\tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i] + \boldsymbol{z}_{\boldsymbol{2}}[i])^2 \leq \varepsilon^2$$

and therefore

$$\boldsymbol{z_1}[i]^2 + \boldsymbol{z_2}[i]^2 \leq \varepsilon^2.$$

If we choose $\varepsilon < c$, we get $\boldsymbol{\lambda}[i] = 0$, due to

$$\boldsymbol{\lambda}[i] = \max\left\{0, \boldsymbol{\lambda}[i] + \gamma\left(\left(\boldsymbol{z_1}[i]^2 + \boldsymbol{z_2}[i]^2\right)^{1/2}\right) - c\right\}.$$

Therefore, we get

$$\tilde{\boldsymbol{\lambda}}[i]^2 = \left(\tilde{\boldsymbol{\lambda}}[i] - \boldsymbol{\lambda}[i]\right)^2 \leq \varepsilon^2.$$

As a consequence, we obtain

$$\tilde{\boldsymbol{v}}[i] = \tilde{\boldsymbol{\lambda}}[i] + \gamma\left(\left(\tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i]^2 + \tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i]^2\right)^{1/2} - c\right) \leq \varepsilon - \gamma c < 0,$$

if we choose $\varepsilon < \gamma c$. Therefore, we get $G_m(\tilde{\boldsymbol{v}})[i,i] = 0$ and hence the case

$$G_m(\tilde{\boldsymbol{v}})[i,i] = 1 \quad \text{and} \quad \tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i] = \tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i] = 0$$

cannot occur. As the Schur complement matrix

$$\begin{pmatrix} \frac{1}{c}\tilde{G}_m^\top(\tilde{\boldsymbol{v}})\mathrm{diag}\left\{\tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i]\right\} & \frac{1}{c}\tilde{G}_m^\top(\tilde{\boldsymbol{v}})\mathrm{diag}\left\{\tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i]\right\} \end{pmatrix}$$
$$\begin{pmatrix} S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\} & -S_{h,2} \\ -S_{h,2}^\top & S_{h,1} + \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{\lambda}}[i]\right\} \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{z}}_{\boldsymbol{1}}[i]\right\}\tilde{G}_m(\tilde{\boldsymbol{v}}) \\ \frac{1}{c}\mathrm{diag}\left\{\tilde{\boldsymbol{z}}_{\boldsymbol{2}}[i]\right\}\tilde{G}_m(\tilde{\boldsymbol{v}}) \end{pmatrix}$$

has full rank, i.e. rank $\tilde{M}^c$, we obtain that the matrix $\tilde{G}(\tilde{\boldsymbol{z}}_{\boldsymbol{1}}, \tilde{\boldsymbol{z}}_{\boldsymbol{2}}, \tilde{\boldsymbol{\lambda}})$ is invertible. Summing up, we have to choose ε such that

$$\varepsilon < cd, \quad \varepsilon < c \quad \text{and} \quad \varepsilon < \gamma c.$$

□

Remark 3.15. *If $G_m(\boldsymbol{v_k})[i,i] = 0$, we have already seen that we obtain $\boldsymbol{\lambda_{k+1}}[i] = 0$. However, if $G_m(\boldsymbol{v_k})[i,i] \neq 0$, we do not get $|\boldsymbol{z_{k+1}}[i]| = c$ in general. This is a main difference to the real valued problem where we have to deal with the simpler box constraint $-c \leq \boldsymbol{z}[i] \leq c$, which causes no additional non-linearity. Then it turns out , see [22], that the resulting algorithm of Newton's method is equal to the primal-dual active set strategy, see [26, 41] for more details.*

In the following we test the algorithm for an example, in which the exact solution is known.

Example. *Let $M \in \mathbb{C}^{n\times n}, n = 100$, be the matrix which is defined by*

$$M := M_1 + M_2^* M_2.$$

$M_1 \in \mathbb{R}^{n\times n}$ is defined by

$$M_1[k,\ell] := \begin{cases} n & \text{if } k = \ell, \\ -\frac{n}{2} & \text{if } |k-\ell| = 1, \\ 0 & \text{else,} \end{cases}$$

$k, \ell \in \{1, \cdots, n\}$. Therefore M_1 is symmetric and positive definite. The second matrix is given by

$$M_2[k,\ell] := \sin(k-1+\ell-1) + i\cos(k-1+l-1),$$

$k, \ell \in \{1, \cdots, n\}$. We use the indices k and ℓ instead of i and j to avoid a mix with the imaginary unit i. One can check that a constant $d > 0$ exists, such that

$$\Re\left(M\boldsymbol{z}, \boldsymbol{z}\right)_{\mathbb{C}^n} \geq d\|\boldsymbol{z}\|^2_{\mathbb{C}^n}$$

holds, for all $\boldsymbol{z} \in \mathbb{C}^n$. The boundedness constant c is equal to 2 and the exact solution is given by $\boldsymbol{z} \in \mathbb{C}^n$

$$\boldsymbol{z}[k] := c\cos\left(\frac{\pi(k-1)}{20}\right)\exp\left(\frac{i\pi(k-1)}{20}\right), \quad k \in \{1, \cdots, n\},$$

and $\boldsymbol{\lambda} \in \mathbb{C}^n$

$$\boldsymbol{\lambda}[k] := \begin{cases} 0 & \text{if } |\boldsymbol{z}[k]| = c \\ |\cos(k-1)| & \text{else,} \end{cases} \quad k \in \{1, \cdots, n\}.$$

The right hand side vector is defined by the formula

$$\boldsymbol{f}[k] := (M\boldsymbol{z})[k] + \frac{1}{c}\boldsymbol{\lambda}[k]\boldsymbol{z}[k], \quad k \in \{1, \cdots, n\}.$$

Using the semi-smooth Newton algorithm, we get superlinear convergence. This can be seen in Table 3.1, where the quotients

$$\frac{\|\boldsymbol{z} - \boldsymbol{z_{k+1}}\|_{\mathbb{C}^n}}{\|\boldsymbol{z} - \boldsymbol{z_k}\|_{\mathbb{C}^n}}$$

and

$$\frac{\left(\sum_{i=1}^{3} \|\boldsymbol{F_i}(\boldsymbol{z_{1,k+1}}, \boldsymbol{z_{2,k+1}}, \boldsymbol{\lambda_{k+1}})\|^2_{\mathbb{C}^n}\right)^{1/2}}{\left(\sum_{i=1}^{3} \|\boldsymbol{F_i}(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k})\|^2_{\mathbb{C}^n}\right)^{1/2}}$$

tend to zero.

It.	$\|\boldsymbol{z} - \boldsymbol{z_k}\|_{\mathbb{C}^n}$	Quotient	$\left(\sum_{i=1}^{3} \|\boldsymbol{F_i}(\boldsymbol{z_{1,k}}, \boldsymbol{z_{2,k}}, \boldsymbol{\lambda_k})\|^2_{\mathbb{C}^n}\right)^{1/2}$	Quotient
1	5.48E+00		2.79E+00	
2	3.14E+00	0.573	2.64E+01	9.441
3	1.67E+00	0.532	2.25E+01	0.854
4	9.53E−01	0.571	1.37E+01	0.608
5	4.97E−01	0.522	6.31E+00	0.461
6	1.47E−01	0.296	1.75E+00	0.277
7	1.63E−03	0.011	3.15E−02	0.018
8	1.28E−06	0.001	1.96E−06	0.000
9	1.20E−12	0.000	8.72E−12	0.000

Table 3.1: Error table to verify superlinear convergence for the semi-smooth Newton method.

3.4 Modified boundary integral equations

In this section we want to see what happens if the single layer boundary integral operator V_κ^{cc} is not invertible. As we have already analyzed in Section 2.4, this is the case if and only if κ^2 is an eigenvalue of the corresponding interior Dirichlet Laplace eigenvalue problem.

The following well known statement will be an important ingredient in this section:

$$\ker V_\kappa^{cc} = \ker\left(\frac{1}{2} - K_{-\kappa}^{cc\,*}\right).$$

A proof can be found in e.g. [56, Section 2]. Due to Fredholm's alternative, we know that if the kernel of V_κ^{cc} is not trivial, we get that the kernel of V_κ^{cc*} is not trivial as well and we obtain

$$\ker V_\kappa^{cc*} = \ker\left(\frac{1}{2} - K_\kappa^{cc*}\right). \tag{3.34}$$

Another important result is discussed in the following lemma.

Lemma 3.16. *Let $\tilde{t}$ be an element of $\ker V_\kappa^{cc}$. The function $\tilde{u} := \left(SL_\kappa^c \tilde{t}\right)(\boldsymbol{x})$ is equal to zero for all points $\boldsymbol{x} \in \Omega^c$.*

Proof. We know that

$$\gamma_0^{\text{ext}} \tilde{u} = \gamma_0^{\text{ext}} SL_\kappa^c \tilde{t} = V_\kappa^{cc} \tilde{t} = 0$$

and therefore $\tilde{u}$ solves the boundary value problem

$$\begin{aligned} \Delta\tilde{u} - \kappa^2\tilde{u} = 0 \quad &\text{in } \Omega^c \\ \gamma_0^{\text{ext}}\tilde{u} = 0 \quad &\text{on } \Gamma_C. \end{aligned}$$

Furthermore, $\tilde{u}$ satisfies the radiation condition of Rellich. As this exterior boundary value problem is uniquely solvable for all $\kappa > 0$, see [39, Theorem 9.11], we get $\tilde{u} = 0$ for $\boldsymbol{x} \in \Omega^c$. □

In the first boundary integral equation of the primal problem (3.7), i.e.

$$V_\kappa^{cc} t = -\left(\frac{1}{2} - K_\kappa^{cc}\right) z \quad \text{on } \Gamma_C,$$

we cannot eliminate the Neumann datum t. However, due to Fredholm's alternative we can determine t up to an element of the kernel of V_κ^{cc}. Using the pseudo inverse $V_\kappa^{cc\dagger}$ of V_κ^{cc}, we get

$$t = -V_\kappa^{cc\dagger}\left(\frac{1}{2} - K_\kappa^{cc}\right) z - \tilde{t},$$

where $\tilde{t}$ is an in general unknown element in the kernel of V_κ^{cc}. Due to the unknown function $\tilde{t}$, we have to be careful in using t. Fortunately, we do not need t but $-V_\kappa^{oc}t$. As $-V_\kappa^{oc}t$ is nothing else than $-SL_\kappa^c t$ restricted to the observation boundary, Γ_O we can use the previous lemma to verify that

$$-V_\kappa^{oc}t = V_\kappa^{oc}\left(V_\kappa^{cc\dagger}\left(\frac{1}{2} - K_\kappa^{cc}\right)z + \tilde{t}\right) = V_\kappa^{oc}V_\kappa^{cc\dagger}\left(\frac{1}{2} - K_\kappa^{cc}\right)z$$

holds and hence this term is independent of $\tilde{t}$. Therefore, we get an expression of u_o without problems by using the point evaluation (3.6). The dual problem (3.10) again causes some troubles. We have to find $q \in \mathrm{H}^{-1/2}(\Gamma_C)$ such that

$$V_\kappa^{cc*}q = V_\kappa^{oc*}u_o \quad \text{on } \Gamma_C$$

holds. As V_κ^{cc} is not invertible, V_κ^{cc*} is neither. Using the pseudo inverse $(V_\kappa^{cc*})^\dagger$ of V_κ^{cc*}, we get

$$q = (V_\kappa^{cc*})^\dagger V_\kappa^{oc*}u_o + \tilde{q},$$

where $\tilde{q}$ is an element in the kernel of V_κ^{cc*}. Again we can benefit from the structure of the optimality system. In the optimality condition we apply the operator $\frac{1}{2} - K_\kappa^{cc*}$ to the dual Neumann datum q. Using (3.34), we get

$$\begin{aligned}\left(\frac{1}{2} - K_\kappa^{cc*}\right)q &= \left(\frac{1}{2} - K_\kappa^{cc*}\right)\left((V_\kappa^{cc*})^\dagger V_\kappa^{oc*}u_o + \tilde{q}\right)\\ &= \left(\frac{1}{2} - K_\kappa^{cc*}\right)(V_\kappa^{cc*})^\dagger V_\kappa^{oc*}u_o\end{aligned}$$

and therefore the variational inequality (3.11), i.e.

$$\begin{aligned}\Re\left(\left(\frac{1}{2} - K_\kappa^{cc*}\right)q + K_\kappa^{oc*}u_o + \varrho\hat{D}_0^{cc}z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}&\\ \geq \Re\,(f, v - z)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)},&\end{aligned}$$

for all $v \in Z_{ad}$, is well defined and independent of $\tilde{t}$ and $\tilde{q}$. Using the same arguments as in Section 3.1, we get the existence and uniqueness of the control z.

Summing up, we have proven that although V_κ^{cc} and V_κ^{cc*} are not invertible, we get existence and uniqueness of z and u_o. Obviously, we cannot expect uniqueness for the Neumann datum t and q. A similar approach was analyzed in [28, 29, 30] for the acoustic-structure-interaction.

Remark 3.17. *For the numerical analysis we get the following two problems. First, if we want to use a Schur complement solver, we have to realize the pseudo inverse, which is more complicated than the standard inverse. Alternatively, we can solve the block system. This block system is not uniquely solvable, which can cause troubles for the solver. The non-uniqueness concerns the approximation of the Neumann datum, i.e. the approximation of t and q respectively. Second, in the discrete setting we cannot guarantee that the property* (3.34) *holds. The same problem occurs when using Lemma 3.16. Hence, we cannot ensure unique solvability neither for the control nor the point evaluation. Therefore, it is not clear how to derive a rigorous numerical analysis.*

Due to the arguments of Remark 3.17, we want to find another approach to avoid problems in case that κ^2 is an eigenvalue of the interior Dirichlet Laplace eigenvalue problem. Additionally, we want to be able to derive a rigorous numerical analysis. This can be done by using modified boundary integral equations. In this thesis we use the approach which was already introduced in Section 2.4. However, using modified boundary integral equations makes the optimality system more complicated. Therefore, solving times are higher compared to the standard approach and preconditioning gets more complicated.

In the following we will use (2.14) for the primal problem, i.e.

$$\begin{pmatrix} D_\kappa^{cc} + i\eta \hat{D}_0^{cc} & \frac{1}{2} + K_{-\kappa}^{cc\,*} \\ \frac{1}{2} + K_\kappa^{cc} & -V_\kappa^{cc} \end{pmatrix} \begin{pmatrix} \tilde{z} \\ t \end{pmatrix} = \begin{pmatrix} i\eta \hat{D}_0^{cc} z \\ z \end{pmatrix} \tag{3.35}$$

instead of (3.7). The constant $\eta \in \mathbb{R} \setminus \{0\}$ can be chosen arbitrary. This operator is $\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)$-coercive and surjective for all $\kappa > 0$. Therefore, this operator is also injective and hence bijective. For more details see [68, Section 5.6].

As is explained in Section 2.4, we get $\tilde{z} = z$. Therefore, we can use the auxiliary variable $\tilde{z}$ in the point evaluation instead of z, i.e.

$$u_o = -V_\kappa^{oc} t + K_\kappa^{oc} \tilde{z} \quad \text{on } \Gamma_O. \tag{3.36}$$

Concerning the dual problem we have already seen that the dual variable q corresponds to

$$p(\boldsymbol{x}) = -SL^c_{-\kappa} q + \int_{\Gamma_O} G_{-\kappa}(\boldsymbol{x}, \boldsymbol{y}) u_o(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y},$$

for $\boldsymbol{x} \in \Omega^c$, if Γ_O is a three dimensional object. For all other dimensions the formula is similar, see Section 3.1. On Γ_C we have seen that $\gamma_0^{\text{ext}} p = 0$ and $\gamma_1^{\text{ext}} p = q$ hold.

The first boundary integral equation for the dual problem is therefore given by

$$V_\kappa^{cc*} q = V_\kappa^{oc*} u_o \quad \text{on } \Gamma_C$$

and for the second boundary integral equation we obtain

$$q = \left(\frac{1}{2} - K_\kappa^{cc*} \right) q + K_\kappa^{oc*} u_o \quad \text{on } \Gamma_C.$$

As the Dirichlet datum is zero, we obtain

$$\begin{pmatrix} D_\kappa^{cc*} & \frac{1}{2} + K_\kappa^{cc*} \\ \frac{1}{2} + K_{-\kappa}^{cc} & -V_\kappa^{cc*} \end{pmatrix} \begin{pmatrix} \tilde{p} \\ q \end{pmatrix} = \begin{pmatrix} K_\kappa^{oc*} u_o \\ -V_\kappa^{oc*} u_o \end{pmatrix} \quad \text{on } \Gamma_C.$$

$\tilde{p}$ is a new auxiliary variable, which is equal to $\gamma_0^{\text{ext}} p = 0$. Again we will use the idea of modified boundary integral equations. Therefore, we modify this system to

$$\begin{pmatrix} D_\kappa^{cc*} + i\eta \hat{D}_0^{cc} & \frac{1}{2} + K_\kappa^{cc*} \\ \frac{1}{2} + K_{-\kappa}^{cc} & -V_\kappa^{cc*} \end{pmatrix} \begin{pmatrix} \tilde{p} \\ q \end{pmatrix} = \begin{pmatrix} K_\kappa^{oc*} u_o \\ -V_\kappa^{oc*} u_o \end{pmatrix} \quad \text{on } \Gamma_C. \tag{3.37}$$

Again this operator is bijective. We get the following relation between the modified operator of the primal problem and the modified operator of the dual problem

$$\begin{pmatrix} D_\kappa^{cc} + i\eta \hat{D}_0^{cc} & \frac{1}{2} + K_{-\kappa}^{cc\,*} \\ \frac{1}{2} + K_\kappa^{cc} & -V_\kappa^{cc} \end{pmatrix}^* = \begin{pmatrix} D_\kappa^{cc*} + i\eta \hat{D}_0^{cc} & \frac{1}{2} + K_\kappa^{cc*} \\ \frac{1}{2} + K_{-\kappa}^{cc} & -V_\kappa^{cc*} \end{pmatrix}.$$

Finally, we transform the variational inequality (3.11): Find $z \in Z_{ad}$ such that

$$\Re\left(\left(\frac{1}{2} - K_\kappa^{cc*}\right) q + K_\kappa^{oc*} u_o + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(f, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)},$$

for all $v \in Z_{ad}$ into the variational inequality: Find $z \in Z_{ad}$, such that

$$\Re\left(i\eta \tilde{D}_0^{cc} \tilde{p} + q + \varrho \hat{D}_0^{cc} z, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(\tilde{f}, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}, \quad (3.38)$$

for all $v \in Z_{ad}$. This is possible, due to $\tilde{p} = 0$ and the second boundary integral equation of the dual problem. The right hand side f was already introduced in Section 3.1. For the modified variational inequality the right hand side is defined by

$$\tilde{f} := \begin{pmatrix} i\eta \tilde{D}_0^{cc} & 1 \end{pmatrix} \begin{pmatrix} D_\kappa^{cc} + i\eta \hat{D}_0^{cc} & \frac{1}{2} + K_{-\kappa}^{cc\,*} \\ \frac{1}{2} + K_\kappa^{cc} & -V_\kappa^{cc} \end{pmatrix}^{*-1} \begin{pmatrix} K_\kappa^{oc*} \\ -V_\kappa^{oc*} \end{pmatrix} \tilde{u}_0.$$

Summing up, we have to solve the modified primal problem (3.35), the modified point evaluation (3.36), the modified dual problem (3.37) and the modified variational inequality (3.38). Therefore, we have to solve the system: Find

$$\begin{pmatrix} \tilde{p} \\ q \end{pmatrix}, \begin{pmatrix} \tilde{z} \\ t \end{pmatrix} \in \mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C), \quad u_o \in \mathrm{L}^2(\Gamma_O) \quad \text{and} \quad z \in Z_{ad},$$

such that

$$\begin{pmatrix} 0 & A & 0 & -B \\ A^* & 0 & -C^* & 0 \\ 0 & -C & 1 & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \tilde{p} \\ q \end{pmatrix} \\ \begin{pmatrix} \tilde{z} \\ t \end{pmatrix} \\ u_o \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (3.39)$$

is satisfied together with the variational inequality

$$\Re\left(-B^*\begin{pmatrix}\tilde{p}\\ q\end{pmatrix}-\varrho\hat{D}_0^{cc}z, v-z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \left(-\tilde{f}, v-z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}, \quad (3.40)$$

for all $v \in Z_{ad}$. The operators are defined by

$$A := \begin{pmatrix} D_\kappa^{cc}+i\eta\hat{D}_0^{cc} & \frac{1}{2}+K_{-\kappa}^{cc\,*}\\ \frac{1}{2}+K_\kappa^{cc} & -V_\kappa^{cc}\end{pmatrix}, \quad B := \begin{pmatrix} i\eta\tilde{D}_0^{cc}\\ 1\end{pmatrix}, \quad C := \begin{pmatrix} K_\kappa^{oc} & -V_\kappa^{oc}\end{pmatrix}.$$

Using these operators, the right hand side has the representation

$$\tilde{f} = B^*A^{*-1}C^*\tilde{u}_0.$$

If we assume that there are no control constraints, we end up with the optimality system

$$\begin{pmatrix} 0 & A & 0 & -B\\ A^* & 0 & -C^* & 0\\ 0 & -C & 1 & 0\\ -B^* & 0 & 0 & -\varrho\hat{D}_0^{cc}\end{pmatrix}\begin{pmatrix}\begin{pmatrix}\tilde{p}\\ q\end{pmatrix}\\ \begin{pmatrix}\tilde{z}\\ t\end{pmatrix}\\ u_o\\ z\end{pmatrix} = \begin{pmatrix} 0\\ 0\\ 0\\ -\tilde{f}\end{pmatrix}. \quad (3.41)$$

In (3.41) we neglected control constraints to illustrate the symmetric structure of the optimality system. From now on we will again consider control constraints.

Due to the fact that the operator A is $\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)$-coercive and bijective, we can use the same arguments as in Section 3.1 to prove unique solvability of the optimality system (3.39)-(3.40) or (3.41).

If κ^2 is not an eigenvalue of the interior Dirichlet Laplace eigenvalue problem, the variables q, t, u_o and z are the same as in the standard approach. In case of an eigenvalue we still get the same control z and point evaluation u_o. But of course we cannot compare the Neumann data q and t since they are not unique in the standard approach.

The Schur complement $S\colon \mathrm{H}^{1/2}(\Gamma_C) \to \mathrm{H}^{-1/2}(\Gamma_C)$ has the representation

$$S := B^* A^{*-1} C^* C A^{-1} B + \varrho \hat{D}_0^{cc}.$$

Therefore, we have to solve the variational inequality: Find $z \in Z_{ad}$ such that

$$\Re\left(Sz, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} \geq \Re\left(\tilde{f}, v - z\right)_{\mathrm{H}^{-1/2}(\Gamma)\times\mathrm{H}^{1/2}(\Gamma)}, \tag{3.42}$$

for all $v \in Z_{ad}$.

Next we want to discretize this optimality system. Using the same discrete spaces as in Section 3.2, we get the following matrices:

$$A_h := \begin{pmatrix} D_{\kappa,h}^{cc} + i\eta \hat{D}_{0,h}^{cc} & \frac{1}{2} M_h^{cc*} + {K_{-\kappa,h}^{cc}}^* \\ \frac{1}{2} M_h^{cc} + K_{\kappa,h}^{cc} & -V_{\kappa,h}^{cc} \end{pmatrix}, \quad B_h := \begin{pmatrix} i\eta \hat{D}_{0,h}^{cc} \\ M_h^{cc} \end{pmatrix}$$

and

$$C_h := \begin{pmatrix} K_{\kappa,h}^{oc} & -V_{\kappa,h}^{oc} \end{pmatrix}.$$

The discrete system is therefore given by: Find

$$\begin{pmatrix} \tilde{\boldsymbol{p}} \\ \boldsymbol{q} \end{pmatrix}, \begin{pmatrix} \tilde{\boldsymbol{z}} \\ \boldsymbol{t} \end{pmatrix} \in \mathbb{C}^{M^c} \times \mathbb{C}^{N^c}, \quad \boldsymbol{u_o} \in \mathbb{C}^{N^o} \quad \text{and} \quad \boldsymbol{z} \in \left\{ \boldsymbol{v} \in \mathbb{C}^{M^c} \colon |\boldsymbol{v}[i]| \leq c \right\},$$

such that

$$\begin{pmatrix} 0 & A_h & 0 & -B_h \\ A_h^* & 0 & -C_h^* & 0 \\ 0 & -C_h & M_h^{oo} & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{p}} \\ \boldsymbol{q} \end{pmatrix} \\ \begin{pmatrix} \tilde{\boldsymbol{z}} \\ \boldsymbol{t} \end{pmatrix} \\ \boldsymbol{u_o} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \end{pmatrix} \tag{3.43}$$

as well as

$$\Re\left(-B_h^* \begin{pmatrix} \tilde{\boldsymbol{p}} \\ \boldsymbol{q} \end{pmatrix} - \varrho \hat{D}_{0,h}^{cc} \boldsymbol{z}, \boldsymbol{v} - \boldsymbol{z} \right)_{\mathbb{C}^{M^c}} \geq \Re\left(-\tilde{\boldsymbol{f}}, \boldsymbol{v} - \boldsymbol{z} \right)_{\mathbb{C}^{M^c}}, \tag{3.44}$$

for all $\boldsymbol{v} \in \mathbb{C}^{M^c}\colon |\boldsymbol{v}[i]| \leq c$. To define the right hand side $\tilde{\boldsymbol{f}}$, we need an approximation of $\tilde{u}_o$. This is done in the following way: Find $\tilde{u}_{o,h} \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O)$ which satisfies

$$(\tilde{u}_{o,h}, w_h)_{\mathrm{L}^2(\Gamma_O)} = (\tilde{u}_o, w_h)_{\mathrm{L}^2(\Gamma_O)},$$

for all $w_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O)$. The corresponding coefficient vector is denoted by $\tilde{\boldsymbol{u}}_{\boldsymbol{o}}$ as in the case of the standard discretization. The right hand side vector of (3.44) is given by

$$\tilde{\boldsymbol{f}} := B_h^* A_h^{*-1} C_h^* \tilde{\boldsymbol{u}}_{\boldsymbol{o}}.$$

If no control constraints are used, the optimality system (3.43)-(3.44) turns into: Find

$$\begin{pmatrix} \tilde{\boldsymbol{p}} \\ \boldsymbol{q} \end{pmatrix}, \begin{pmatrix} \tilde{\boldsymbol{z}} \\ \boldsymbol{t} \end{pmatrix} \in \mathbb{C}^{M^c} \times \mathbb{C}^{N^c}, \quad \boldsymbol{u}_{\boldsymbol{o}} \in \mathbb{C}^{N^o} \quad \text{and} \quad \boldsymbol{z} \in \mathbb{C}^{M^c},$$

such that

$$\begin{pmatrix} 0 & A_h & 0 & -B_h \\ A_h^* & 0 & -C_h^* & 0 \\ 0 & -C_h & M_h^{oo} & 0 \\ -B_h^* & 0 & 0 & -\varrho \hat{D}_{0,h}^{cc} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{p}} \\ \boldsymbol{q} \end{pmatrix} \\ \begin{pmatrix} \tilde{\boldsymbol{z}} \\ \boldsymbol{t} \end{pmatrix} \\ \boldsymbol{u}_{\boldsymbol{o}} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \\ -\tilde{\boldsymbol{f}} \end{pmatrix}.$$

Using the discrete Schur complement S_h,

$$S_h := B_h^* A_h^{*-1} C_h^* M_h^{oo-1} C_h A_h^{-1} B_h + \varrho \hat{D}_{0,h}^{cc},$$

we end up with the variational inequality: Find

$$\boldsymbol{z} \in \left\{ \boldsymbol{v} \in \mathbb{C}^{M^c}\colon |\boldsymbol{v}[i]| \leq c \right\},$$

such that

$$\Re\left(S_h \boldsymbol{z}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}} \geq \Re\left(\tilde{\boldsymbol{f}}, \boldsymbol{v} - \boldsymbol{z}\right)_{\mathbb{C}^{M^c}},$$

for all $\boldsymbol{v} \in \mathbb{C}^{M^c}\colon |\boldsymbol{v}[i]| \leq c$.

Concerning the numerical analysis, we can use the same arguments as in Section 3.2 and therefore omit the details. The only difference is that we have two additional approximations of the auxiliary variables $\tilde{p}$ and $\tilde{z}$. As for the discretization of the standard optimality system, the symmetric structure guarantees unique solvability of the discrete system.

3.5 Numerical examples

3.5.1 Convergence study with exact solution

In general it is not easy to construct an analytic solution to check the theoretical results. Therefore, we apply our theory to a very simple problem, where the Helmholtz equation is replaced by the Laplace equation. Furthermore, we skip control constraints and modify the minimization problem to

$$\min_{z\in \mathrm{H}^{1/2}(\Gamma_C)} \frac{1}{2}\left\|u_o-\tilde{u}_o\right\|^2_{\mathrm{L}^2(\Gamma_O)} + \frac{\varrho}{2}\left(S_0^{cc}z,z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)} - \frac{1}{2}\left(S_0^{cc}g,z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)},$$

subject to

$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega^c, \\ \gamma_0^{\mathrm{ext}} u &= z \quad \text{on } \Gamma_C \end{aligned}$$

and $u(\boldsymbol{x}) \in \mathcal{O}\left(\frac{1}{|\boldsymbol{x}|}\right)$ for $|\boldsymbol{x}| \to \infty$. For this minimization problem we use the Steklov-Poincaré operator S_0^{cc} instead of the stabilized hypersingular operator. Additionally to the given desired state $\tilde{u}_0$, we use the function $g \in \mathrm{H}^{1/2}(\Gamma_C)$ as input. The control boundary Γ_C is the boundary of the sphere with center in $\mathbf{0}$ and radius 1 and the observation boundary Γ_O is the boundary of the sphere with center in $\left(\frac{1}{2},0,0\right)^\top$ and radius 2.

Applying the theory of the previous sections, we have to solve an optimality system containing a primal problem, a dual problem, a point evaluation and an optimality condition. Due to the additional term $-\frac{1}{2}\left(S_0^{cc}g,z\right)_{\mathrm{H}^{-1/2}(\Gamma_C)\times\mathrm{H}^{1/2}(\Gamma_C)}$, the optimality condition turns into

$$\left(\frac{1}{2}-K_0^{cc*}\right)q + K_0^{oc*}u_o + \varrho S_0^{cc}z = f + S_0^{cc}g.$$

We introduce the auxiliary dual variable $\tilde{p}$, which solves

$$\begin{aligned} -\Delta\tilde{p} &= 0 && \text{in } \Omega^c \setminus \bar{\Gamma}_O, \\ \gamma_0^{ext}\tilde{p} &= g && \text{on } \Gamma_C, \\ \left[\gamma_{0,O}\tilde{p}\right] &= 0 && \text{on } \Gamma_O, \\ \left[\gamma_{1,O}\tilde{p}\right] &= u_o - \tilde{u}_o && \text{on } \Gamma_O \end{aligned}$$

and $\tilde{p} \in \mathcal{O}\left(\frac{1}{|\boldsymbol{x}|}\right)$ for $|\boldsymbol{x}| \to \infty$. The representation formula is given by

$$\tilde{p}(\boldsymbol{x}) = -\left(SL_0^c\tilde{q}\right)(\boldsymbol{x}) + \left(DL_0^c g\right)(\boldsymbol{x}) + \int_{\Gamma_O} G_0(\boldsymbol{x},\boldsymbol{y})\left[u_o(\boldsymbol{y}) - \tilde{u}_0(\boldsymbol{y})\right] \mathrm{d}\mu_{\boldsymbol{y}},$$

for points $\boldsymbol{x} \in \Omega^c$. The Neumann datum of $\tilde{p}$ is denoted by $\tilde{q}$. The first boundary integral equation is given by

$$g = -V_0^{cc}\tilde{q} + \left(\frac{1}{2} + K_0^{cc}\right) g + V_0^{oc*}\left(u_o - \tilde{u}_o\right) \quad \text{on } \Gamma_C$$

and the second boundary integral equation by

$$\tilde{q} = \left(\frac{1}{2} - K_0^{cc*}\right)\tilde{q} - D_0^{cc} g + K_0^{oc*}\left(u_o - \tilde{u}_o\right) \quad \text{on } \Gamma_C.$$

Using these two formulas, the definitions of q, f and the Steklov-Poincaré operator, we get

$$\tilde{q} = -S_0^{cc} g - f + \left(\frac{1}{2} - K_0^{cc*}\right) q + K_o^{oc*} u_o \quad \text{on } \Gamma_C.$$

Therefore, the optimality condition is equivalent to

$$\tilde{q} + \varrho t = 0 \quad \text{on } \Gamma_C$$

and it follows that

$$\tilde{q} = -S_0^{cc} g - f + q.$$

Let $\boldsymbol{x} \in \mathbb{R}^3$ be a point with components x_1, x_2, x_3. Then the desired state is given by the constant

$$\tilde{u}_o(\boldsymbol{x}) \equiv \frac{1+\varrho}{2}$$

and the function g is given by

$$g = \varrho \left(r(\boldsymbol{x})^{-1} - 1 \right),$$

where the function $r(\boldsymbol{x})$ is defined by

$$r(\boldsymbol{x}) = \left(\left(x_1 - \frac{1}{2} \right)^2 + x_2^2 + x_3^2 \right)^{1/2}.$$

The solution of the primal problem is given by the primal variable

$$u(\boldsymbol{x}) = r(\boldsymbol{x})^{-1}$$

and the solution of the dual problem is given by

$$p(\boldsymbol{x}) = \begin{cases} \varrho \left(r(\boldsymbol{x})^{-1} - 1 \right) & 1 < r(\boldsymbol{x}) < 2, \\ -\varrho r(\boldsymbol{x})^{-1} & 2 < r(\boldsymbol{x}), \\ -\frac{\varrho}{2} & 2 = r(\boldsymbol{x}). \end{cases}$$

In this example we use $\varrho = 1\text{E}{-6}$ for the cost coefficient. In Table 3.2 we can see the $\mathrm{L}^2(\Gamma_C)$-error of the control. In Section 3.2 error estimates were proven in $\mathrm{H}^{1/2}(\Gamma_C)$. However, as the implementation of the $\mathrm{L}^2(\Gamma_C)$-norm is easier to realize, this norm is used. In the $\mathrm{H}^{1/2}(\Gamma_C)$-norm we expect a convergence rate of 1.50. Therefore, a convergence rate of 2.00 in the $\mathrm{L}^2(\Gamma_C)$-norm seems to be natural.

Level	Elements		Nodes		$\|z - z_h\|_{\mathrm{L}^2(\Gamma_C)}$	Eoc	GMRES
	Γ_C	Γ_O	Γ_C	Γ_O			
0	32	232	18	118	2.97E−1	–	18
1	128	928	66	466	2.29E−1	0.38	59
2	5124	3712	258	1858	5.41E−2	2.08	69
3	2048	14848	1026	7426	1.31E−2	2.04	56
4	8192	59392	4098	29698	3.26E−3	2.01	53
5	32768	237568	16386	118786	8.14E−4	2.00	54

Table 3.2

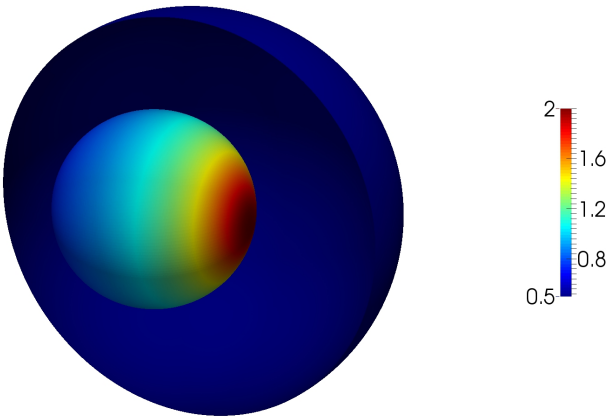


Figure 3.4: Control and point evaluation.

For assembling the boundary element matrices the software BEM++ Version 2.0 was used, see [53]. The ACA option was enabled. The corresponding options were ACAOPTIONS.EPS = 6.4E-7; and ACAOPTIONS.ETA = 0.9;

A Schur complement solver was used to solve the optimality system. For inverting the single layer boundary integral operators $V_{0,h}^{cc}$ and $V_{0,h}^{cc\,*}$ the GMRES method was used, see [49]. The solving of the Schur complement system was also done by the GMRES method.

For preconditioning the Schur complement, the matrix

$$\left(\tilde{M}_h^{cc}\right)^{-1} \tilde{V}_{0,h}^{cc} \left(\tilde{M}_h^{cc}\right)^{-1}$$

was used. The matrices $\tilde{V}_{0,h}^{cc}$ and $\tilde{M}_h^{cc}$ are the single layer boundary integral operator and the mass matrix defined on Γ_C with piecewise linear and globally continuous test and ansatz functions. Further details can be found in e.g. [57, Section 13.2.1]. For preconditioning the two matrices $V_{\kappa,h}^{cc}$ and $V_{\kappa,h}^{cc\,*}$, the BEM++ method ACAOPERATORAPPROXIMATELUINVERSE was used.

The control and the point evaluation are plotted in Figure 3.4.

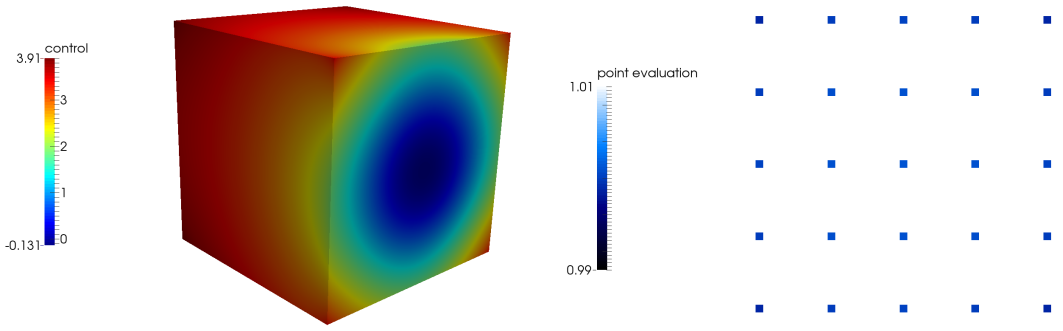


Figure 3.5: $\kappa = 0$, no control constraints, Γ_O ... points.

3.5.2 Convergence study without exact solution

In this section we analyze optimal control problems, where the exact solution is not known. To get a convergence study, all discrete solutions are prolongated to the finest mesh level, i.e. to the fifth mesh level. These prolongated solutions are compared with the discrete solution of level five.

The control takes place on the boundary of the cube $(-1,1)^3$. For the observation two cases are considered. Either we observe on the manifold

$$\left\{ \boldsymbol{x} \in \mathbb{R}^3 \colon x_1 = 3, x_2, x_3 \in \left(-\frac{1}{2}, \frac{1}{2} \right) \right\}$$

or on 25 points, which are uniformly distributed on the previous defined manifold. In the following examples we choose $\varrho = 1\text{E}{-5}$.

In the first example we consider $\kappa = 0$, $\tilde{u}_o \equiv 1$ and no control constraints are used. Furthermore, we observe on the 25 points, which were introduced above. In Figure 3.5 the control and the point observation are plotted and in Table 3.3 we see a convergence rate of 1.66 in the $\mathrm{L}^2(\Gamma_C)$-norm. As in Section 3.5.1 we use the $\mathrm{L}^2(\Gamma_C)$-norm although the theoretical results were proven in the $\mathrm{H}^{1/2}(\Gamma_C)$-norm. Due to the reentrant corner we expect a convergence rate of 1.16 in the $\mathrm{H}^{1/2}(\Gamma_C)$-norm. The solution z is expected to be an element of $\mathrm{H}^{5/3-\varepsilon}(\Gamma_C)$. Therefore, it seems natural to get a convergence rate of 1.66 in the $\mathrm{L}^2(\Gamma_C)$-norm.

In the second example we choose $\kappa = 5$, $\tilde{u}_o = e^{i\kappa\sqrt{x_1^2+x_2^2+x_3^2}}$ and again we do not consider control constraints. In contrast to the first example we observe on

Level	Elements		Nodes		$\|z - z_h\|_{L^2(\Gamma_C)}$	Eoc
	Γ_C	Γ_O	Γ_C	Γ_O		
0	96	–	50	25	5.82E−1	–
1	384	–	194	25	1.68E−1	1.79
2	1536	–	770	25	5.68E−2	1.57
3	6144	–	3074	25	2.04E−2	1.48
4	24576	–	12290	25	6.44E−3	1.66
5	98304	–	49154	25	–	–

Table 3.3: $\kappa = 0$, no control constraints, Γ_O ... points.

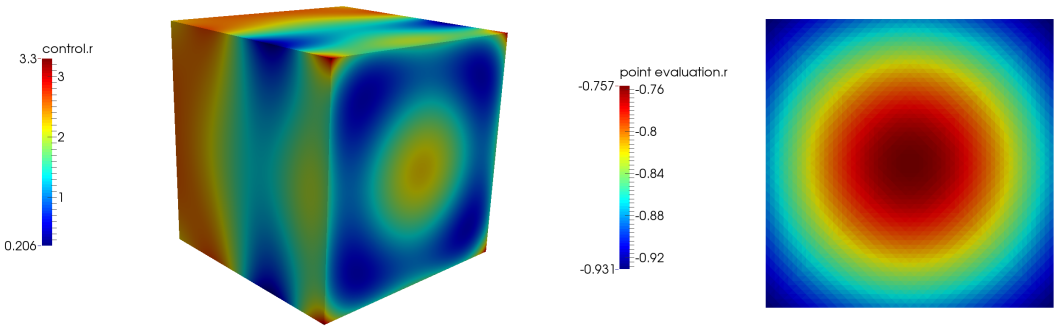


Figure 3.6: Real part, $\kappa = 5$, no control constraints, Γ_O ... manifold.

the manifold. The real and the imaginary part of the solution as well as the absolute value of the solution are plotted in Figure 3.6, 3.7 and 3.8. We can see in Table 3.4 that a convergence rate has not yet been reached. This is due to the lack of an exact solution to which the discrete solution could be compared. It is likely that we again get the convergence rate of 1.66, which is motivated due to the reentrant corner.

In the last example we use the configuration of the second example. Additionally, we claim that $|z(\boldsymbol{x})| \leq 3$ for almost all points $\boldsymbol{x} \in \Gamma_O$. In Figure 3.9 and 3.10 the real and the imaginary part are plotted. Furthermore, we can see the absolute value of the solution in Figure 3.11. Observing a convergence rate with the results of Table 3.5 is difficult. This is due to the comparison with the finest solution.

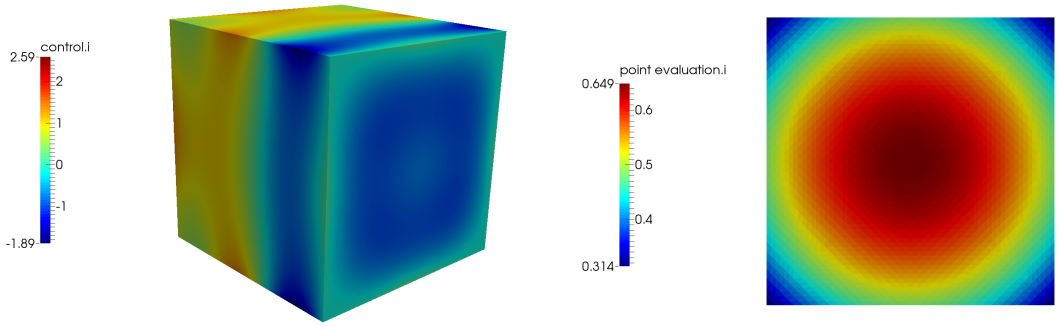


Figure 3.7: Imaginary part, $\kappa = 5$, no control constraints, Γ_O ... manifold.

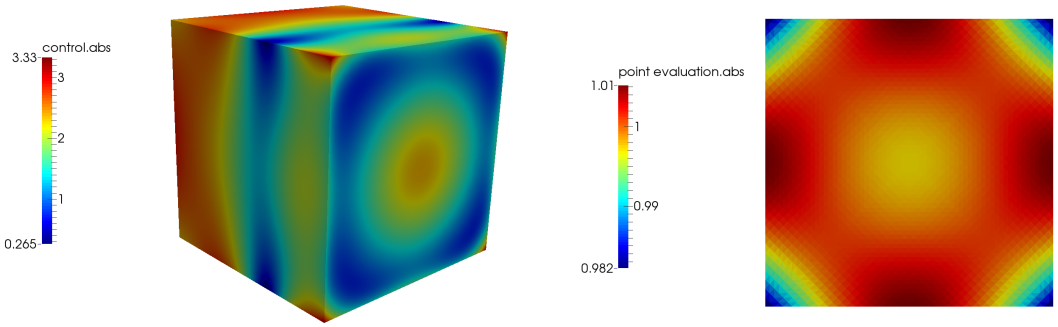


Figure 3.8: Absolute value, $\kappa = 5$, no control constraints, Γ_O ... manifold.

Level	Elements		Nodes		$\|z - z_h\|_{L^2(\Gamma_C)}$	Eoc
	Γ_C	Γ_O	Γ_C	Γ_O		
0	96	4	50	5	8.34E+0	–
1	384	16	194	13	2.06E+0	2.02
2	1536	64	770	41	3.18E+1	2.70
3	6144	256	3074	145	8.54E−2	1.90
4	24576	1024	12290	545	2.46E−2	1.80
5	98304	4096	49154	2113	–	–

Table 3.4: $\kappa = 5$, no control constraints, Γ_O ... manifold.

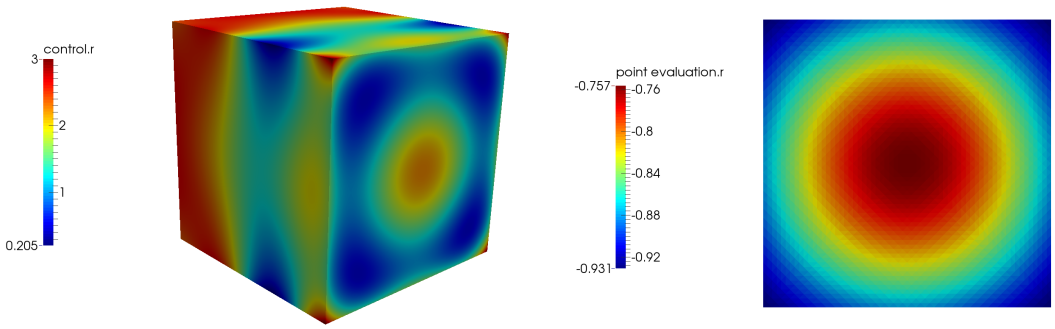


Figure 3.9: Real part, $\kappa = 5$, control constraints, Γ_O ... manifold.

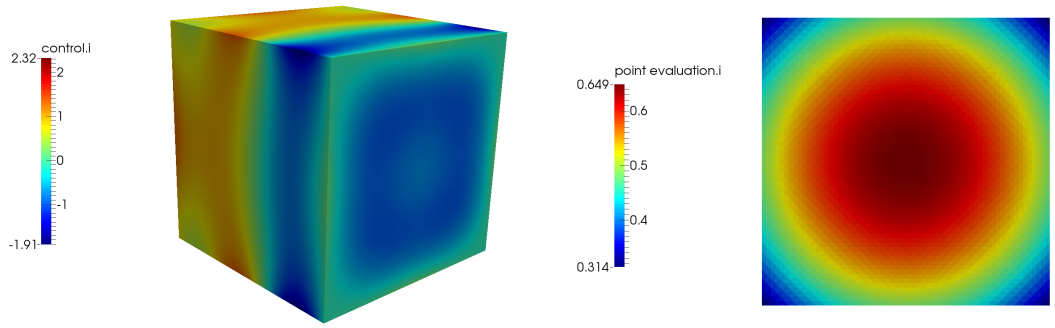


Figure 3.10: Imaginary part, $\kappa = 5$, control constraints, Γ_O ... manifold.

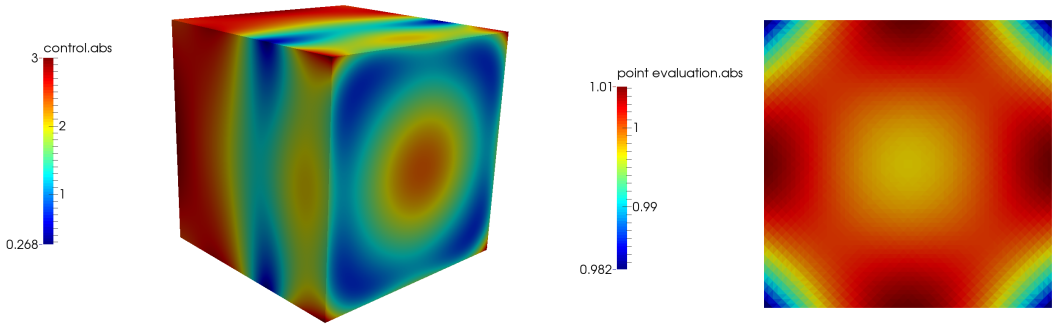


Figure 3.11: Absolute value, $\kappa = 5$, control constraints, Γ_O ... manifold.

Level	Elements		Nodes		$\|z - z_h\|_{\mathrm{L}^2(\Gamma_C)}$	Eoc	Newton it.
	Γ_C	Γ_O	Γ_C	Γ_O			
0	96	4	50	5	8.29E+0	–	9
1	384	16	194	13	1.61E+0	2.36	10
2	1536	64	770	41	2.52E−1	2.68	12
3	6144	256	3074	145	6.94E−2	1.86	12
4	24576	1024	12290	545	3.33E−2	1.06	14
5	98304	4096	49154	2113	–	–	16

Table 3.5: $\kappa = 5$, control constraints, Γ_O ... manifold.

4 Exterior Neumann boundary control problems

The theory of exterior Neumann boundary control problems is similar to the theory of exterior Dirichlet boundary control problems. Therefore, only the differences and the main results are discussed in this chapter. First, the optimal control problem will be introduced and analyzed. Afterwards the discretization will be discussed. In the third section modified boundary integral equations are used to overcome difficulties due to eigenvalues of the interior Neumann Laplace eigenvalue problem. In the last section two numerical examples will be shown and analyzed.

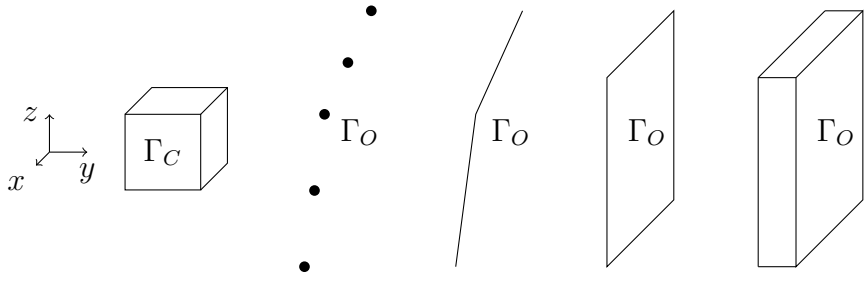
4.1 The optimal control problem

In this chapter we consider exterior Neumann boundary control problems. In acoustics the Neumann datum of the pressure p has the following relation to the normal component of the velocity $\boldsymbol{v}$:

$$\boldsymbol{v} \cdot \boldsymbol{n} = \frac{i}{\omega \varrho_0} \frac{\partial}{\partial \boldsymbol{n}} p.$$

In this formula ϱ_0 is the constant part of the density ϱ. This relation can be obtained by using a linearization of Euler's equations. Further details can be found in e.g. [27]. This is one motivation for controlling the Neumann datum. One possible application of this Neumann boundary control problem is given by the sound source reconstruction problem, see e.g. [19, 34, 52, 63, 70].

The main ideas are the same as in Chapter 3. We again consider a three dimensional bounded Lipschitz domain Ω with the corresponding unbounded



Control boundary. Different observation domains.

Figure 4.1: Geometric setting.

exterior domain Ω^c. The boundary is denoted by Γ_C and as for the Dirichlet control this boundary is used for controlling the state. The set for observation is denoted by Γ_O and the dimension of Γ_O can be any natural number between zero and three, see Figure 4.1.

In case of Γ_O is a set of finitely many points, the desired state $\tilde{u}_o$ is defined by complex values $\tilde{u}_o(\boldsymbol{x_i})$, $\boldsymbol{x_i} \in \Gamma_O$. Otherwise, the desired state $\tilde{u}_o$ is an element of $\mathrm{L}^2(\Gamma_O)$. Furthermore, $\varrho \in \mathbb{R}^+$ is a given cost coefficient and $\kappa \in \mathbb{R}^+$ is a given wave number.

The minimization problem we are interested in is given by: Find $(z,u) \in Z_{ad} \times \mathrm{H}^1_{\mathrm{loc}}(\Omega^c) = \mathrm{H}^{-1/2}(\Gamma_C) \times \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ which is a minimizer of the cost functional

$$J(z,u) := \frac{1}{2} \|u|_{\Gamma_O} - \tilde{u}_o\|^2_{\mathrm{L}^2(\Gamma_O)} + \frac{\varrho}{2} (V_0^{cc} z, z)_{\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)} \tag{4.1}$$

subject to

$$-\Delta u - \kappa^2 u = 0 \quad \text{in } \Omega^c, \tag{4.2}$$

$$\gamma_1^{\mathrm{ext}} u = z \quad \text{on } \Gamma_C \tag{4.3}$$

in the distributional sense. If Γ_O is given by a set of finitely many points, the functional is given by

$$J(z,u) := \frac{1}{2} \sum_{\boldsymbol{x_i} \in \Gamma_O} \left(u(\boldsymbol{x_i}) - \tilde{u}_o(\boldsymbol{x_i})\right)^2 + \frac{\varrho}{2} (V_0^{cc} z, z)_{\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)}. \tag{4.4}$$

Additionally, u has to satisfy the radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla u - i\kappa u \right|^2 \mathrm{d}\mu = 0. \tag{4.5}$$

For this kind of minimization problem we do not use additional constraints for the control.

In contrast to the Dirichlet boundary control problem, the regularization $\frac{\varrho}{2} \|z\|^2_{\mathrm{L}^2(\Gamma_C)}$ is also possible as it is a stronger regularization than the

$$\frac{\varrho}{2} \left(V_0^{cc} z, z\right)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)}$$

regularization.

We use the abbreviation $u_o := u|_{\Gamma_O}$ and $u_c := u|_{\Gamma_c}$ to make notation easier. Using the local maximal regularity theorem, we get that u_o is well defined for any dimension of Γ_O.

The control to state operator is denoted by H and is defined by $H\colon \mathrm{H}^{-1/2}(\Gamma_C) \to \mathrm{L}^2(\Gamma_O)$

$$Hz := u_o \quad \text{on } \Gamma_O.$$

Using the representation formula (2.9), we get

$$Hz = \left(-SL_\kappa^c z + DL_\kappa^c u_c\right)|_{\Gamma_O}.$$

Next we use the operators V_κ^{oc} and K_κ^{oc}, which were introduced in Chapter 3. The result is given by

$$u_o = -V_\kappa^{oc} z + K_\kappa^{oc} u_c \quad \text{on } \Gamma_O. \tag{4.6}$$

Instead of the first boundary integral equation (2.10) we use the second boundary integral equation (2.11), i.e.

$$D_\kappa^{cc} u_c + \left(\frac{1}{2} + K_{-\kappa}^{cc\,*}\right) z = 0. \tag{4.7}$$

To be able to eliminate the variable u_c, we have to make the following assumption:

Assumption 4.1. *We assume that the wave number $\kappa \in \mathbb{R}^+$ is chosen, such that the hypersingular boundary integral operator is invertible. This is equivalent to: κ^2 is not an eigenvalue of the interior Neumann Laplace eigenvalue problem, see Theorem 2.27.*

Later we will use modified boundary integral equations to overcome this problem. By using the inverse hypersingular boundary integral operator we can eliminate the variable u_c. We then end up with

$$Hz = -V_\kappa^{oc} z - K_\kappa^{oc} \left(D_\kappa^{cc}\right)^{-1} \left(\frac{1}{2} + K_{-\kappa}^{cc\,*}\right) z \quad \text{on } \Gamma_O.$$

Therefore, the operator H has the representation

$$H = -V_\kappa^{oc} - K_\kappa^{oc} \left(D_\kappa^{cc}\right)^{-1} \left(\frac{1}{2} + K_{-\kappa}^{cc\,*}\right).$$

Using the reduced cost functional

$$\hat{J}(z) = J(z, Hz),$$

we can prove that a unique solution of the Neumann boundary control problem exists.

Theorem 4.2. *A unique solution $(z, u) \in Z_{ad} \times \mathrm{H}^1_{\mathrm{loc}}(\Omega^c)$ of the exterior Neumann boundary control problem* (4.1)-(4.5) *exists.*

The proof of Theorem 4.2 is similar to the one of Theorem 3.3, i.e. we use [64, Theorem 2.14]. As the set Z_{ad} is unbounded, we restrict the set of all admissible controls to the set

$$\left\{ z \in Z_{ad} \colon \left(V_0^{cc} z, z\right)_{\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)} \leq 2\varrho^{-1} \hat{J}(\tilde{z}) \right\}.$$

In the definition of the previous set $\tilde{z}$ can be an arbitrary but fixed element of Z_{ad}. In the following we are interested in first order optimality conditions.

Theorem 4.3. *$z \in Z_{ad}$ is a minimizer of* (4.1)-(4.5)*, if and only if $z \in Z_{ad}$ is a solution of*

$$H^*(Hz - \tilde{u}_o) + \varrho V_0^{cc} z = 0 \quad \text{on } \Gamma_C. \tag{4.8}$$

The proof of Theorem 4.3 is similar to the proof of the Dirichlet control and is therefore omitted. The adjoint operator of H has the representation

$$H^* = -V_\kappa^{oc*} - \left(\frac{1}{2} + K_{-\kappa}^{cc}\right)\left(D_\kappa^{cc*}\right)^{-1} K_\kappa^{oc*}.$$

In case of the Neumann boundary control problem the dual variable is denoted by p_c. We define $p_c \in \mathrm{H}^{1/2}(\Gamma_C)$ as the unique solution of

$$D_\kappa^{cc*} p_c = K_\kappa^{oc*} u_o \quad \text{on } \Gamma_C. \tag{4.9}$$

The function $f \in \mathrm{H}^{1/2}(\Gamma_C)$ is defined by

$$f = -V_\kappa^{oc*}\tilde{u}_o - \left(\frac{1}{2} + K_{-\kappa}^{cc}\right)\left(D_\kappa^{cc*}\right)^{-1} K_\kappa^{oc*}\tilde{u}_o \quad \text{on } \Gamma_C.$$

Corollary 4.4. *Using the dual variable p_c,* (4.8) *turns into*

$$-V_\kappa^{oc*} u_o - \left(\frac{1}{2} + K_{-\kappa}^{cc}\right) p_c + \varrho V_0^{cc} z = f \quad \textit{on } \Gamma_C. \tag{4.10}$$

The corresponding dual partial differential equation is given by: Find the distributional solution of

$$\begin{aligned} -\Delta p - \kappa^2 p &= u_o \delta_{\Gamma_O} && \text{in } \Omega^c, \\ \gamma_1^{\mathrm{ext}} p &= 0 && \text{on } \Gamma_C. \end{aligned}$$

Furthermore, p has to satisfy the following radiation condition of Rellich

$$\lim_{|\boldsymbol{x}|=R\to\infty} \int_{\partial B_R} \left| \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla p + i\kappa p \right|^2 \mathrm{d}\mu = 0,$$

where the sign has changed in the second term compared to the radiation condition (4.5).

Summing up, we have to solve the optimality system, i.e. the primal problem (4.7), the point evaluation (4.6), the dual problem (4.9) and the optimality condition (4.10). For a given $\tilde{u}_o \in \mathrm{L}^2(\Gamma_O)$ we have to find $p_c, u_c \in \mathrm{H}^{1/2}(\Gamma_C)$, $u_o \in \mathrm{L}^2(\Gamma_O)$ and $z \in Z_{ad}$, such that

$$\begin{pmatrix} 0 & D_\kappa^{cc} & 0 & \frac{1}{2} + K_{-\kappa}^{cc\,*} \\ D_\kappa^{cc*} & 0 & -K_\kappa^{oc*} & 0 \\ 0 & -K_\kappa^{oc} & 1 & V_\kappa^{oc} \\ \frac{1}{2} + K_{-\kappa}^{cc} & 0 & V_\kappa^{oc*} & -\varrho V_0^{cc} \end{pmatrix} \begin{pmatrix} p_c \\ u_c \\ u_o \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -f \end{pmatrix}. \tag{4.11}$$

Theorem 4.5. *Let us assume that Assumption 4.1 is satisfied. Then the operator $H^*H + \varrho V_0^{cc}$ is $\mathrm{H}^{-1/2}(\Gamma_C)$-elliptic, i.e. a constant $c_1 > 0$ exists such that*

$$\Re\left(\left(H^*H + \varrho V_0^{cc}\right) z, z\right)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)} \geq \varrho c_1 \|z\|^2_{\mathrm{H}^{-1/2}(\Gamma_C)}$$

holds, for all $z \in \mathrm{H}^{-1/2}(\Gamma_C)$.

We immediately get the following corollary:

Corollary 4.6. *Let us assume that Assumption 4.1 is satisfied. Then the optimality system 4.11 has a unique solution.*

Finally, we define the Schur complement operator S by

$$S := H^*H + \varrho V_0^{cc}.$$

The operator S has the representation

$$S = \left(V_\kappa^{oc*} + \left(\frac{1}{2} + K_{-\kappa}^{cc}\right)\left(D_\kappa^{cc*}\right)^{-1} K_\kappa^{oc*}\right) \left(V_\kappa^{oc} + K_\kappa^{oc}\left(D_\kappa^{cc}\right)^{-1}\left(\frac{1}{2} + K_{-\kappa}^{cc\,*}\right)\right) + \varrho V_0^{cc}.$$

Therefore, the optimality system was transformed into the operator equation: Find $z \in Z_{ad}$ such that

$$Sz = f \quad \text{on } \Gamma_C.$$

4.2 Discretization

In this section we discretize the optimality system for the Neumann boundary control problem, which was derived in Section 4.1.

We assume that κ^2 is not an eigenvalue of the interior Neumann Laplace eigenvalue problem. Therefore, the optimality system has a unique solution

$$(p_c, u_c, u_o, z) \in \mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{L}^2(\Gamma_O) \times \mathrm{H}^{-1/2}(\Gamma_C).$$

In Section 4.3 we will analyze the case, if this assumption is not satisfied.

Again a standard Galerkin approach is used for the discretization. As most proofs are similar to the proofs of Section 3.2, we only want to analyze the differences and state the main results.

To be able to derive a numerical analysis, we assume that all assumption, which were used in Section 2.6 are satisfied.

The control $z \in \mathrm{H}^{-1/2}(\Gamma_C)$ will be discretized by $z_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$. To get an error estimate for the control, we introduce the auxiliary variable $\tilde{z}_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$. $\tilde{z}_h$ is the unique solution of: Find $\tilde{z}_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$, such that

$$(S\tilde{z}_h, v_h)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)} = (f, v_h)_{\mathrm{H}^{1/2}(\Gamma_C)\times\mathrm{H}^{-1/2}(\Gamma_C)},$$

for all $v_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$. As the operator S is $\mathrm{H}^{-1/2}(\Gamma_C)$-elliptic and therefore also $\mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$-elliptic, we immediately obtain unique solvability by using Theorem 2.8. To get an a priori error estimate, we use Theorem 2.28 and 2.36.

Lemma 4.7. *For the semi discrete approximation the error estimate*

$$\|z - \tilde{z}_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq ch^{s+1/2} \|z\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}$$

holds, if $z \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)$, $s \in [-\frac{1}{2}, 1]$.

In the next step the variables u_c, p_c and u_o are discretized too. The used discrete functions belong to the following spaces

$$\mathrm{H}^{1/2}(\Gamma_C) \ni p_c \approx p_{c,h} \in \mathrm{S}^1_{\mathrm{h}}(\Gamma_C), \quad \mathrm{H}^{1/2}(\Gamma_C) \ni u_c \approx u_{c,h} \in \mathrm{S}^1_{\mathrm{h}}(\Gamma_C)$$

and

$$\mathrm{L}^2(\Gamma_O) \ni u_o \approx u_{o,h} \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_O).$$

Therefore, we have to find the corresponding coefficient vectors $\boldsymbol{u_c}, \boldsymbol{p_c} \in \mathbb{C}^{M^c}$, $\boldsymbol{u_o} \in \mathbb{C}^{N^o}$ and $\boldsymbol{z} \in \mathbb{C}^{N^c}$, such that

$$\begin{pmatrix} 0 & D^{cc}_{\kappa,h} & 0 & \frac{1}{2}M^{cc*}_h + K^{cc}_{-\kappa,h}{}^* \\ D^{cc}_{\kappa,h}{}^* & 0 & -K^{oc}_{\kappa,h}{}^* & 0 \\ 0 & -K^{oc}_{\kappa,h} & M^{oo}_h & V^{oc}_{\kappa,h} \\ \frac{1}{2}M^{cc}_h + K^{cc}_{-\kappa,h} & 0 & V^{oc}_{\kappa,h}{}^* & -\varrho V^{cc}_{0,h} \end{pmatrix} \begin{pmatrix} \boldsymbol{p_c} \\ \boldsymbol{u_c} \\ \boldsymbol{u_o} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \\ -\boldsymbol{f} \end{pmatrix}. \tag{4.12}$$

The right hand side vector $\boldsymbol{f} \in \mathbb{C}^{N^c}$ is defined by

$$\boldsymbol{f} := -V_{\kappa,h}^{oc\,*}\tilde{\boldsymbol{u}}_{\boldsymbol{o}} - \left(\frac{1}{2}M_h^{cc} + K_{-\kappa,h}^{cc}\right)\left(D_{\kappa,h}^{cc\,*}\right)^{-1} K_{\kappa,h}^{oc\,*}\tilde{\boldsymbol{u}}_{\boldsymbol{o}}.$$

The corresponding Schur complement matrix S_h is given by

$$S_h := \left(V_{\kappa,h}^{oc\,*} + \left(\frac{1}{2}M_h^{cc} + K_{-\kappa,h}^{cc}\right)\left(D_{\kappa,h}^{cc\,*}\right)^{-1} K_{\kappa,h}^{oc\,*}\right)(M_h^{oo})^{-1} \left(V_{\kappa,h}^{oc} + K_{\kappa,h}^{oc}\left(D_{\kappa,h}^{cc}\right)^{-1}\left(\frac{1}{2}M_h^{cc*} + K_{-\kappa,h}^{cc\,*}\right)\right) + \varrho V_{0,h}^{cc}.$$

Therefore, the discrete optimality system (4.12) is equivalent to: Find $\boldsymbol{z} \in \mathbb{C}^{N^c}$ such that

$$S_h\boldsymbol{z} = \boldsymbol{f}. \tag{4.13}$$

The approximation S_h of S is invertible and does not disturb the error estimate of Lemma 4.7. For details see Section 3.2. Therefore, we can state the following theorem:

Theorem 4.8. *Let $z \in \mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)$, for $s \in [-\frac{1}{2}, 1]$. Furthermore, let us assume that $p_c, u_c \in \mathrm{H}^{\tilde{s}}(\Gamma_C)$, $\tilde{s} = s + 1$. The unique solution $z_h \in \mathrm{S}^0_{\mathrm{h}}(\Gamma_C)$ to (4.13) satisfies the a priori error estimate*

$$\|z - z_h\|_{\mathrm{H}^{-1/2}(\Gamma_C)} \leq ch^{s+1/2}\|z\|_{\mathrm{H}^{\mathrm{s}}_{\mathrm{pw}}(\Gamma_C)}.$$

4.3 Modified boundary integral equations

As the boundary integral formulation suffers from eigenvalues of the interior Neumann Laplace eigenvalue problem, we will use modified boundary integral equations to overcome this problem. In Section 3.4 two approaches were described. It turned out that only the second approach had the advantage of a rigorous numerical analysis. Therefore, we will consider only the second approach in this chapter.

In the following we will use (2.15), i.e.

$$\begin{pmatrix} -D_\kappa^{cc} & \frac{1}{2} - K_{-\kappa}^{cc\,*} \\ \frac{1}{2} - K_\kappa^{cc} & V_\kappa^{cc} + i\eta V_0^{cc} \end{pmatrix} \begin{pmatrix} u_c \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} z \\ i\eta V_0^{cc} z \end{pmatrix} \quad \text{on } \Gamma_C \tag{4.14}$$

instead of (4.7). The constant $\eta \in \mathbb{R} \setminus \{0\}$ can be chosen arbitrary. This operator is $\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)$-coercive and surjective for all $\kappa > 0$. Hence, we conclude that this operator is bijective. For details see [68, Section 5.7].

As in the Dirichlet case, we get $\tilde{z} = z$. Therefore, we can use the auxiliary variable $\tilde{z}$ in the point evaluation instead of z, i.e.

$$u_o = -V_\kappa^{oc} \tilde{z} + K_\kappa^{oc} u_c \quad \text{on } \Gamma_O. \tag{4.15}$$

For the dual problem we again use a modified formulation:

$$\begin{pmatrix} -D_\kappa^{cc} & \frac{1}{2} - K_{-\kappa}^{cc\,*} \\ \frac{1}{2} - K_\kappa^{cc} & V_\kappa^{cc} + i\eta V_0^{cc} \end{pmatrix}^* \begin{pmatrix} p_c \\ \tilde{q} \end{pmatrix} = \begin{pmatrix} -K_\kappa^{oc*} u_o \\ V_\kappa^{oc*} u_o \end{pmatrix} \quad \text{on } \Gamma_C, \tag{4.16}$$

where $\tilde{q}$ is a new auxiliary variable, which is equal to zero.

Finally, we transform the optimality condition into: Find $z \in \mathrm{H}^{-1/2}(\Gamma_C)$, such that

$$p_c + i\eta V_0^{cc} \tilde{q} + \varrho V_0^{cc} z = \tilde{f} \quad \text{on } \Gamma_C. \tag{4.17}$$

This is valid because $\tilde{q} = 0$ holds. The right hand side $\tilde{f}$ is defined by

$$\tilde{f} := \begin{pmatrix} 1 & i\eta V_0^{cc} \end{pmatrix} \begin{pmatrix} -D_\kappa^{cc} & \frac{1}{2} - K_{-\kappa}^{cc\,*} \\ \frac{1}{2} - K_\kappa^{cc} & V_\kappa^{cc} + i\eta V_0^{cc} \end{pmatrix}^{*-1} \begin{pmatrix} -K_\kappa^{oc*} \\ V_\kappa^{oc*} \end{pmatrix} \tilde{u}_0.$$

Summing up, we have to solve the modified primal problem (4.14), the modified point evaluation (4.15), the modified dual problem (4.16) and the modified optimality condition (4.17). Therefore, we have to solve the system: Find

$$\begin{pmatrix} p_c \\ \tilde{q} \end{pmatrix}, \begin{pmatrix} u_c \\ \tilde{z} \end{pmatrix} \in \mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C), \quad u_o \in \mathrm{L}^2(\Gamma_O) \quad \text{and} \quad z \in \mathrm{H}^{-1/2}(\Gamma_C),$$

such that

$$\begin{pmatrix} 0 & A & 0 & -B \\ A^* & 0 & -C^* & 0 \\ 0 & -C & 1 & 0 \\ -B^* & 0 & 0 & -\varrho V_0^{cc} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} p_c \\ \tilde{q} \end{pmatrix} \\ \begin{pmatrix} u_c \\ \tilde{z} \end{pmatrix} \\ u_o \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\tilde{f} \end{pmatrix}. \tag{4.18}$$

The operators are defined by

$$A := \begin{pmatrix} -D_\kappa^{cc} & \frac{1}{2} - K_{-\kappa}^{cc\,*} \\ \frac{1}{2} - K_\kappa^{cc} & V_\kappa^{cc} + i\eta V_0^{cc} \end{pmatrix}, \quad B := \begin{pmatrix} 1 \\ i\eta V_0^{cc} \end{pmatrix}, \quad C := \begin{pmatrix} K_\kappa^{oc} & -V_\kappa^{oc} \end{pmatrix}.$$

Using these operators, the right hand side has the representation

$$\tilde{f} = -B^* A^{*-1} C^* \tilde{u}_0.$$

Due to the fact that the operator A is $\mathrm{H}^{1/2}(\Gamma_C) \times \mathrm{H}^{-1/2}(\Gamma_C)$-coercive and bijective, we can use the same arguments as in Section 4.1 to prove unique solvability of the optimality system (4.18).

The Schur complement $S\colon \mathrm{H}^{-1/2}(\Gamma_C) \to \mathrm{H}^{1/2}(\Gamma_C)$ has the representation

$$S := B^* A^{*-1} C^* C A^{-1} B + \varrho V_0^{cc}.$$

Therefore, we have to solve: Find $z \in Z_{ad}$, such that

$$Sz = \tilde{f} \quad \text{on } \Gamma_C. \tag{4.19}$$

For the discretization we use the matrices

$$A_h := \begin{pmatrix} -D_{\kappa,h}^{cc} & \frac{1}{2} M_h^{cc*} - K_{-\kappa,h}^{cc\,*} \\ \frac{1}{2} M_h^{cc} - K_{\kappa,h}^{cc} & V_{\kappa,h}^{cc} + i\eta V_{0,h}^{cc} \end{pmatrix}, \quad B_h := \begin{pmatrix} M_h^{cc*} \\ i\eta V_{0,h}^{cc} \end{pmatrix}$$

and

$$C_h := \begin{pmatrix} K_{\kappa,h}^{oc} & -V_{\kappa,h}^{oc} \end{pmatrix}.$$

The discrete system is therefore given by: Find

$$\begin{pmatrix} \boldsymbol{p_c} \\ \tilde{\boldsymbol{q}} \end{pmatrix}, \begin{pmatrix} \boldsymbol{u_c} \\ \tilde{\boldsymbol{z}} \end{pmatrix} \in \mathbb{C}^{M^c} \times \mathbb{C}^{N^c}, \quad \boldsymbol{u_o} \in \mathbb{C}^{N^o} \quad \text{and} \quad \boldsymbol{z} \in \mathbb{C}^{N^c},$$

such that

$$\begin{pmatrix} 0 & A_h & 0 & -B_h \\ A_h^* & 0 & -C_h^* & 0 \\ 0 & -C_h & M_h^{oo} & 0 \\ -B_h^* & 0 & 0 & -\varrho V_{0,h}^{cc} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \boldsymbol{p_c} \\ \tilde{\boldsymbol{q}} \end{pmatrix} \\ \begin{pmatrix} \boldsymbol{u_c} \\ \tilde{\boldsymbol{z}} \end{pmatrix} \\ \boldsymbol{u_o} \\ \boldsymbol{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \\ -\tilde{\boldsymbol{f}} \end{pmatrix}. \tag{4.20}$$

The right hand side vector is defined by

$$\tilde{\boldsymbol{f}} := -B_h^* A_h^{*-1} C_h^* \tilde{\boldsymbol{u}}_{\boldsymbol{o}}.$$

Using the discrete Schur complement S_h

$$S_h := B_h^* A_h^{*-1} C_h^* M_h^{oo-1} C_h A_h^{-1} B_h + \varrho V_{0,h}^{cc},$$

we end up with: Find $\boldsymbol{z} \in \mathbb{C}^{M^c}$, such that

$$S_h \boldsymbol{z} = \tilde{\boldsymbol{f}}$$

holds. We can use the same arguments which were used in Section 4.2 to obtain a similar error estimate for the control. As it was mentioned in the Dirichlet case, we have to approximate the two auxiliary variables $\tilde{q}$ and $\tilde{z}$.

4.4 Numerical examples

In this section we want to analyze two convergence studies. The setting is almost similar to the setting in Section 3.5.2. The exact solution is not known. Hence, all discrete solutions are prolongated to the finest mesh level, i.e. to the fifth mesh level.

The Neumann control takes place on the boundary of the cube $(-1,1)^3$. For the observation two cases are considered. In the first case, Γ_O is the manifold

$$\left\{ \boldsymbol{x} \in \mathbb{R}^3 \colon x_1 = 3, x_2, x_3 \in \left(-\frac{1}{2}, \frac{1}{2} \right) \right\}.$$

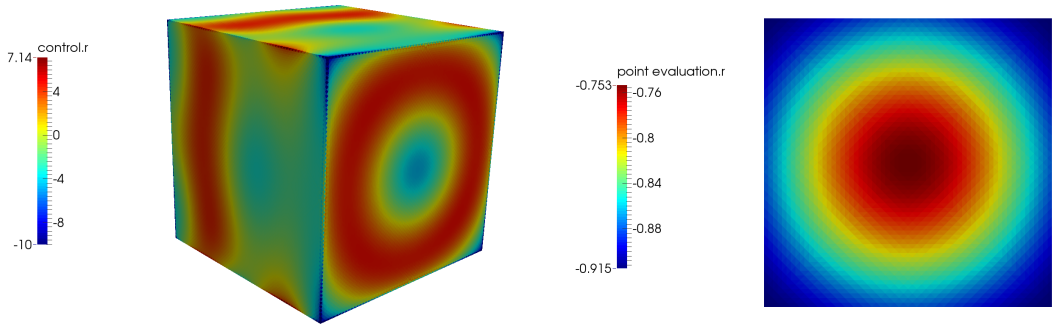


Figure 4.2: Real part, $\kappa = 5$, Γ_O ... manifold.

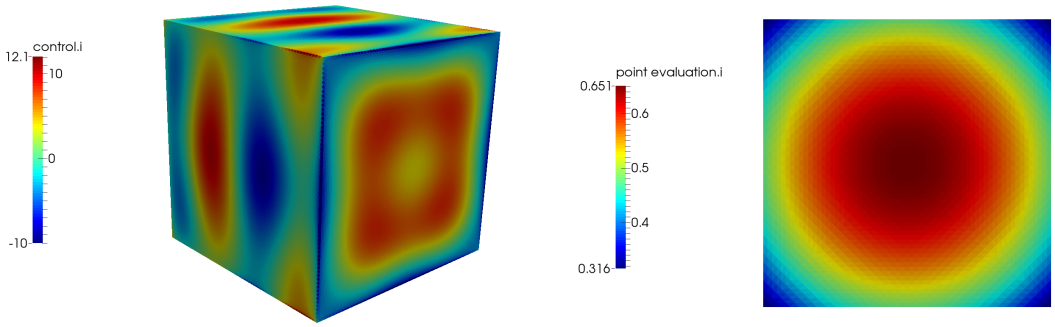


Figure 4.3: Imaginary part, $\kappa = 5$, Γ_O ... manifold.

In the second case, 25 points uniformly distributed on the previously defined manifold are used for observations. In the following examples we choose $\varrho = 1\text{E}{-5}$, $\kappa = 5$ and $\tilde{u}_0$ is defined by the function $\tilde{u}_o = e^{i\kappa\sqrt{x_1^2+x_2^2+x_3^2}}$.

First, we observe on the manifold. The real and the imaginary part of the solution as well as the absolute value of the solution are plotted in Figure 4.2, 4.3 and 4.4. In Table 4.1 we can see a convergence rate for the control of around 0.66 in the $\mathrm{L}^2(\Gamma_C)$-norm and a convergence rate of around 1.16 in the $\mathrm{H}^{-1/2}(\Gamma_C)$-norm, which fits together with the reentrant corner.

In the last example we observe on the 25 points, which were introduced above. In Figure 4.5 and 4.6 the real and the imaginary part are plotted. Furthermore, we can see the absolute value of the solution in Figure 4.7.

In Table 4.2 we can again observe a convergence rate for the control of 0.66 in case of the $\mathrm{L}^2(\Gamma_C)$-norm and a convergence rate of 1.16 in case of the

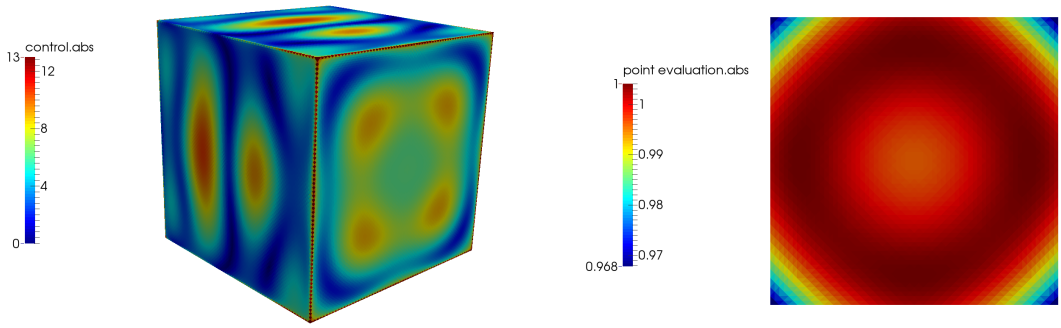


Figure 4.4: Absolute value, $\kappa = 5$, Γ_O ... manifold.

Level	Elements		Nodes		$\|\cdot\|_{L^2(\Gamma_C)}$	Eoc	$\|\cdot\|_{H^{-1/2}(\Gamma_C)}$	Eoc
	Γ_C	Γ_O	Γ_C	Γ_O				
0	96	4	50	5	2.29E+1	–	6.95E+0	–
1	384	16	194	13	1.37E+1	0.73	3.04E+0	1.19
2	1536	64	770	41	6.52E+0	1.07	7.08E−1	2.10
3	6144	256	3074	145	4.10E+0	0.67	3.13E−1	1.18
4	24576	1024	12290	545	2.62E+0	0.64	1.49E−1	1.07
5	98304	4096	49154	2113	–	–	–	–

Table 4.1: $\kappa = 5$, Γ_O ... manifold.

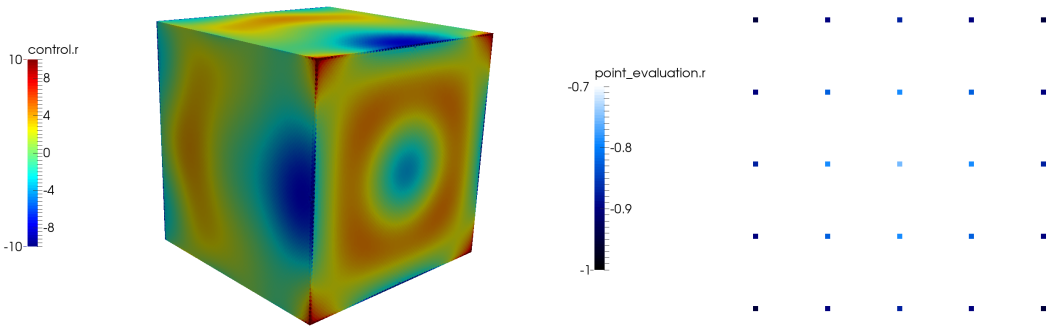


Figure 4.5: Real part, $\kappa = 5$, Γ_O ... manifold.

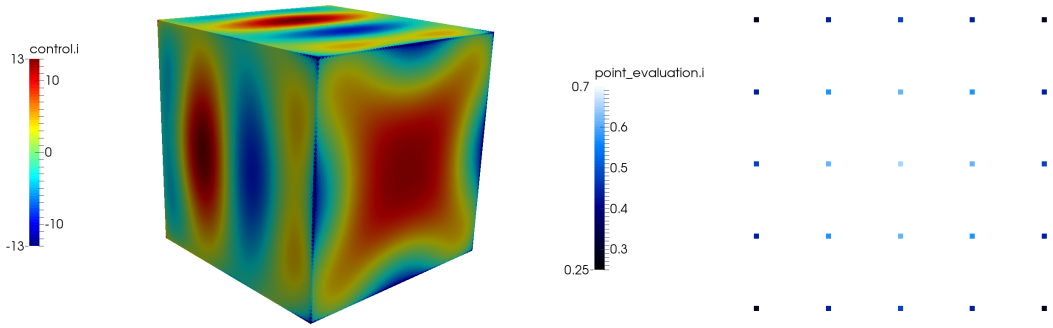


Figure 4.6: Imaginary part, $\kappa = 5$, Γ_O ... manifold.

$\mathrm{H}^{-1/2}(\Gamma_C)$-norm.

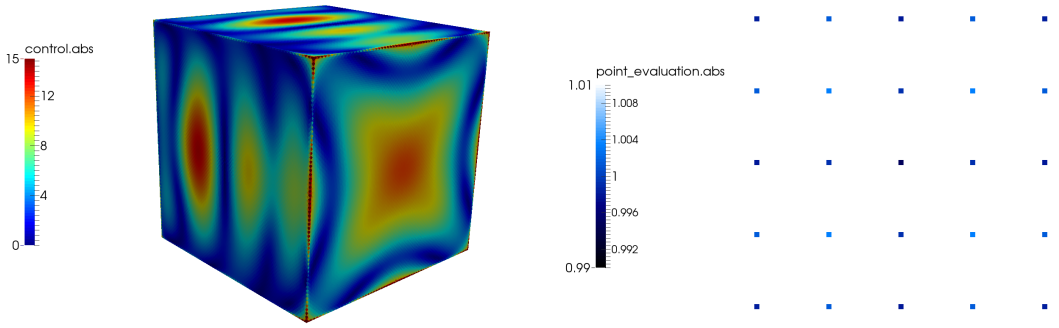


Figure 4.7: Absolute value, $\kappa = 5$, Γ_O ... manifold.

Level	Elements		Nodes		$\|\cdot\|_{L^2(\Gamma_C)}$	Eoc	$\|\cdot\|_{H^{-1/2}(\Gamma_C)}$	Eoc
	Γ_C	Γ_O	Γ_C	Γ_O				
0	96	–	50	25	3.51E+1	–	9.86E+0	–
1	384	–	194	25	1.74E+1	1.01	4.32E+0	1.19
2	1536	–	770	25	7.08E+0	1.29	7.57E−1	2.51
3	6144	–	3074	25	4.38E+0	0.69	3.35E−1	1.18
4	24576	–	12290	25	2.78E+0	0.66	1.59E−1	1.08
5	98304	–	49154	25	–	–	–	–

Table 4.2: $\kappa = 5$, Γ_O ... points.

5 Conclusions and outlook

In this work Dirichlet and Neumann boundary control problems have been studied. The state equation was given by the Helmholtz equation, which was motivated by acoustics. Therefore, we assumed that all excitations were time harmonic and that all assumptions concerning linear acoustics were satisfied.

In many applications the Helmholtz equation has to be solved in unbounded exterior domains. This was the motivation for using boundary integral equations and the corresponding boundary element method. When using boundary integral equations, the fundamental solution has to be known. For the Helmholtz equation this is the case and as the control takes place on the boundary of the unbounded exterior domain, the boundary element method turned out to be a very effective method for this kind of optimal control problems. However, the standard method is not stable for all wave numbers. Therefore, modified boundary integral equations were suggested. As a result, it was possible to solve the Helmholtz equation for all wave numbers without additional restrictions to the regularity of the domain.

In contrast to common literature the control was considered in the energy spaces $\mathrm{H}^{1/2}(\Gamma_C)$ and $\mathrm{H}^{-1/2}(\Gamma_C)$ instead of $\mathrm{L}^2(\Gamma_C)$. When using boundary integral equations, it turned out that this kind of regularization is more practicable. To solve the minimization problems first order optimality conditions were derived and analyzed. These optimality conditions were given by a variational inequality or a boundary integral equation, depending on the usage of control constraints. It was possible to show that the minimization problem has a unique solution.

A standard Galerkin-Bubnov method was used for the discretization. Using a symmetric formulation and standard assumptions, it was possible to guarantee unique solvability of the resulting system of linear equations. Furthermore, error estimates were derived for the control. The software library BEM++ was used for assembling the occurring matrices. To solve the occurring discrete

variational inequality a semi-smooth Newton method was used and finally some examples were considered. It turned out that these numerical examples verify the theoretical results.

It would be very interesting to use this approach for more practical applications concerning the optimization of acoustic behavior. Another suitable application could be found in sound source reconstruction problems. As more practical problems lead to large linear systems, another important topic would be the use of fast block solvers. This implies the usage of block preconditioners, which is a challenging topic too. Further applications could also be in the field of electromagnetism. It is possible to use boundary integral equations in the case of Maxwell's equations. Therefore, it seems that this approach could be extended to this area.

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