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Boundary Element Methods for Boundary Control Problems

DISSERTATION

written to obtain the academic degree of
a Doctor of Engineering

Technische Universität Graz

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Graz, in January 2011

Acknowledgment

First, I would like to express my special appreciation to my supervisor, Professor Olaf Steinbach, for his guidance and encouragement throughout my study. I would like also to thank Professor Le Hung Son for his recommendation to Professor Olaf Steinbach. I am grateful to Dr. Günther Of for his help in numerics and computations. I also want to thank Professor Arnd Rösch for being a reviewer of this work.

Furthermore, I would like to thank all my colleagues at the Institute of Computational Mathematics at Graz University of Technology, who have been helping me not only in my work but also in getting used to the life in Austria.

I gratefully acknowledge the financial support by the Austrian Science Fund (FWF) under the grant SFB Mathematical Optimization and Applications in Biomedical Sciences, Subproject Fast Finite Element and Boundary Element Methods for Optimality Systems.

Finally, during my study, I always get the support and encouragement from my family and friends. Thank you all.

Abstract

In this thesis we consider the application of boundary integral equation methods to the solution of boundary control problems governed by boundary value problems of linear second order elliptic and parabolic partial differential equations. A difficulty when dealing with Dirichlet control problems is the choice of the control space. In the literature almost all contributions consider $L_2(\Gamma)$ as the control space. But these approaches require to consider the state equation within an ultra-weak variational formulation, and an adjoint state variable to be sufficiently regular. Hence the considered domain has to be either polygonal or polyhedral but convex, or sufficiently smooth. In this work the controls are considered in the related energy spaces. This approach allows to consider a standard variational formulation. Moreover, it shows the proper mapping properties which link the Dirichlet and Neumann data in the optimality condition by using some appropriate operators. In the case of box constraints the optimality condition is a variational inequality in $H^{1/2}(\Gamma)$ which can be written as a Signorini boundary value problem with bilateral constraints.

Since the unknown function in boundary control problems is to be found on the boundary of the computational domain, the use of boundary element methods seems to be a natural choice. To the best of our knowledge, there are only few results known on the use of boundary integral equations to solve optimal boundary control problems. The most popular approaches are based on the use of finite element methods which require a discretization of the computational domain. In contrast, the use of boundary element methods requires only a discretization of the boundary. In principle, the use of boundary integral equations is based on an explicit knowledge of fundamental solutions of the considered partial differential equations. Then, the solutions of both the state and adjoint boundary value problems are represented by surface and volume potentials. Since the state enters the adjoint problem as volume density, we apply integration by parts to replace these volume potentials by surface potentials. This results in a system of boundary integral equations which involve the standard Laplace and Bi-Laplace boundary integral operators. In the case of parabolic boundary control problems we first transfer the adjoint state equations to the heat equations and then use an auxiliary function which relates to the fundamental solution of the heat equation, to get rid of volume potentials. The obtained system of boundary integral equations is similar to the system in the elliptic case. We prove the unique solvability and study the boundary element discretizations of the optimality system. Piecewise linear boundary elements are used to approximate the Dirichlet control and piecewise constant approximations for Neumann control. We prove stability and related error estimates. While the non-symmetric boundary integral formulation needs an additional condition on the discretization to ensure stability, we can prove the stability of the symmetric boundary element approach without any condition on the discretization. We consider only the symmetric formulation in the case of parabolic boundary control problems. Note that the primal-dual active set strategy is employed to solve related variational inequalities. Some numerical examples are tested to confirm the theoretical results.

Zusammenfassung

In dieser Arbeit betrachten wir die Anwendung von Randintegralmethoden zur Lösung von Randkontrollproblemen, wobei die Nebenbedingungen durch lineare partielle elliptische und parabolische Differentialgleichungen zweiter Ordnung beschrieben werden. Eine Schwierigkeit besteht dabei in der Wahl des Funktionenraumes für die Kontrolle. Fast alle Beiträge in der Literatur verwenden $L_2(\Gamma)$ als Kontrollraum. Diese Ansätze benötigen aber eine ultraschwache Formulierung der Zustandsgleichung und genügend Regularität der adjungierten Zustandsvariablen. Dementsprechend muss das betrachtete Gebiet entweder polygonal oder polyhedral und konvex, oder glatt genug sein. In dieser Arbeit wird die Kontrolle im entsprechenden Energieraum betrachtet. Dieser Ansatz erlaubt es, die übliche Variationsformulierung zu verwenden. Weiters enthält die Optimalitätsbedingung eine Dirichlet zu Neumann Abbildung welche die korrekten Abbildungseigenschaften widerspiegelt.

Für die Lösung von Randkontrollproblemen erscheint die Randelementmethode als ein geeignetes Diskretisierungsverfahren. Im Gegensatz zu Finiten Element Methoden verlangt die Randelementmethode nur eine Diskretisierung des Randes. Bei Kenntnis einer Fundamentallösung können die Lösungen der Zustandsgleichung und der adjungierten Zustandsgleichung durch Oberflächenpotentiale und Volumenpotentiale beschrieben werden. Da die Zustandsvariable jedoch in der adjungierten Gleichung als Volumenpotential zu berücksichtigen ist, erfolgt durch partielle Integration eine Rückführung auf Oberflächenpotentiale. Dies resultiert in einem System von Randintegralgleichungen mit Laplace und Bi-Laplace Randintegraloperatoren. Im Falle eines parabolischen Randkontrollproblems wird die adjungierte Zustandsgleichung zunächst in eine Wärmeleitgleichung transformiert. Um das Volumenpotential zu vermeiden, wird im Anschluss eine auf der Fundamentallösung der Wärmeleitgleichung basierende Hilfsfunktion verwendet. Das resultierende System entspricht dem System für den elliptischen Fall. Wir beweisen die eindeutige Lösbarkeit und studieren die Randelementdiskretisierung des Optimalitätssystems. Die Dirichletkontrolle wird mittels linearer Formfunktionen approximiert und die Neumannkontrolle wird durch stückweise konstante Formfunktionen. Wir beweisen Stabilität und zugehörige Fehlerabschätzungen. Während für die Stabilität der nicht-symmetrischen Formulierung zusätzliche Anforderungen an die Diskretisierung gestellt werden müssen, kann die Stabilität der symmetrischen Formulierung ohne zusätzliche Anforderungen bewiesen werden. Für parabolische Probleme beschränken wir uns auf die symmetrische Formulierung. Für die Lösung der auftretenden Variationsungleichungen verwenden wir die primal-dual aktive Mengen-Strategie. Numerische Beispiele bestätigen die theoretischen Ergebnisse.

CONTENTS

1 INTRODUCTION

Optimal control problems subject to partial differential equations (PDEs) with additional constraints on the controls play an important role in many practical applications, see [28, 38, 66] and references given therein. In particular, for Dirichlet boundary control problems in fluid mechanics, consult [22, 25]. Here, let us consider some examples of optimal heating problems, [66].

Optimal stationary heating. Consider the equilibrium distribution of the absolute temperature $u : \Omega \to \mathbb{R}^+$ inside a body $\Omega \subset \mathbb{R}^3$ which is determined by the stationary heat equation

$$-\mathrm{div}(\kappa \nabla u) = f, \tag{1.1}$$

where κ is the body's thermal conductivity, and f represents possible heat sources. In the simplest case, κ is a positive constant. We can apply a heat source $f = z$ (the *control*) in the domain Ω. The goal is to find the control z in such a way that the temperature distribution u in Ω (the *state*) is the best possible approximation to a desired temperature distribution $\bar{u}$ in Ω. Problems of this kind arise if the body Ω is heated by electromagnetic induction or by microwaves. Assuming that the boundary temperature vanishes, we can model an optimal control problem as follows:

$$\text{Minimize} \quad J(u,z) = \frac{1}{2}\int_\Omega [u(x) - \bar{u}(x)]^2\,dx + \frac{\alpha}{2}\int_\Omega [z(x)]^2\,dx \tag{1.2}$$

subject to the PDE constraints, for $\kappa = 1$,

$$-\Delta u(x) = z(x) \quad \text{in } \Omega, \tag{1.3}$$

$$u(x) = 0 \quad \text{on } \Gamma = \partial\Omega, \tag{1.4}$$

and the pointwise control constraints

$$z_1(x) \le z(x) \le z_2(x) \quad \text{in } \Omega. \tag{1.5}$$

The constant $\alpha \ge 0$ can be seen as a regularization parameter. It has the effect that possible optimal controls show improved regularity properties. The *cost functional* $J(u,z)$ to be minimized is called the *objective functional*. Observe that the control acts in the volume domain Ω. Hence we have a *distributed control problem*.

In a similar way, the control can act at each point of the boundary Γ. The control is no longer distributed in the domain Ω, we have now a *boundary control problem*. The problem leads to the minimization of the objective functional

$$J(u,z) = \frac{1}{2}\int_{\Omega} [u(x) - \overline{u}(x)]^2\,dx + \frac{\alpha}{2}\|z\|^2_{\mathcal{V}} \tag{1.6}$$

subject to the PDE constraints

$$-\Delta u(x) = f(x) \quad \text{in } \Omega, \tag{1.7}$$
$$u(x) = z(x) \quad \text{on } \Gamma, \tag{1.8}$$

and

$$z_1(x) \le z(x) \le z_2(x) \quad \text{on } \Gamma. \tag{1.9}$$

Here $f(x)$ is a given function. The second term in (1.6), $\|z\|^2_{\mathcal{V}}$ describes either the costs of the control or represents some regularization, where $\mathcal{V}$ is an appropriate Hilbert space to be specified. In a slightly more realistic application, one might only be able to control the temperature on some part Γ_c of Γ with $\Gamma_c \subsetneq \Gamma$. In this case, we need an additional boundary condition on the remaining part $\Gamma \setminus \Gamma_c$ of the boundary, e.g., a homogeneous Neumann boundary condition which describes an isolation.

Optimal nonstationary heating. The temperature is now changing with the time t. Then the temperature distribution is modeled by the transient heat equation

$$\partial_t u - \operatorname{div}(\kappa \nabla u) = f, \tag{1.10}$$

where the heat sources f and the temperature u, in general, depend on time as well as on the space coordinates. They are defined in the space-time cylinder $Q := \Omega \times (0,T)$, where $T > 0$ represents a final time. We know the temperature distribution at the initial time $t = 0$, $u(\cdot,0) = u_0$, and we want to reach a temperature $\overline{u}$ at the final time $t = T$. The problem then reads as follows:

$$\text{Minimize} \quad J(u,z) = \frac{1}{2}\int_{\Omega} [u(x,T) - \overline{u}(x)]^2\,dx + \frac{\alpha}{2}\|z\|^2_{\mathcal{V}}, \tag{1.11}$$

subject to

$$\partial_t u - \Delta u = 0 \quad \text{in } Q, \tag{1.12}$$
$$u = z \quad \text{on } \Sigma := \Gamma \times (0,T), \tag{1.13}$$
$$u(\cdot,0) = u_0 \quad \text{in } \Omega, \tag{1.14}$$

and

$$z_1(x,t) \le z(x,t) \le z_2(x,t) \quad \text{on } \Sigma. \tag{1.15}$$

Here the control z is considered in an appropriate Hilbert space $\mathcal{V}$, e.g., $\mathcal{V} = L_2(\Sigma)$. The temperature distribution u fulfills a parabolic partial differential equation, where z controls the temperature on the boundary. We thus have to deal with a *linear-quadratic parabolic boundary control problem.*

The numerical analysis of the distributed control problems (1.2)-(1.5) by finite element methods (FEMs) was considered in [46, 47, 55]. In particular, Meyer and Rösch derived error estimates of order h^2 for the controls in the L_2 norm by using piecewise constant controls, and of linear convergence in the L_∞ norm by using piecewise linear controls. For the approximation of the discretization for semilinear elliptic optimal control problems, see, e.g., [2, 9]. We refer to [13, 27, 54] for general linear-quadratic optimal control problems.

For the Dirichlet boundary control problem, the choice of the function space for the control is crucial. In [25], the Dirichlet boundary condition is considered in $\mathcal{V} \subset H^{1/2}(\Gamma)$, where the objective functional is the domain integral over the strain tensor of the velocity field u satisfying the steady Navier-Stokes equations. To obtain smoother optimal solutions one may consider $H^2(\Gamma)$ as a control space, see [30]. Note that such an approach requires a sufficient regularity of the domain Ω which is assumed to be of the class $C^{2,1}$. In [36], several variational formulations of Dirichlet control problems are discussed. The most popular choice is to consider L_2 as control space. However, the associated partial differential equation of the state has to be considered within an ultra-weak variational formulation. To include a Dirichlet boundary condition in $L_2(\Gamma)$ in a standard variational formulation, one may approximate Dirichlet boundary control problems by a regularization which is based on Robin boundary controls, see [7, 10, 29]. For the problem (1.6)-(1.9), a finite element approach is considered in [51], where the energy norm is realized by using the Steklov-Poincaré operator which links the Dirichlet control with the normal derivative of the adjoint variable.

Numerical solutions of $L_2(\Gamma)$ Dirichlet boundary control problems by finite element approximations are considered in [11, 19, 42]. Casas and Raymond [11] present a finite element analysis for piecewise linear approximations of the Dirichlet controls governed by semilinear elliptic equations on two-dimensional convex polygonal domains Ω. They prove an error estimate of the optimal control of order $\mathcal{O}(h^{1-1/p})$ for some $p > 2$ in the $L_2(\Gamma)$ norm. In [42] May, Rannacher and Vexler consider the Dirichlet boundary control without control constraints (1.6)-(1.8) in a L_2 setting. They present error estimates for the state and adjoint state and derive optimal error estimates in $H^{-1/2}(\Gamma)$ for the Dirichlet control. For two- and three-dimensional smooth domains, an $\mathcal{O}(h\sqrt{|\log h|})$ bound for the L_2 error of the optimal control and state is proved in [19], which can be improved to $\mathcal{O}(h^{\frac{3}{2}})$ under additional conditions in two space dimensions. In the case of a finite dimensional Dirichlet control [67], Vexler derives an error estimate of the optimal control of quadratic order for two-dimensional bounded polygonal domains.

In a recent contribution [12], the Dirichlet and Neumann boundary control problems governed by a semilinear elliptic equation on a curved convex domain $\Omega \subset \mathbb{R}^2$ are analyzed. Casas and Sokolowski approximate the curved domain Ω by a polygonal domain Ω_h and consider the corresponding infinite dimensional control problems in Ω_h. Some error estimates for the related controls are derived. While for the Neumann control the order of the approximation is $\mathcal{O}(h^{\frac{5}{3}})$, a linear order is proved in the case of Dirichlet control only.

Let us briefly recall some publications of parabolic optimal control problems. Such optimal control problems with observations in the domain Ω or on the boundary Γ are considered in [38] from an analytic point of view. In [44, 45], distributed parabolic optimal control problems without and with control constraints were considered. The authors established several a priori error estimates which correspond to various types of control discretizations. For the analysis of the parabolic Dirichlet boundary control problems, we cite [3, 4], see also [36, 38]. In [68, 69], a numerical Galerkin method was proposed to solve a parabolic Neumann control problem. This approximation was based on a backward discretization with respect to time, and for every time level $t = nh_t$, the author proved the order $\mathcal{O}((\log \frac{T}{h_t})^2(h_t + h_x^2))$ of the error of the control in $L_\infty(\Gamma)$. For the control and/or state constrained case of the parabolic Neumann control problems, see [53, 56].

This thesis is concerned with the application of boundary integral equation methods to optimal boundary control problems. The controls are considered in the related energy spaces. This approach allows to consider the standard variational formulation. There are several papers to deal with optimal boundary control problems by FEMs, see the discussion above. But to our knowledge there are only few results on the use of boundary integral equations to solve optimal boundary control problems, see, e.g., [70] for the problem with point observations. While the finite element approaches require a discretization of the computational domain, the use of boundary integral formulations and boundary element methods (BEMs) requires only a discretization of the boundary. Hence, BEMs can be easier to deal with a complicated domain. Moreover, the boundary element solution exactly fulfills the considered partial differential equation inside the domain. Since the unknown function in the optimal boundary control problems is to be sought on the boundary of the computational domain, the use of boundary element methods seems to be a natural choice. However, this approach can only be employed if a fundamental solution of the underlying partial differential equation is available.

Then, by using the potential theory, the solutions of the related state and adjoint partial differential equations can be represented by surface and volume potentials. Applying the proper limiting processes, a system of boundary integral equations is obtained. The first approach is based on the first boundary integral equations of the state and the adjoint partial differential equations. The system of boundary integral equations results in a non-symmetric variational formulation. We prove unique solvability of the related elliptic variational inequality of the first kind. Note that the cost term of the control in the energy space $H^{1/2}(\Gamma)$ is characterized by using the Steklov-Poincasé operator S which links the Dirichlet with the Neumann data. For Galerkin boundary element methods, we use a non-symmetric representation of the operator S. This results in a non-symmetric Galerkin boundary element approximation which requires the use of appropriate boundary element spaces to ensure stability. As a second approach, we consider the second boundary integral equation of the adjoint problem. The obtained system of boundary integral equations results in a symmetric variational formulation which is stable for standard boundary element discretization. Moreover, we use the symmetric Galerkin boundary element approximation of the Steklov-Poincasé S. We then derive error estimates which are confirmed by numerical examples. For the mixed boundary control problems where the control acts on a part $\Gamma_0 \subset \Gamma$ of the boundary Γ, we consider the symmetric variational formulation by using the so-called Dirichlet to Neumann map S. For an overview on boundary integral equations and boundary element methods, see, e.g., [31, 43, 57, 59, 64].

For parabolic boundary control problems, similarly, the related state and the adjoint state can be represented by some layer heat potentials, and Newton heat potentials. Since the final state appears in a representation of the adjoint boundary value problem, we modify the representation by using an auxiliary function which relates to the fundamental solution of the heat equation. This results in a system of boundary integral equations. We consider only the Galerkin boundary element approximation of the symmetric formulation which is stable for standard boundary trial spaces. In particular, we choose an approximation for the Dirichlet control which is piecewise linear and continuous in space and piecewise constant in time, and for the Neumann control an approximation which is piecewise constant both in space and in time, see [15]. We derive related error estimates and test some numerical examples.

Outline

In *Chapter* 2 we present some mathematical preliminaries. We recall the concept of Sobolev spaces which are used for boundary and finite element methods. Then we introduce some finite dimensional trial spaces and discuss their approximation properties.

In *Chapter* 3 we consider a Dirichlet boundary control problem associated to the Poisson equation with box control constraints. The Dirichlet control is considered in the energy space $H^{1/2}(\Gamma)$, where the energy norm is realized by using the Steklov-Poincaré operator. The primal and adjoint equations are written as boundary integral equations. The optimality condition results in a variational inequality which is studied in a non-symmetric or a symmetric formulation. We also discuss related Galerkin boundary element methods.

In *Chapter* 4 an elliptic mixed boundary control problem is considered with control constraints. The Dirichlet control acts on a part Γ_D of the boundary Γ where the Neumann boundary condition is given on the remaining part $\Gamma_N := \Gamma \setminus \Gamma_D$. In order to avoid volume potentials, the idea of integration by parts as in *Chapter* 3 is used. We investigate a system of boundary integral equations which is related to the Steklov-Poincaré operator.

Chapter 5 is devoted to the analysis of a parabolic Dirichlet boundary control problem with control constraints. We setup a system of boundary integral equations in a symmetric formulation which is similar to the elliptic version as discussed in *Chapter* 3. The unique solvability of the related variational inequality and a related error analysis of the Galerkin discretization are based on the mapping properties of the standard heat potentials and new “bi-heat” potentials. In addition, the boundary element approach can be applied to a parabolic Neumann boundary control problem as well. Then we give some main results for this problem.

Finally, in *Chapter* 6 we give some conclusions and discussions.

2 MATHEMATICAL PRELIMINARIES

2.1 Sobolev spaces and trace theory

In this section we recall some relevant Sobolev spaces as used for the analysis of boundary and finite element methods. A brief summary of the basic definitions and results of Sobolev spaces are presented which suffice for our purposes. The main references of this section are the standard books [1, 31, 39, 40, 43].

2.1.1 Isotropic Sobolev spaces

Definition 2.1. *Let Ω be an open subset of $\mathbb{R}^d$. For $k \in \mathbb{N}_0$ the Sobolev space $W_2^k(\Omega)$ is defined by*

$$W_2^k(\Omega) := \{u \in L_2(\Omega)\colon\ D^\alpha u \in L_2(\Omega) \text{ for all multi-indices } \alpha \in \mathbb{N}_0^d \text{ with } |\alpha| \le k\}.$$

The Sobolev space $W_2^k(\Omega)$ is equipped with the norm

$$\|u\|_{W_2^k(\Omega)} := \left(\sum_{|\alpha|\le k} \int_\Omega |D^\alpha u(x)|^2\, dx \right)^{1/2} \tag{2.1}$$

and it is a Hilbert space with respect to the inner product

$$\langle u, v\rangle_{W_2^k(\Omega)} := \sum_{|\alpha|\le k} \int_\Omega D^\alpha u(x)\overline{D^\alpha v(x)}\, dx.$$

For the case of a fractional order $s = k + \mu$ with $k \in \mathbb{N}_0$ and $\mu \in (0,1)$, the Sobolev space $W_2^s(\Omega)$ is defined by

$$W_2^s(\Omega) := \{u \in W_2^k(\Omega)\colon\ \|u\|_{W_2^s(\Omega)} < \infty\}$$

where

$$\|u\|_{W_2^s(\Omega)} := \left(\|u\|^2_{W_2^k(\Omega)} + \sum_{|\alpha|=k} \int_\Omega \int_\Omega \frac{|D^\alpha u(x) - D^\alpha u(y)|^2}{|x-y|^{d+2\mu}}\, dx\, dy \right)^{1/2} \tag{2.2}$$

is the *Sobolev-Slobodetskii norm*. Again, $W_2^s(\Omega)$ is a Hilbert space with respect to the inner product

$$\langle u,v\rangle_{W_2^s(\Omega)} := \langle u,v\rangle_{W_2^k(\Omega)} + \sum_{|\alpha|=k} \int_\Omega \int_\Omega \frac{(D^\alpha u(x) - D^\alpha u(y))\overline{(D^\alpha v(x) - D^\alpha v(y))}}{|x-y|^{d+2\mu}}\, dx\, dy.$$

Clearly, for $k=0$ we have $W_2^0(\Omega) = L_2(\Omega)$.

In what follows we introduce Sobolev spaces $H^s(\Omega)$ which may be equivalent to the Sobolev spaces $W_2^s(\Omega)$ when some regularity assumptions on Ω are satisfied. The definition of the Sobolev spaces $H^s(\Omega)$ is based on the Fourier transform

$$\widehat{u}(\xi) := (\mathcal{F}u)(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{-i\langle x,\xi\rangle} u(x)\, dx, \quad \xi \in \mathbb{R}^d,$$

for $u \in L_1(\mathbb{R}^d)$. Now let $\mathcal{S}(\mathbb{R}^d)$ be the Schwartz space of rapidly decreasing functions in $C^\infty(\mathbb{R}^d)$,

$$\mathcal{S}(\mathbb{R}^d) := \{\varphi \in C^\infty(\mathbb{R}^d) \colon \sup_{x\in\mathbb{R}^d} |x^\alpha D^\beta \varphi(x)| < \infty \quad \text{for all multi-indices } \alpha \text{ and } \beta\},$$

and let $\mathcal{S}'(\mathbb{R}^d)$ be its dual space. The Sobolev space $H^s(\mathbb{R}^d)$ is defined by

$$H^s(\mathbb{R}^d) := \{u \in \mathcal{S}'(\mathbb{R}^d) \colon \mathcal{J}^s u \in L_2(\mathbb{R}^d)\},$$

where $\mathcal{J}^s : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d)$ is the Bessel potential operator

$$\mathcal{J}^s u(x) := (2\pi)^{d/2} \int_{\mathbb{R}^d} (1+|\xi|^2)^{s/2} \widehat{u}(\xi) e^{i\langle x,\xi\rangle}\, d\xi, \quad x \in \mathbb{R}^d.$$

The Sobolev space $H^s(\mathbb{R}^d)$ is equipped with the norm

$$\|u\|_{H^s(\mathbb{R}^d)} := \|\mathcal{J}^s u\|_{L_2(\mathbb{R}^d)} = \left(\int_{\mathbb{R}^d} (1+|\xi|^2)^s |\widehat{u}(\xi)|^2\, d\xi \right)^{1/2}. \qquad (2.3)$$

For all $0 \le s \in \mathbb{R}$, the Sobolev spaces $H^s(\mathbb{R}^d)$ and $W_2^s(\mathbb{R}^d)$ coincide, see for example [43, Theorem 3.16].

For a domain $\Omega \subset \mathbb{R}^d$ we introduce the following definitions of Sobolev spaces.

Definition 2.2. *Let Ω be an open subset of $\mathbb{R}^d$. We define the Sobolev space $H^s(\Omega)$ for $s \in \mathbb{R}$ by restriction,*

$$H^s(\Omega) := \{u = \widetilde{u}_{|\Omega} \colon \widetilde{u} \in H^s(\mathbb{R}^d)\},$$

with the norm

$$\|u\|_{H^s(\Omega)} := \inf_{\widetilde{u}\in H^s(\mathbb{R}^d),\widetilde{u}_{|\Omega}=u} \|\widetilde{u}\|_{H^s(\mathbb{R}^d)}.$$

Further,

$$\widetilde{H}^s(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\mathbb{R}^d)}}, \quad H_0^s(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\Omega)}}.$$

To see the connection of the above definitions of Sobolev spaces, we need to make some regularity assumptions on the domain Ω. Let us recall the definition of the classes $C^{k,\kappa}$, $k\in\mathbb{N}_0$, $\kappa\in[0,1]$ as in [31, Section 3.3]. Given a point $y=(y_1,...,y_d)\in\mathbb{R}^d$, we shall write

$$y=(y',y_d)$$

where

$$y'=(y_1,...,y_{d-1})\in\mathbb{R}^{d-1}.$$

Definition 2.3. *A bounded domain Ω in $\mathbb{R}^d$ is said to be of class $C^{k,\kappa}$ (in short $\Omega\in C^{k,\kappa}$) if the following properties are satisfied:*

i. *There exists a finite number p of orthogonal linear transformations $T_{(r)}$ (i.e. $d\times d$ orthogonal matrices) and the same number of points $x_{(r)}\in\Gamma$ and functions $a_{(r)}(y')$, $r=1,...,p$, defined on the closures of the $(d-1)$-dimensional ball,*

$$Q=\{y'\in\mathbb{R}^{d-1}:\ |y'|<\delta\} \tag{2.4}$$

where $\delta>0$ is a fixed constant. For each $x\in\Gamma$ there is at least one $r\in\{1,...,p\}$ such that

$$x=x_{(r)}+T_{(r)}(y',a_{(r)}(y')). \tag{2.5}$$

ii. *The functions $a_{(r)}$ belong to $C^{k,\kappa}(Q)$.*

iii. *There exists a positive number ε such that for any $r\in\{1,...,p\}$ the open set*

$$B_{(r)} := \{x_{(r)}+T_{(r)}y:\ y=(y',y_d), y'\in Q \text{ and } |y_d|<\varepsilon\}$$

is the union of the sets

$$\begin{aligned}\mathcal{U}_{(r)}^- &= B_{(r)}\cap\Omega\\ &= \{x=x_{(r)}+T_{(r)}y:\ y=(y',y_d), y'\in Q \text{ and } a_{(r)}(y')-\varepsilon<y_d<a_{(r)}(y')\},\\ \mathcal{U}_{(r)}^+ &= B_{(r)}\cap(\mathbb{R}^d\setminus\overline{\Omega})\\ &= \{x=x_{(r)}+T_{(r)}y:\ y=(y',y_d), y'\in Q \text{ and } a_{(r)}(y')<y_d<a_{(r)}(y')+\varepsilon\},\end{aligned}$$

and

$$\Gamma_{(r)}=B_{(r)}\cap\partial\Omega=\{x=x_{(r)}+T_{(r)}(y',a_{(r)}(y')):\ y'\in Q\}.$$

The boundary surface $\Gamma = \partial\Omega$ is said to be in the class $C^{k,\kappa}$ if $\Omega \in C^{k,\kappa}$, and in short we write $\Gamma \in C^{k,\kappa}$. In the special case, when $\Gamma \in C^{0,1}$, the boundary is called a *Lipschitz boundary* and Ω is called a *Lipschitz domain*. Note that a Lipschitz domain may be unbounded. For example, if Ω is a Lipschitz domain, then its complement $\mathbb{R}^d \setminus \overline{\Omega}$ is also a Lipschitz domain.

The relations among the above Sobolev spaces can be seen from the following theorem, see for example [43, Section 3].

Theorem 2.1. *Let Ω be a Lipschitz domain. For $s \geq 0$ we have*

i. $W_2^s(\Omega) = H^s(\Omega)$.

ii. $\widetilde{H}^s(\Omega) \subset H_0^s(\Omega)$.

iii. $\widetilde{H}^s(\Omega) = H_0^s(\Omega)$ *for* $s \notin \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\}$.

Moreover, for all $s \in \mathbb{R}$

$$\widetilde{H}^s(\Omega) = [H^{-s}(\Omega)]', \quad H^s(\Omega) = [\widetilde{H}^{-s}(\Omega)]'.$$

Sobolev spaces on the boundary

In what follows, we assume that Ω is a Lipschitz domain, unless stated otherwise.

Let $L_2(\Gamma)$, $s = 0$, be the completion of $C^0(\Gamma)$, the space of all continuous functions on Γ, with respect to the norm

$$\|u\|_{L_2(\Gamma)} := \left(\int_\Gamma |u(x)|^2 \, ds_x \right)^{1/2}. \tag{2.6}$$

This is a Hilbert space with the inner product

$$\langle u, v \rangle_{L_2(\Gamma)} := \int_\Gamma u(x)\overline{v(x)} \, ds_x.$$

For $0 < s < 1$ we define $H^s(\Gamma)$ to be the completion of $C^0(\Gamma)$ with respect to the Sobolev-Slobodetskii norm

$$\|u\|_{H^s(\Gamma)} := \left(\|u\|_{L_2(\Gamma)}^2 + \int_\Gamma \int_\Gamma \frac{|u(x) - u(y)|^2}{|x - y|^{d-1+2s}} \, ds_x \, ds_y \right)^{1/2}. \tag{2.7}$$

Again, $H^s(\Gamma)$ is a Hilbert space equipped with the inner product

$$\langle u, v \rangle_{H^s(\Gamma)} := \langle u, v \rangle_{L_2(\Gamma)} + \int_\Gamma \int_\Gamma \frac{(u(x) - u(y))\overline{(v(x) - v(y))}}{|x - y|^{d-1+2s}} \, ds_x \, ds_y.$$

For general $s \in \mathbb{R}$, a regularity assumption for the boundary $\Omega \in C^{k,\kappa}$ is required. Let us recall the parametric representation (2.5)

$$x = x_{(r)} + T_{(r)}(y', a_{(r)}(y')) \quad \text{for } y' \in Q, r = 1, ..., p.$$

Then, for $s \in \mathbb{R}$ with $0 \le s < k+\kappa$ for noninteger $k+\kappa$ or $0 \le s \le k+\kappa$ for integer $k+\kappa$ we define the Sobolev space $H^s(\Gamma)$ by

$$H^s(\Gamma) := \{u \in L_2(\Gamma) : \; u(x_{(r)} + T_{(r)}(y', a_{(r)}(y'))) \in H^s(Q), r = 1, ..., p\}$$

equipped with the norm

$$\|u\|_{H^s(\Gamma)} := \left(\sum_{r=1}^{p} \|u(x_{(r)} + T_{(r)}(y', a_{(r)}(y')))\|^2_{H^s(Q)} \right)^{1/2}. \tag{2.8}$$

This space is a Hilbert space with the inner product

$$\langle u, v \rangle_{H^s(\Gamma)} := \sum_{r=1}^{p} \langle u(x_{(r)} + T_{(r)}(y', a_{(r)}(y'))), v(x_{(r)} + T_{(r)}(y', a_{(r)}(y'))) \rangle_{H^s(Q)},$$

see [31, Section 4.2].

Note that, for $0 < s < 1$, the Sobolev norms as defined in (2.7) and (2.8) are equivalent.

For negative order, the Sobolev space $H^s(\Gamma)$ for $s < 0$ is defined as the dual space of $H^{-s}(\Gamma)$,

$$H^s(\Gamma) := [H^{-s}(\Gamma)]'$$

with respect to the $L_2(\Gamma)$ inner product, i.e., the completion of $L_2(\Gamma)$ with respect to the associated norm

$$\|u\|_{H^s(\Gamma)} := \sup_{0 \neq v \in H^{-s}(\Gamma)} \frac{\langle u, v \rangle_{L_2(\Gamma)}}{\|v\|_{H^{-s}(\Gamma)}}, \tag{2.9}$$

and to the duality pairing

$$\langle u, v \rangle_\Gamma := \langle u, v \rangle_{L_2(\Gamma)} = \int_\Gamma u(x) \overline{v(x)} \, ds_x. \tag{2.10}$$

For the study of the mixed boundary control problems we further need to define some Sobolev spaces on an open part of the boundary Γ, see [64, p.37]. Let $\Gamma_0 \subset \Gamma$ be some open part of a sufficient smooth boundary $\Gamma = \partial\Omega$. For $s \geq 0$ we define the Sobolev spaces

$$H^s(\Gamma_0) := \{v = \widetilde{v}_{|\Gamma_0} : \; \widetilde{v} \in H^s(\Gamma)\},$$
$$\widetilde{H}^s(\Gamma_0) := \{v = \widetilde{v}_{|\Gamma_0} : \; \widetilde{v} \in H^s(\Gamma), \; \text{supp}\widetilde{v} \subset \Gamma_0\}$$

with the norm

$$\|v\|_{H^s(\Gamma_0)} := \inf_{\widetilde{v}\in H^s(\Gamma):\widetilde{v}_{|\Gamma_0}=v} \|\widetilde{v}\|_{H^s(\Gamma)}.$$

For $s < 0$ we define the appropriate Sobolev spaces by duality with respect to the $L_2(\Gamma_0)$ inner product,

$$H^s(\Gamma_0) := [\widetilde{H}^{-s}(\Gamma_0)]', \quad \widetilde{H}^s(\Gamma_0) := [H^{-s}(\Gamma_0)]'.$$

Remark 2.1. *For a Lipschitz domain Ω, we have to assume $|s| \le 1$ to ensure the above definitions and statements concerning the Sobolev spaces defined on subsets of the boundary $\Gamma = \partial\Omega$. For the case $|s| > 1$ stronger regularity conditions of the boundary need to be assumed, i.e., $\Gamma \in C^{k,1}$, $k \in \mathbb{N}_0$ for $|s| \le k+1$, see [31, Section 4.3].*

Moreover, let Γ be a closed boundary which is piecewise smooth,

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

We define for $s > 0$ the space $H^s_{pw}(\Gamma)$ as the space of piecewise smooth functions

$$H^s_{pw}(\Gamma) := \{v \in L_2(\Gamma) \colon\ v_{|\Gamma_i} \in H^s(\Gamma_i), i = 1, \ldots, J\}$$

with the norm

$$\|v\|_{H^s_{pw}(\Gamma)} := \left\{ \sum_{i=1}^{J} \|v_{|\Gamma_i}\|^2_{H^s(\Gamma_i)} \right\}^{1/2}$$

while for $s < 0$ we have

$$H^s_{pw}(\Gamma) := \prod_{j=1}^{J} \widetilde{H}^s(\Gamma_j)$$

with the norm

$$\|w\|_{H^s_{pw}(\Gamma)} := \sum_{j=1}^{J} \|w_{|\Gamma_j}\|_{\widetilde{H}^s(\Gamma_j)}.$$

Lemma 2.1. *For $w \in H^s_{pw}(\Gamma)$ and $s < 0$ we have*

$$\|w\|_{H^s(\Gamma)} \le \|w\|_{H^s_{pw}(\Gamma)}.$$

Proof. See [64, Lemma 2.20]. □

2.1.2 Anisotropic Sobolev spaces

In this subsection, we briefly recall some definitions and properties of anisotropic Sobolev spaces for studying parabolic boundary control problems, see [15, 40].

Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain with boundary $\Gamma = \partial\Omega$. For a fixed real number $T > 0$, we write

$$I := (0,T), \quad Q := \Omega \times I, \quad \Sigma := \Gamma \times I.$$

Let X be a Banach space with the norm $\|\cdot\|_X$. We define $L_2(I;X)$ as the space of all measurable functions $u : [0,T] \to X$ with

$$\|u\|_{L_2(I;X)} := \left(\int_0^T \|u(\cdot,t)\|_X^2 \, dt \right)^{1/2} < \infty.$$

Let

$$\hat{u}(x,\tau) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-it\tau} u(x,t)\, dt$$

be the Fourier transform of u with respect to the time variable, we have

$$u \in H^s(\mathbb{R};L_2(\Omega)) \quad \Leftrightarrow \quad (1+|\tau|^2)^{s/2}\hat{u} \in L_2(\mathbb{R};L_2(\Omega)) = L_2(\Omega\times\mathbb{R}).$$

The Sobolev space $H^{r,s}(\mathbb{R}^d \times \mathbb{R})$ for $r,s \geq 0$, is defined by

$$H^{r,s}(\mathbb{R}^d \times \mathbb{R}) := L_2(\mathbb{R};H^r(\mathbb{R}^d)) \cap H^s(\mathbb{R};L_2(\mathbb{R}^d)),$$

see [15], with the natural norms defined in these spaces of Hilbert space valued distributions. We have

$$\|u\|^2_{H^{r,s}(\Omega\times\mathbb{R})} := \int_{\mathbb{R}} \left(\|\hat{u}(\cdot,\tau)\|^2_{H^r(\Omega)} + (1+|\tau|^2)^s \|\hat{u}(\cdot,\tau)\|^2_{L_2(\Omega)} \right) d\tau.$$

With $r \geq 0$ and $s \in (0,1)$, an equivalent norm is given by

$$\|u\|^2_{H^{r,s}(\Omega\times\mathbb{R})} = \int_{\mathbb{R}} \|u(\cdot,t)\|^2_{H^r(\Omega)}\, dt + \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{\|u(\cdot,t)-u(\cdot,\tau)\|^2_{L_2(\Omega)}}{|t-\tau|^{1+2s}}\, dt\, d\tau.$$

For $r,s \leq 0$ we define by duality $H^{r,s}(\mathbb{R}^d \times \mathbb{R}) := [H^{-r,-s}(\mathbb{R}^d \times \mathbb{R})]'$. By $H^{r,s}(Q)$ we denote the space of restrictions of elements of $H^{r,s}(\mathbb{R}^d \times \mathbb{R})$ to Q, equipped with the obvious quotient norm.

Moreover, we define the following subspaces:

$$\widetilde{H}^{r,s}(Q) := \{u \in H^{r,s}(\Omega \times (-\infty, T)) \colon \ u(x,t) = 0 \text{ for } t < 0\} \subset H^{r,s}(\Omega \times (-\infty, T)),$$
$$\overset{(T)}{H}{}^{r,s}(Q) := \{u \in H^{r,s}(\Omega \times (0, \infty)) \colon \ u(x,t) = 0 \text{ for } t > T\},$$

and

$$H^{r,s}_{0,}(Q) := L_2(I; H^r_0(\Omega)) \cap H^s(I; L_2(\Omega)) \subset H^{r,s}(Q).$$

It can be verified that the space $H^{r,s}_{0,}(Q)$ coincides with the closure in $H^{r,s}(Q)$ of the subspace of functions which vanish in a (spatial variable) neighbourhood of Σ;

$$H^{r,s}_{,0}(Q) := L_2(I; H^r(\Omega)) \cap H^s_0(I; L_2(\Omega)) \subset H^{r,s}(Q),$$

which is the closure in $H^{r,s}(Q)$ of the subspace of functions which vanish in the neighbourhood of $t = 0$ and of $t = T$; and

$$H^{r,s}_{0,0}(Q) := H^{r,s}_{0,}(Q) \cap H^{r,s}_{,0}(Q),$$

which is the closure of $\mathcal{D}(Q)$ in $H^{r,s}(Q)$. Similarly, $\widetilde{H}^{r,s}_0(Q)$ or $\overset{(T)}{H}{}^{r,s}_0(Q)$ are defined as the closure in $H^{r,s}(Q)$ of the subspace of functions which vanish in the (spatial variable) neighbourhood of Σ and the neighbourhood of $t = 0$ or $t = T$, respectively.

The negative indexed Sobolev spaces are defined as the dual spaces with respect to the $L_2(\Sigma)$ inner product as following, see [40, p.41], [15]:

$$H^{-r,-s}(Q) := [H^{r,s}_{0,0}(Q)]' \quad \text{for } r, s \geq 0,$$

and

$$\widetilde{H}^{-r,-s}(Q) := [\overset{(T)}{H}{}^{r,s}_0(Q)]' \quad \text{for all } r, s \text{ with } r - \frac{1}{2} \notin \mathbb{Z}.$$

Another important space is

$$\mathcal{V}(Q) := L_2(I; H^1(\Omega)) \cap H^1(I; H^{-1}(\Omega)) = \{u \in L_2(I; H^1(\Omega)) \colon \ \partial_t u \in L_2(I; H^{-1}(\Omega))\}.$$

The subspaces $\widetilde{\mathcal{V}}(Q) \subset \mathcal{V}(\Omega \times (-\infty, 0))$ and $\mathcal{V}_0(Q) \subset \mathcal{V}(Q)$ are defined analogously. It is true that, see [15, 39],

$$\mathcal{V}(Q) \text{ is a dense subspace of } H^{1,\frac{1}{2}}(Q).$$

Sobolev spaces on the boundary

Analogously we may first define the spaces $H^{r,s}(\Gamma\times\mathbb{R})$ and then $H^{r,s}(\Sigma)$ by restriction to Σ, see [40, Section 13.3].

The Sobolev space $H^{r,s}(\Gamma\times\mathbb{R})$ for $r,s\geq 0$, is defined by

$$H^{r,s}(\Gamma\times\mathbb{R}) = \{u:\ u\in L_2(\mathbb{R};H^r(\Gamma)), |\tau|^s\hat{u}\in L_2(\mathbb{R};H^0(\Gamma))\}, \tag{2.11}$$

equipped with the norm

$$\|u\|_{H^{r,s}(\Gamma\times\mathbb{R})} := \left(\|u\|^2_{L_2(\mathbb{R};H^r(\Gamma))} + \||\tau|^s\hat{u}\|^2_{L_2(\mathbb{R};H^0(\Gamma))}\right)^{1/2}.$$

We define $H^{r,s}(\Sigma)$ as the restriction of $H^{r,s}(\Gamma\times\mathbb{R})$ to Σ, equipped with the corresponding quotient norm. This definition is equivalent to

$$H^{r,s}(\Sigma) = L_2(I;H^r(\Gamma))\cap H^s(I;L_2(\Gamma)).$$

For $0<r,s<1$, an equivalent norm in $H^{r,s}(\Sigma)$ is given by

$$\begin{aligned}\|u\|^2_{H^{r,s}(\Sigma)} = \|u\|^2_{L_2(\Sigma)} \ &+ \int_0^T\int_\Gamma\int_\Gamma \frac{|u(x,t)-u(y,t)|^2}{|x-y|^{d-1+2r}}\,dt\,ds_x\,ds_y \\ &+ \int_0^T\int_0^T \frac{\|u(\cdot,t)-u(\cdot,\tau)\|^2_{L_2(\Gamma)}}{|t-\tau|^{1+2s}}\,dt\,d\tau.\end{aligned}$$

Since $H^r_0(\Gamma) = H^r(\Gamma)$, there is no distinction between $H^{r,s}_{0,}(\Sigma)$ and $H^{r,s}(\Sigma)$, but we may set

$$H^{r,s}_{,0}(\Sigma) = L_2(I;H^r(\Gamma))\cap H^s_0(I;H^0(\Gamma)).$$

The space $\widetilde{H}^{r,s}(\Sigma)$ is defined analogously. By duality, for $r,s\geq 0$,

$$H^{-r,-s}(\Sigma) = [H^{r,s}_{,0}(\Sigma)]'.$$

Remark 2.2. *As discussed in Remark 2.1, for Lipschitz boundary Γ we have to assume $|r|\leq 1$ ($s\in\mathbb{R}$ arbitrary) to define the above anisotropic Sobolev spaces on the boundary. For $|r|>1$ stronger regularity assumptions on the boundary need to be assumed, first to formulate $H^r(\Gamma)$, then to define $H^{r,s}(\Gamma\times\mathbb{R})$ as in (2.11).*

Trace theorem

Theorem 2.2. *For $u \in H^{r,s}(Q)$ with $r > \frac{1}{2}, s \geq 0$, we may define:*

$$\frac{\partial^j}{\partial n^j} u \quad on \quad \Sigma \quad if \quad j < r - \frac{1}{2} \quad (integer\ j \geq 0), \quad \frac{\partial^j}{\partial n^j} u \in H^{\mu_j, \nu_j}(\Sigma),$$

where

$$\frac{\mu_j}{r} = \frac{\nu_j}{s} = \frac{r - j - \frac{1}{2}}{r} \quad (\nu_j = 0 \quad if \quad s = 0).$$

The linear map $u \to \frac{\partial^j}{\partial n^j} u$ is continuous,

$$H^{r,s}(Q) \to H^{\mu_j, \nu_j}(\Sigma).$$

Here $\frac{\partial}{\partial n}$ is the normal derivative on Σ, oriented toward the interior of Q.

We may also define, for $s > \frac{1}{2}, r \geq 0$,

$$\frac{\partial^k}{\partial t^k} u(x,0) \quad on \quad \Omega \quad if \quad k < s - \frac{1}{2} \quad (integer\ k \geq 0), \quad \frac{\partial^k}{\partial t^k} u(x,0) \in H^{p_k}(\Omega),$$

where

$$p_k = \frac{r}{s}\left(s - k - \frac{1}{2}\right).$$

The linear map $u \to \frac{\partial^k}{\partial t^k} u(x,0)$ is continuous,

$$H^{r,s}(Q) \to H^{p_k}(\Omega).$$

Proof. See [40, Theorem 2.1]. □

Next we consider the trace of $\widetilde{H}^{1,\frac{1}{2}}(Q)$ on the boundary Σ, see [15, Lemma 2.4].

Lemma 2.2. *The trace map $\gamma_0 : u \mapsto u_{|\Sigma}$ is continuous and surjective from $\widetilde{H}^{1,\frac{1}{2}}(Q)$ to $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$.*

Remark 2.3. *The traces on Σ have to be understood in a distributional sense, i.e., they are defined by continuous extensions of the traces defined in the pointwise sense for smooth functions.*

2.2 Boundary elements

For the approximate solution of boundary integral equations let us summarize some appropriate finite dimensional trial spaces. We recall some approximation properties in various Sobolev spaces. We refer to [48, 64] for more details.

Let $\Gamma = \partial\Omega$ be a piecewise smooth Lipschitz boundary with $\overline{\Gamma} = \cup_{j=1}^{J} \overline{\Gamma}_j$ where any boundary part Γ_j can be smoothly mapped in a 1 to 1 fashion onto some parameter domain $\mathcal{Q} \subset \mathbb{R}^{d-1}$: $\Gamma_j = \chi_j(\mathcal{Q})$. The domain $\mathcal{Q}$ can be $(0,1)$ in the two dimensional case or a unit square in the three dimensional case. We consider a decomposition of the parameter domain $\mathcal{Q}$ into finite elements q_ℓ^j which correspond to an admissible decomposition of the boundary part Γ_j into boundary elements $\tau_\ell = \chi_j(q_\ell^j)$. We denote by

$$\Delta_\ell := \int_{\tau_\ell} ds_x, \quad h_\ell := \Delta_\ell^{1/(d-1)}$$

the volume and the local mesh size of the boundary element τ_ℓ, respectively. The (global) mesh size is defined by

$$h := \max_\ell h_\ell.$$

The boundary decomposition is called globally quasi-uniform if

$$\frac{h}{\min_\ell h_\ell} \le c_G$$

is satisfied with a global constant $c_G \ge 1$. Note, in the three dimensional case, the boundary decomposition is called admissible if two neighboring boundary elements share either a node or an edge, and it is called shape regular if there exists a constant c_B such that

$$d_\ell \le c_B h_\ell \quad \text{for all boundary elements } \tau_\ell,$$

where $d_\ell := \sup_{x,y\in\tau_\ell} |x-y|$.

Trial spaces
Let us recall some trial spaces $S_h^{d_x}(\Gamma)$ of local polynomials of degree d_x. In particular we will consider the trial space $S_h^0(\Gamma)$ of piecewise constant functions and the trial space $S_h^1(\Gamma)$ of piecewise linear continuous functions:

$$S_h^0(\Gamma) := \mathrm{span}\{\varphi_k^0\}_{k=1}^N, \quad S_h^1(\Gamma) := \mathrm{span}\{\varphi_i^1\}_{i=1}^M,$$

where the basis functions $\varphi_k^0(x)$ are given by

$$\varphi_k^0(x) = \begin{cases} 1 & \text{for } x \in \tau_k, \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, a function $v_h \in S_h^1(\Gamma)$ is determined by the nodal values which are described at the M nodes x_k, i.e., a basis of $S_h^1(\Gamma)$ is given by

$$\varphi_i^1(x) = \begin{cases} 1 & \text{for } x = x_i, \\ 0 & \text{for } x = x_j \neq x_i, \\ \text{linear} & \text{otherwise.} \end{cases}$$

If $u \in L_2(\Gamma)$ is a given function, the L_2 projection $\mathcal{P}_h^0 u \in S_h^0(\Gamma)$ is defined as the unique solution of the variational problem

$$\langle \mathcal{P}_h^0 u, v_h \rangle_{L_2(\Gamma)} = \langle u, v_h \rangle_{L_2(\Gamma)} \quad \text{for all } v_h \in S_h^0(\Gamma).$$

In addition, we define the L_2 projection $\mathcal{P}_h^1 u \in S_h^1(\Gamma)$ as the unique solution of the variational problem

$$\langle \mathcal{P}_h^1 u, v_h \rangle_{L_2(\Gamma)} = \langle u, v_h \rangle_{L_2(\Gamma)} \quad \text{for all } v_h \in S_h^1(\Gamma).$$

The following error estimates for the projection operator $\mathcal{P}_h^{d_x}$, when assuming sufficient smoothness on Γ, can be found in, e.g., [48, 64].

Lemma 2.3. *Let $u \in H^s(\Gamma)$ be given for some $s \in [0,1]$. For $\sigma \in [-1,0]$ there holds the error estimate*

$$\|u - \mathcal{P}_h^0 u\|_{H^\sigma(\Gamma)} \leq c\, h^{s-\sigma} |u|_{H^s(\Gamma)}. \tag{2.12}$$

Lemma 2.4. *Let $u \in H^s(\Gamma)$ be given for some $s \in [0,2]$. For $\sigma \in [-1,0]$ there holds the error estimate*

$$\|u - \mathcal{P}_h^1 u\|_{H^\sigma(\Gamma)} \leq c\, h^{s-\sigma} |u|_{H^s(\Gamma)}. \tag{2.13}$$

Moreover, the following approximation properties of the trial spaces are available as shown in [64, Section 10.2].

Theorem 2.3. *Let $\sigma \in [-1,0]$. For $u \in H^s(\Gamma)$ with some $s \in [0,1]$ there holds the approximation property of $S_h^0(\Gamma)$,*

$$\inf_{v_h \in S_h^0(\Gamma)} \|u - v_h\|_{H^\sigma(\Gamma)} \leq c\, h^{s-\sigma} |u|_{H^s(\Gamma)}. \tag{2.14}$$

Theorem 2.4. *Let $\Gamma = \partial\Omega$ be sufficiently smooth. For $\sigma \in [0,1]$ and for some $s \in [\sigma,2]$ we assume $u \in H^s(\Gamma)$. Then there holds the approximation property of $S_h^1(\Gamma)$,*

$$\inf_{v_h \in S_h^1(\Gamma)} \|u - v_h\|_{H^\sigma(\Gamma)} \leq c\, h^{s-\sigma} |u|_{H^s(\Gamma)}. \tag{2.15}$$

To construct the trial spaces for parabolic boundary control problems, we use a uniform partition of the interval $[0,T]$ with a time stepsize h_t. We define $T_{h_t}^{d_t}$ as the space of locally polynomials of degree d_t in time. For example, $T_{h_t}^{0}$ is the space of piecewise constant functions. This space is conveniently described as the span of the following basis functions, see [48],

$$\psi_k^0(t) = \begin{cases} 1 & \text{if } kh_t < t < (k+1)h_t, \\ 0 & \text{otherwise,} \end{cases}, \quad k = 0,1,...,N-1. \tag{2.16}$$

We describe a standard class of tensor product spaces $Q_h^{d_x,d_t}(\Sigma) = S_{h_x}^{d_x}(\Gamma) \otimes T_{h_t}^{d_t}$. We would like to estimate

$$\inf\{\|u - v_h\|_{H^{p,q}(\Sigma)} \colon v_h \in Q_h^{d_x,d_t}(\Sigma)\}$$

for $u \in H^{r,s}(\Sigma)$ with $0 \le r$, $0 \le s$ and $p \le r$, $q \le s$. The following approximation properties are recalled from [15, 48].

Theorem 2.5. *Let*

$$-d_x \le p \le 0 \le r \le d_x + 1, \quad 0 \le s \le d_t + 1.$$

Then there is a constant $C > 0$ which depends on (p,r,s) such that

$$\inf\{\|u - v_h\|_{H^{p,\frac{p}{2}}(\Sigma)} \colon v_h \in Q_h^{d_x,d_t}(\Sigma)\} \le C(h_x^{-p} + h_t^{-\frac{p}{2}})(h_x^r + h_t^s)\|u\|_{H^{r,s}(\Sigma)} \tag{2.17}$$

for all $u \in H^{r,s}(\Sigma)$.

Theorem 2.6. *Let*

$$0 \le p \le r \le d_x + 1, \quad p < d_x + 1/2,$$
$$0 \le q \le s \le d_t + 1, \quad q < d_t + 1/2,$$

and

$$\frac{r}{s} = \frac{p}{q}.$$

Then there is a constant $C(r,s) > 0$ such that

$$\inf\{\|u - v_h\|_{H^{p,q}(\Sigma)} \colon v_h \in Q_h^{d_x,d_t}(\Sigma)\} \le C(r,s)(h_x^{r-p} + h_t^{s-q})\|u\|_{H^{r,s}(\Sigma)} \tag{2.18}$$

for all $u \in H^{r,s}(\Sigma)$.

In the simplest finite element approximations compatible with the energy norm, i.e., $p = \frac{1}{2}$ ($p = -\frac{1}{2}$), $q = \frac{p}{2}$, we choose the approximations of piecewise linear and continuous (or piecewise constant) in space and piecewise constant in time. It results in the following corollary.

Corollary 2.1. *Assume that there are constants* $c_1, c_2 > 0$ *such that*

$$c_1 h_x^2 \leq h_t \leq c_2 h_x^2.$$

Then, for $0 \leq r \leq 1$, $\frac{1}{2} \leq s \leq 2$, *we have*

$$\inf\{\|u - v_h\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} : v_h \in Q_h^{0,0}(\Sigma)\} \leq C h_x^{r+\frac{1}{2}} \|u\|_{H^{r,\frac{r}{2}}(\Sigma)}, \tag{2.19}$$

$$\inf\{\|u - v_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} : v_h \in Q_h^{1,0}(\Sigma)\} \leq C h_x^{s-\frac{1}{2}} \|u\|_{H^{s,\frac{s}{2}}(\Sigma)}. \tag{2.20}$$

3 ELLIPTIC DIRICHLET BOUNDARY CONTROL PROBLEMS

This chapter is devoted to study Dirichlet boundary control problems subject to elliptic partial differential equations. The Karush-Kuhn-Tucker (KKT) system [28], which comprises the state equation, the adjoint equation, and the optimality condition is rewritten as either a system of boundary integral equations in a non-symmetric or in a symmetric formulation. The unique solvability of these systems can be derived from the properties of the standard boundary integral operators of the Laplace and of the Bi-Laplace equations. We discuss stability and error estimates of the related Galerkin boundary element methods. While the non-symmetric formulation leads to a non-symmetric matrix representation of a self-adjoint operator in which we need an additional condition on the discretization to guarantee the stability, we can prove the stability of the symmetric boundary element approach by using the hypersingular Bi-Laplace boundary integral operator. In the case of box constraints on the Dirichlet control, we obtain an elliptic variational inequality of the first kind to be solved. It will be treated by using semi-smooth Newton methods which give superlinear convergence.

This chapter is based on our paper [52]. It is organized as follows. In the first section, the model problem is described where we also discuss the adjoint problem which characterizes the solution of the reduced minimization problem. In Section 3.2 we present the representation formulae to describe the solutions of both the primal and adjoint Dirichlet boundary value problems. We formulate the weakly singular boundary integral equations. Since the state enters the adjoint boundary value problem as a volume density, an additional volume integral has to be considered. By using integration by parts, this Newton potential can be reformulated by using boundary potentials of the Bi-Laplace operator. Some properties of boundary integral operators for the Bi-Laplace operator are presented. We analyze a non-symmetric formulation of boundary integral equations to solve the Dirichlet boundary control problem, and we discuss stability and error estimates of the related Galerkin boundary element method in Section 3.4. By using the so-called hypersingular boundary integral equation in the optimality condition, we get a symmetric formulation. This is presented in Section 3.5, again we discuss a related stability and error analysis. In Section 3.6, we use a semi-smooth Newton method as in [18, 24, 33, 35] to solve the variational inequality. Finally, in Section 3.7 we describe some numerical examples.

3.1 Dirichlet boundary control problems

Let $\Omega \subset \mathbb{R}^d$, $d = 2,3$ be a bounded Lipschitz domain with boundary $\Gamma = \partial\Omega$. As a model problem, we consider the Dirichlet boundary control problem to minimize

$$J(u,z) = \frac{1}{2}\int_\Omega [u(x) - \overline{u}(x)]^2\,dx + \frac{1}{2}\alpha\langle Sz, z\rangle_\Gamma \quad \text{for } (u,z) \in H^1(\Omega) \times H^{1/2}(\Gamma) \tag{3.1}$$

subject to

$$-\Delta u(x) = f(x) \quad \text{for} \quad x \in \Omega, \quad u(x) = z(x) \quad \text{for } x \in \Gamma \tag{3.2}$$

with box constraints

$$z_1(x) \le z(x) \le z_2(x) \quad \text{for } x \in \Gamma, \tag{3.3}$$

where $\overline{u} \in L_2(\Omega)$ is a given target; $z_1, z_2 \in H^{1/2}(\Gamma)$ are given functions satisfying $z_1 \le z_2$ on Γ; $f \in L_2(\Omega)$ is a given volume density; $\alpha \in \mathbb{R}_+$ is a fixed parameter. Moreover, we use the Steklov-Poincaré operator $S : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ to describe the cost, or some regularization term, via a semi-norm in $H^{1/2}(\Gamma)$, see [51, 63]. Note that $\langle \cdot, \cdot \rangle_\Gamma$ denotes the related duality pairing, see (2.10).

To rewrite the Dirichlet boundary control problem (3.1), (3.2) and (3.3) by using a reduced cost functional we introduce a linear solution operator describing the application of the constraint (3.2). Let u_f be a particular weak solution of the homogeneous Dirichlet boundary value problem

$$-\Delta u_f(x) = f(x) \quad \text{for } x \in \Omega, \quad u_f(x) = 0 \quad \text{for } x \in \Gamma.$$

The solution of the Dirichlet boundary value problem (3.2) is then given by $u = u_z + u_f$, where $u_z \in H^1(\Omega)$ is the unique solution of the Dirichlet boundary value problem

$$-\Delta u_z(x) = 0 \quad \text{for } x \in \Omega, \quad u_z(x) = z(x) \quad \text{for } x \in \Gamma. \tag{3.4}$$

In particular, by using Green's first formula, we have

$$\int_\Omega |\nabla u_z(x)|^2\,dx = \int_\Gamma \frac{\partial}{\partial n_x} u_z(x) u_z(x)\,ds_x = \langle Sz, z\rangle_\Gamma =: |z|^2_{H^{1/2}(\Gamma)},$$

where the Steklov-Poincaré operator $S : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$,

$$(Sz)(x) := \frac{\partial}{\partial n_x} u_z(x) \quad \text{for } x \in \Gamma,$$

characterizes the Dirichlet to Neumann map related to the Dirichlet boundary value problem (3.4). This motivates the use of the Steklov-Poincaré operator S to describe the cost term in (3.1). In addition, one may think of using the hypersingular operator D in (3.1) to realize a semi-norm in $H^{1/2}(\Gamma)$, see [64].

Note that the solution of the Dirichlet boundary value problem (3.4) defines a linear map $u_z = \mathcal{H}z$. Then, by using $u = \mathcal{H}z + u_f$, instead of (3.1) we now consider the problem to find the minimizer $z \in \mathcal{U}_{ad}$ of the reduced cost functional

$$\begin{aligned}\widetilde{J}(z) &= \frac{1}{2}\int_\Omega [(\mathcal{H}z)(x) + u_f(x) - \overline{u}(x)]^2\,dx + \frac{\alpha}{2}\langle Sz, z\rangle_\Gamma \\ &= \frac{1}{2}\langle \mathcal{H}z + u_f - \overline{u}, \mathcal{H}z + u_f - \overline{u}\rangle_\Omega + \frac{\alpha}{2}\langle Sz, z\rangle_\Gamma \\ &= \frac{1}{2}\langle \mathcal{H}^*\mathcal{H}z, z\rangle_\Gamma + \langle \mathcal{H}^*(u_f - \overline{u}), z\rangle_\Gamma + \frac{1}{2}\|u_f - \overline{u}\|^2_{L_2(\Omega)} + \frac{\alpha}{2}\langle Sz, z\rangle_\Gamma,\end{aligned}$$

where

$$\mathcal{U}_{ad} := \{w \in H^{1/2}(\Gamma) \colon z_1(x) \le w(x) \le z_2(x) \text{ for } x \in \Gamma\} \tag{3.5}$$

is the admissible set, and $\mathcal{H}^* : L_2(\Omega) \to H^{-1/2}(\Gamma)$ is the adjoint operator of $\mathcal{H} : H^{1/2}(\Gamma) \to L_2(\Omega)$, i.e.,

$$\langle \mathcal{H}^*\psi, \varphi\rangle_\Gamma = \langle \psi, \mathcal{H}\varphi\rangle_\Omega \quad \text{for all } \varphi \in H^{1/2}(\Gamma), \psi \in L_2(\Omega).$$

Since the reduced cost functional $\widetilde{J}(\cdot)$ is convex, the minimizer $z \in \mathcal{U}_{ad}$ can be found from the variational inequality

$$\langle \alpha Sz + \mathcal{H}^*\mathcal{H}z - g, w - z\rangle_\Gamma \ge 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{3.6}$$

where we define

$$g := \mathcal{H}^*(\overline{u} - u_f) \in H^{-1/2}(\Gamma). \tag{3.7}$$

Note that the operator

$$T_\alpha := \alpha S + \mathcal{H}^*\mathcal{H} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma) \tag{3.8}$$

is bounded and $H^{1/2}(\Gamma)$-elliptic, see [51, 50]. Hence, the elliptic variational inequality of the first kind (3.6) admits a unique solution $z \in H^{1/2}(\Gamma)$, see, e.g., [23, 38, 41].

The application of the adjoint operator $\tau = \mathcal{H}^*(u - \overline{u})$ is characterized by the Neumann datum

$$\tau(x) = -\frac{\partial}{\partial n_x} p(x) \quad \text{for almost all } x \in \Gamma,$$

where p is the unique solution of the adjoint Dirichlet boundary value problem

$$-\Delta p(x) = u(x) - \overline{u}(x) \quad \text{for } x \in \Omega, \quad p(x) = 0 \quad \text{for } x \in \Gamma. \tag{3.9}$$

Hence the variational inequality (3.6) is rewritten as

$$\langle \alpha Sz - \frac{\partial}{\partial n} p, w - z\rangle_\Gamma \ge 0 \quad \text{for all } w \in \mathcal{U}_{ad}. \tag{3.10}$$

Proposition 3.1 ([51]). *Let Ω be either a convex two-dimensional polygonal bounded domain or a bounded domain with a smooth boundary. Let z be the unique solution of the variational inequality* (3.10). *For $\overline{u}, f \in L_2(\Omega)$, $z_1, z_2 \in H^{3/2}(\Gamma)$, we have the regularity $z \in H^{3/2}(\Gamma)$.*

Proof. Let us consider the variational inequality (3.10). We introduce

$$\lambda := T_\alpha z - g = \alpha S z - \frac{\partial}{\partial n} p = \alpha \frac{\partial}{\partial n} u_z - \frac{\partial}{\partial n} p \in H^{-1/2}(\Gamma),$$

where p is the unique solution of the homogeneous Dirichlet boundary value problem (3.9), and where u_z is the harmonic extension of z, see (3.4). Then we can rewrite the variational inequality (3.10) as

$$\langle \lambda, w - z \rangle_\Gamma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}.$$

Let

$$\mathcal{I} := \{x \in \Gamma \colon z_1(x) < z(x) < z_2(x)\}$$

be the inactive set. We can choose $\phi \in H^{1/2}(\Gamma)$ arbitrarily, with $\phi(x) \geq 0$ for $x \in \Gamma$, $\phi(x) > 0$ for $x \in \mathcal{I}$ and

$$w_1 = z - \phi \in \mathcal{U}_{ad}, \quad w_2 = z + \phi \in \mathcal{U}_{ad}.$$

Then we find

$$\langle \lambda, \phi \rangle_\Gamma = 0,$$

i.e., $\lambda = 0$ on $\mathcal{I}$. Hence we have

$$\lambda (z - z_1)(z_2 - z) = 0 \quad \text{on } \Gamma. \tag{3.11}$$

Moreover,

$$\lambda \leq 0 \quad \text{for } z = z_2 \quad \text{and} \quad \lambda \geq 0 \quad \text{for } z = z_1 \tag{3.12}$$

in the sense of $H^{-1/2}(\Gamma)$. Therefore we conclude that $u_z \in H^1(\Omega)$ is the unique solution of the Signorini boundary value problem

$$-\Delta u_z = 0 \quad \text{in } \Omega \tag{3.13}$$

with the bilateral constraints on Γ

$$z_1 \leq z \leq z_2, \quad \alpha \frac{\partial}{\partial n} u_z \leq \frac{\partial}{\partial n} p \quad \text{for } u_z = z_2, \quad \alpha \frac{\partial}{\partial n} u_z \geq \frac{\partial}{\partial n} p \quad \text{for } u_z = z_1, \tag{3.14}$$

and

$$\left[\alpha \frac{\partial}{\partial n} u_z - \frac{\partial}{\partial n} p \right] [u_z - z_1][z_2 - u_z] = 0 \quad \text{on } \Gamma. \tag{3.15}$$

For $\overline{u} \in L_2(\Omega)$ and $u = \mathcal{H}z + u_f \in L_2(\Omega)$ we have $p \in H^2(\Omega)$ for the solution of the adjoint problem (3.9), see e.g., [20]. Let $z_1, z_2 \in H^{3/2}(\Gamma)$, for the solution of the bilateral Signorini problem (3.13)-(3.15) we then have $u_z \in H^2(\Omega)$, and therefore $z \in H^{3/2}(\Gamma)$, see e.g., [5, Theorem 1] in the case of a bounded domain Ω with a smooth boundary. For a two-dimensional polygonal bounded domain it remains to consider the behaviour of the solution at a corner point when it coincides with a boundary point of the active zones, i.e., where $u_z = z_1$ or $u_z = z_2$ is satisfied. In particular, by using local polar coordinates

$$x_1 = x_1(r,\varphi) = r\cos\varphi, \;\; x_2 = x_2(r,\varphi) = r\sin\varphi, \;\; u_z(x_1,x_2) = u_z(r\cos\varphi, r\sin\varphi) = \widetilde{u}(r,\varphi),$$

we have

$$\begin{aligned} \frac{\partial}{\partial x_1} u_z(x_1,x_2) &= \cos\varphi \frac{\partial}{\partial r}\widetilde{u}(r,\varphi) - \frac{1}{r}\sin\varphi \frac{\partial}{\partial \varphi}\widetilde{u}(r,\varphi), \\ \frac{\partial}{\partial x_2} u_z(x_1,x_2) &= \sin\varphi \frac{\partial}{\partial r}\widetilde{u}(r,\varphi) + \frac{1}{r}\cos\varphi \frac{\partial}{\partial \varphi}\widetilde{u}(r,\varphi). \end{aligned}$$

The Laplace equation in polar coordinates reads

$$\Delta u_z(x_1,x_2) = \frac{\partial^2}{\partial x_1^2} u_z(x_1,x_2) + \frac{\partial^2}{\partial x_2^2} u_z(x_1,x_2) = \frac{1}{r}\frac{\partial}{\partial r}\left[r \frac{\partial}{\partial r}\widetilde{u}(r,\varphi)\right] + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\widetilde{u}(r,\varphi) = 0.$$

Let $\widetilde{u}(r,\varphi) = U(r)V(\varphi)$. We then obtain

$$\frac{r}{U(r)}\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}U(r)\right] + \frac{1}{V(\varphi)}\frac{\partial^2}{\partial \varphi^2}V(\varphi) = 0.$$

This implies

$$\frac{r}{U(r)}\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}U(r)\right] = c, \quad \frac{1}{V(\varphi)}\frac{\partial^2}{\partial \varphi^2}V(\varphi) = -c$$

for some constant c. The second ordinary differential equation of the last expression can be solved for $c = \alpha^2 > 0$,

$$V(\varphi) = A\cos(\alpha\varphi) + B\sin(\alpha\varphi).$$

For the first ordinary differential equation

$$r\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}U(r)\right] = \alpha^2 U(r),$$

we use the ansatz $U(r) = r^\gamma$. Then it follows that $\gamma = \pm\alpha$. Due to the boundedness of the solution for $r \to 0$ we finally obtain

$$\widetilde{u}(r,\varphi) = r^\alpha (A\cos(\alpha\varphi) + B\sin(\alpha\varphi)).$$

Now we consider the Signorini boundary conditions

$$\frac{\partial}{\partial n}u_z(x_1,x_2)=0, \quad u_z(x_1,x_2)\geq 0 \quad \text{for } \varphi=0$$

and

$$u_z(x_1,x_2)=0, \quad \frac{\partial}{\partial n}u_z(x_1,x_2)\geq 0 \quad \text{for } \varphi=\varphi_0,$$

where φ_0 is angle at the considered corner point.
For $\varphi=0$ and the normal vector $n=(0,-1)^\top$, we have

$$\begin{aligned}
\frac{\partial}{\partial n}u_z(x_1,x_2) &= n\cdot\nabla u_z(x_1,x_2)=-\frac{\partial}{\partial x_2}u_z(x_1,x_2)\\
&= -\sin\varphi\frac{\partial}{\partial r}\widetilde{u}(r,\varphi)-\frac{1}{r}\cos\varphi\frac{\partial}{\partial\varphi}\widetilde{u}(r,\varphi)\\
&= -\sin\varphi\frac{\partial}{\partial r}[r^\alpha(A\cos(\alpha\varphi)+B\sin(\alpha\varphi))]\\
&\qquad -\frac{1}{r}\cos\varphi\frac{\partial}{\partial\varphi}[r^\alpha(A\cos(\alpha\varphi)+B\sin(\alpha\varphi))]\\
&= -\sin\varphi[\alpha r^{\alpha-1}(A\cos(\alpha\varphi)+B\sin(\alpha\varphi))]\\
&\qquad -\cos\varphi[\alpha r^{\alpha-1}(-A\sin(\alpha\varphi)+B\cos(\alpha\varphi))]\\
&= \alpha r^{\alpha-1}[A\sin((\alpha-1)\varphi)-B\cos((\alpha-1)\varphi)].
\end{aligned}$$

The Neumann boundary condition for $\varphi=0$ reads then

$$\frac{\partial}{\partial n}u_z(x_1,x_2)|_{\varphi=0}=-B\alpha r^{\alpha-1}=0 \quad\Rightarrow\quad B=0.$$

Hence,

$$\widetilde{u}(r,\varphi)=Ar^\alpha\cos(\alpha\varphi).$$

For the Dirichlet boundary condition for $\varphi=\varphi_0$, we further obtain

$$\widetilde{u}(r,\varphi_0)=Ar^\alpha\cos(\alpha\varphi_0)=0 \quad\Rightarrow\quad \alpha\varphi_0=\frac{\pi}{2} \quad\Rightarrow\quad \alpha_0=\frac{\pi}{2\varphi_0}.$$

Moreover, the complementary Dirichlet boundary condition for $\varphi=0$ results in

$$\widetilde{u}(r,0)=Ar^{\alpha_0}\geq 0 \quad\Rightarrow\quad A\geq 0.$$

We now consider the normal derivative $\frac{\partial}{\partial n}u_z(x_1,x_2)$ for $\varphi=\varphi_0$ with the normal vector

$$
\begin{aligned}
&n = (-\sin\varphi_0,\ \cos\varphi_0)^\top,\\
\frac{\partial}{\partial n}u_z(x_1,x_2) &= -\sin\varphi_0\frac{\partial}{\partial x_1}u_z(x_1,x_2)+\cos\varphi_0\frac{\partial}{\partial x_2}u_z(x_1,x_2)\\
&= -\sin\varphi_0\left[\cos\varphi\frac{\partial}{\partial r}(Ar^{\alpha_0}\cos(\alpha_0\varphi))-\frac{1}{r}\sin\varphi\frac{\partial}{\partial\varphi}(Ar^{\alpha_0}\cos(\alpha_0\varphi))\right]\\
&\qquad+\cos\varphi_0\left[\sin\varphi\frac{\partial}{\partial r}(Ar^{\alpha_0}\cos(\alpha_0\varphi))+\frac{1}{r}\cos\varphi\frac{\partial}{\partial\varphi}(Ar^{\alpha_0}\cos(\alpha_0\varphi))\right]\\
&= -\sin\varphi_0\left[\cos\varphi(A\alpha_0r^{\alpha_0-1}\cos(\alpha_0\varphi))-\frac{1}{r}\sin\varphi(-Ar^{\alpha_0}\alpha_0\sin(\alpha_0\varphi))\right]\\
&\qquad+\cos\varphi_0\left[\sin\varphi(A\alpha_0r^{\alpha_0-1}\cos(\alpha_0\varphi))+\frac{1}{r}\cos\varphi(-Ar^{\alpha_0}\alpha_0\sin(\alpha_0\varphi))\right]\\
&= -A\alpha_0r^{\alpha_0-1}\sin\varphi_0\cos((\alpha_0-1)\varphi)-A\alpha_0r^{\alpha_0-1}\cos\varphi_0\sin((\alpha_0-1)\varphi)\\
&= -A\alpha_0r^{\alpha_0-1}\sin[(\alpha_0-1)\varphi+\varphi_0].
\end{aligned}
$$

The complementary Neumann boundary condition for $\varphi=\varphi_0$ now reads

$$\frac{\partial}{\partial n}u_z(x_1,x_2)|_{\varphi=\varphi_0} = -A\alpha_0r^{\alpha_0-1}\sin(\alpha_0\varphi_0) = -A\alpha_0r^{\alpha_0-1}\geq 0 \quad\Rightarrow\quad A\leq 0.$$

Therefore we conclude $A=0$. It turns out that no singularity functions appear in the case of Signorini boundary conditions. This implies $u_z\in H^2(\Omega)$ also for a two-dimensional convex polygonal domain. □

3.2 Boundary integral equations

To find the control $z\in H^{1/2}(\Gamma)$ on the boundary, we discuss in this section the use of boundary integral equations for the solution of the state equation and of the adjoint equation. Some properties of boundary integral operators are included.

Firstly, for the solution of the state equation (3.2)

$$-\Delta u(x) = f(x)\quad\text{for}\quad x\in\Omega,\quad u(x)=z(x)\quad\text{for } x\in\Gamma,$$

we obtain a representation formula for $\widetilde{x}\in\Omega$,

$$u(\widetilde{x}) = \int_\Gamma U^*(\widetilde{x},y)\frac{\partial}{\partial n_y}u(y)\,ds_y - \int_\Gamma\frac{\partial}{\partial n_y}U^*(\widetilde{x},y)z(y)\,ds_y + \int_\Omega U^*(\widetilde{x},y)f(y)\,dy, \tag{3.16}$$

where $U^*(x,y)$ is the fundamental solution of the Laplace operator, see [64],

$$U^*(x,y) = \begin{cases} -\dfrac{1}{2\pi}\log|x-y| & \text{for } d=2,\\ \dfrac{1}{4\pi}\dfrac{1}{|x-y|} & \text{for } d=3.\end{cases} \tag{3.17}$$

For a given Dirichlet datum $z \in H^{1/2}(\Gamma)$, the related Neumann datum $\omega := \frac{\partial}{\partial n} u \in H^{-1/2}(\Gamma)$ can be found by considering the representation formula (3.16) for $\Omega \ni \widetilde{x} \to x \in \Gamma$. Due to the jump relation of the double layer potential, we obtain the boundary integral equation

$$z(x) = u(x) = \int_\Gamma U^*(x,y)\omega(y)\,ds_y + \frac{1}{2}z(x) - \int_\Gamma \frac{\partial}{\partial n_y} U^*(x,y)z(y)\,ds_y + \int_\Omega U^*(x,y)f(y)\,dy$$

for almost all $x \in \Gamma$, which can be written as

$$(V\omega)(x) = (\frac{1}{2}I + K)z(x) - (N_0 f)(x) \quad \text{for almost all } x \in \Gamma. \tag{3.18}$$

Here,

$$(V\omega)(x) = \int_\Gamma U^*(x,y)\omega(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the Laplace single layer potential $V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ satisfying

$$\|V\omega\|_{H^{1/2}(\Gamma)} \le c_2^V \|\omega\|_{H^{-1/2}(\Gamma)} \quad \text{for all } \omega \in H^{-1/2}(\Gamma),$$

and

$$(Kz)(x) = \int_\Gamma \frac{\partial}{\partial n_y} U^*(x,y)z(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the Laplace double layer potential $K : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)$ satisfying

$$\|(\frac{1}{2}I + K)z\|_{H^{1/2}(\Gamma)} \le c_2^K \|z\|_{H^{1/2}(\Gamma)} \quad \text{for all } z \in H^{1/2}(\Gamma).$$

Moreover,

$$(N_0 f)(x) = \int_\Omega U^*(x,y)f(y)\,dy \quad \text{for } x \in \Gamma$$

is the related Newton potential $N_0 : \widetilde{H}^{-1}(\Omega) \to H^{1/2}(\Gamma)$. For the properties of these operators, see, e.g., [14, 31, 64].

Note that the single layer potential V is $H^{-1/2}(\Gamma)$-elliptic, see [64], where for $d = 2$ we assume the scaling condition $diam\Omega < 1$ to ensure this:

$$\langle V\omega, \omega \rangle_\Gamma \ge c_1^V \|\omega\|^2_{H^{-1/2}(\Gamma)} \quad \text{for all } \omega \in H^{-1/2}(\Gamma).$$

Hence, we can solve the boundary integral equation (3.18) to obtain

$$\omega = V^{-1}(\frac{1}{2}I + K)z - V^{-1}N_0 f. \tag{3.19}$$

Secondly, the solution of the adjoint Dirichlet boundary value problem (3.9),

$$-\Delta p(x) = u(x) - \overline{u}(x) \quad \text{for } x \in \Omega, \quad p(x) = 0 \quad \text{for } x \in \Gamma,$$

is given correspondingly by the representation formula for $\widetilde{x} \in \Omega$,

$$p(\widetilde{x}) = \int_\Gamma U^*(\widetilde{x},y)\frac{\partial}{\partial n_y}p(y)\,ds_y + \int_\Omega U^*(\widetilde{x},y)[u(y) - \overline{u}(y)]\,dy. \tag{3.20}$$

As in (3.18) we obtain the boundary integral equation

$$(Vq)(x) = (N_0\overline{u})(x) - (N_0u)(x) \quad \text{for } x \in \Gamma \tag{3.21}$$

to determine the unknown Neumann datum $q := \frac{\partial}{\partial n}p \in H^{-1/2}(\Gamma)$.

Hence we conclude a system of boundary integral equations (3.18), (3.21) and the optimality condition (3.10) to be solved. However, since the solution u of the primal Dirichlet boundary value problem (3.2) enters the volume potential N_0u in the boundary integral equation (3.21), we also need to include the representation formula (3.16). Hence we have to solve a coupled system of boundary and domain integral equations. Instead, we will describe a system of only boundary integral equations to solve the adjoint boundary value problem (3.9).

In doing so, instead of (3.20), we introduce a modified representation formula for the adjoint state p as follows. First we note that

$$V^*(x,y) = \begin{cases} -\dfrac{1}{8\pi}|x-y|^2(\log|x-y| - 1) & \text{for } d = 2, \\ \dfrac{1}{8\pi}|x-y| & \text{for } d = 3 \end{cases} \tag{3.22}$$

is a solution of the Poisson equation

$$\Delta_y V^*(x,y) = U^*(x,y) \quad \text{for } x \neq y, \tag{3.23}$$

i.e., $V^*(x,y)$ is the fundamental solution of the Bi-Laplacian. Hence, by using Green's second formula, we can rewrite the volume integral for u in (3.20), as follows

$$\begin{aligned}\int_\Omega U^*(\widetilde{x},y)u(y)\,dy &= \int_\Omega [\Delta_y V^*(\widetilde{x},y)]u(y)\,dy \\ &= \int_\Gamma \frac{\partial}{\partial n_y}V^*(\widetilde{x},y)u(y)\,ds_y - \int_\Gamma V^*(\widetilde{x},y)\frac{\partial}{\partial n_y}u(y)\,ds_y \\ &\qquad + \int_\Omega V^*(\widetilde{x},y)[\Delta u(y)]\,dy \\ &= \int_\Gamma \frac{\partial}{\partial n_y}V^*(\widetilde{x},y)z(y)\,ds_y - \int_\Gamma V^*(\widetilde{x},y)\omega(y)\,ds_y - \int_\Omega V^*(\widetilde{x},y)f(y)\,dy.\end{aligned}$$

Therefore, from (3.20) we now obtain the modified representation formula for $\widetilde{x} \in \Omega$,

$$\begin{aligned} p(\widetilde{x}) = \int_\Gamma U^*(\widetilde{x},y)q(y)\,ds_y + \int_\Gamma \frac{\partial}{\partial n_y} V^*(\widetilde{x},y)z(y)\,ds_y - \int_\Gamma V^*(\widetilde{x},y)\omega(y)\,ds_y \\ - \int_\Omega U^*(\widetilde{x},y)\overline{u}(y)\,dy - \int_\Omega V^*(\widetilde{x},y)f(y)\,dy, \end{aligned} \tag{3.24}$$

where the volume potentials involve given data only.
Due to the regularity of the fundamental solution of the Bi-Laplacian $V^*(x,y)$, there is no jump relation occuring across the boundary Γ, see, e.g., [59]. Hence, when taking the limit $\Omega \ni \widetilde{x} \to x \in \Gamma$, the representation formula (3.24) results in the boundary integral equation

$$\begin{aligned} 0 = p(x) = \int_\Gamma U^*(x,y)q(y)\,ds_y + \int_\Gamma \frac{\partial}{\partial n_y} V^*(x,y)z(y)\,ds_y - \int_\Gamma V^*(x,y)\omega(y)\,ds_y \\ - \int_\Omega U^*(x,y)\overline{u}(y)\,dy - \int_\Omega V^*(x,y)f(y)\,dy \end{aligned}$$

for almost all $x \in \Gamma$, which can be written as

$$(Vq)(x) = (V_1\omega)(x) - (K_1 z)(x) + (N_0\overline{u})(x) + (M_0 f)(x) \quad \text{for } x \in \Gamma. \tag{3.25}$$

Note that

$$(V_1\omega)(x) = \int_\Gamma V^*(x,y)\omega(y)\,ds_y$$

is the Bi-Laplace single layer potential $V_1 : H^{-3/2}(\Gamma) \to H^{3/2}(\Gamma)$ satisfying, see, e.g., [31, Theorem 5.7.3],

$$\|V_1\omega\|_{H^{3/2}(\Gamma)} \le c_2^{V_1} \|\omega\|_{H^{-3/2}(\Gamma)} \quad \text{for all } \omega \in H^{-3/2}(\Gamma), \tag{3.26}$$

and

$$(K_1 z)(x) = \int_\Gamma \frac{\partial}{\partial n_y} V^*(x,y)z(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the Bi-Laplace double layer potential $K_1 : H^{-1/2}(\Gamma) \to H^{3/2}(\Gamma)$ satisfying

$$\|K_1 z\|_{H^{3/2}(\Gamma)} \le c_2^{K_1} \|z\|_{H^{-1/2}(\Gamma)} \quad \text{for all } z \in H^{-1/2}(\Gamma). \tag{3.27}$$

In addition, we have introduced a second Newton potential which is related to the fundamental solution of the Bi-Laplace operator,

$$(M_0 f)(x) = \int_\Omega V^*(x,y)f(y)\,dy \quad \text{for } x \in \Gamma.$$

By inserting (3.19) into the boundary integral equation (3.25), this gives

$$Vq = V_1V^{-1}(\frac{1}{2}I+K)z - K_1z + N_0\overline{u} + M_0f - V_1V^{-1}N_0f,$$

and therefore

$$q = V^{-1}V_1V^{-1}(\frac{1}{2}I+K)z - V^{-1}K_1z + V^{-1}N_0\overline{u} + V^{-1}M_0f - V^{-1}V_1V^{-1}N_0f. \tag{3.28}$$

Now we are in a position to rewrite the variational inequality (3.10) to find $z \in \mathcal{U}_{ad}$ such that

$$\langle T_\alpha z - g, w - z\rangle_\Gamma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{3.29}$$

where

$$T_\alpha := \alpha S + V^{-1}K_1 - V^{-1}V_1V^{-1}(\frac{1}{2}I+K) \tag{3.30}$$

is a boundary integral representation of the operator T_α as defined in (3.8), and

$$g := V^{-1}N_0\overline{u} + V^{-1}M_0f - V^{-1}V_1V^{-1}N_0f \tag{3.31}$$

is the related right hand side as defined in (3.7).

Mapping properties

The operator T_α as defined in (3.30) is composed of the standard Laplace and Bi-Laplace boundary integral operators. To investigate the unique solvability of the variational inequality (3.29), we next recall some mapping properties of these boundary integral operators. We first start with the related Bi-Laplace partial differential equation.

Consider the Bi-Laplace equation

$$\Delta^2 u(x) = 0 \quad \text{for } x \in \Omega. \tag{3.32}$$

This equation can be written as a system

$$\Delta w(x) = 0, \quad \Delta u(x) = w(x) \quad \text{for } x \in \Omega.$$

For the Laplace equation we obtain two boundary integral equations of the associated Cauchy data on Γ: $\{w, \tau := \frac{\partial}{\partial n}w\}$, see [64, section 6]

$$\begin{pmatrix} w \\ \tau \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix} \begin{pmatrix} w \\ \tau \end{pmatrix}, \tag{3.33}$$

where

$$(K'\tau)(x) = \int_\Gamma \frac{\partial}{\partial n_x} U^*(x,y)\tau(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the adjoint Laplace double layer potential $K' : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)$, and

$$(Dw)(x) = -\frac{\partial}{\partial n_x} \int_\Gamma \frac{\partial}{\partial n_y} U^*(x,y) w(y)\, ds_y \quad \text{for } x \in \Gamma$$

is the related hypersingular boundary integral operator $D : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$.

To obtain a representation formula for the solution u of the Bi-Laplace equation (3.32), we first consider Green's first formula

$$\int_\Omega \Delta u(y) \Delta v(y)\, dy = \int_\Gamma \frac{\partial}{\partial n_y} u(y) \Delta v(y)\, ds_y - \int_\Gamma \frac{\partial}{\partial n_y} \Delta v(y) u(y)\, ds_y + \int_\Omega [\Delta^2 v(y)] u(y)\, dy, \tag{3.34}$$

and in the sequel Green's second formula,

$$\begin{aligned}\int_\Gamma \frac{\partial}{\partial n_y} u(y) \Delta v(y)\, ds_y - \int_\Gamma \frac{\partial}{\partial n_y} \Delta v(y) u(y)\, ds_y + \int_\Omega [\Delta^2 v(y)] u(y)\, dy \\ = \int_\Gamma \frac{\partial}{\partial n_y} v(y) \Delta u(y)\, ds_y - \int_\Gamma \frac{\partial}{\partial n_y} \Delta u(y) v(y)\, ds_y + \int_\Omega [\Delta^2 u(y)] v(y)\, dy.\end{aligned}$$

When choosing $v(y) = V^*(\widetilde{x}, y)$ for $\widetilde{x} \in \Omega$ as the Bi-Laplace fundamental solution (3.22), the solution of the Bi-Laplace partial differential equation (3.32) is given by the representation formula for $\widetilde{x} \in \Omega$,

$$\begin{aligned}u(\widetilde{x}) = \int_\Gamma \frac{\partial}{\partial n_y} u(y) \Delta_y V^*(\widetilde{x}, y)\, ds_y - \int_\Gamma \frac{\partial}{\partial n_y} \Delta_y V^*(\widetilde{x}, y) u(y)\, ds_y \\ - \int_\Gamma \frac{\partial}{\partial n_y} V^*(\widetilde{x}, y) \Delta u(y)\, ds_y + \int_\Gamma \frac{\partial}{\partial n_y} \Delta u(y) V^*(\widetilde{x}, y)\, ds_y.\end{aligned}$$

By using (3.23) this can be written as

$$\begin{aligned}u(\widetilde{x}) = \int_\Gamma U^*(\widetilde{x}, y) \omega(y)\, ds_y - \int_\Gamma \frac{\partial}{\partial n_y} U^*(\widetilde{x}, y) u(y)\, ds_y \\ - \int_\Gamma \frac{\partial}{\partial n_y} V^*(\widetilde{x}, y) w(y)\, ds_y + \int_\Gamma V^*(\widetilde{x}, y) \tau(y)\, ds_y.\end{aligned} \tag{3.35}$$

Hence, by taking the trace and the normal derivative of the representation formula (3.35), we get two additional boundary integral equations for almost all $x \in \Gamma$,

$$u(x) = (V\omega)(x) + \frac{1}{2} u(x) - (Ku)(x) - (K_1 w)(x) + (V_1 \tau)(x), \tag{3.36}$$

$$\omega(x) = \frac{1}{2} \omega(x) + (K'\omega)(x) + (Du)(x) + (D_1 w)(x) + (K'\tau)(x), \tag{3.37}$$

where

$$(K_1'\tau)(x) = \int_\Gamma \frac{\partial}{\partial n_x} V^*(x,y)\tau(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the adjoint Bi-Laplace double layer potential, and

$$(D_1 w)(x) = -\frac{\partial}{\partial n_x}\int_\Gamma \frac{\partial}{\partial n_y} V^*(x,y)w(y)\,ds_y \quad \text{for } x \in \Gamma$$

is the Bi-Laplace hypersingular boundary integral operator.

Altogether, we obtain a system of boundary integral equations for the Bi-Laplace equation (3.32), including the so-called Calderon projection $\mathcal{C}$,

$$\begin{pmatrix} u \\ \omega \\ w \\ \tau \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V & -K_1 & V_1 \\ D & \frac{1}{2}I + K' & D_1 & K_1' \\ & & \frac{1}{2}I - K & V \\ & & D & \frac{1}{2}I + K' \end{pmatrix} \begin{pmatrix} u \\ \omega \\ w \\ \tau \end{pmatrix}. \tag{3.38}$$

Lemma 3.1. *The Calderon projection $\mathcal{C}$ as defined in* (3.38) *is a projection, i.e., $\mathcal{C}^2 = \mathcal{C}$.*

Proof. Let $\omega, \psi \in H^{-1/2}(\Gamma)$, $\varphi, \phi \in H^{1/2}(\Gamma)$ be arbitrary but fixed. The function

$$u(\widetilde{x}) := (\widetilde{V}\omega)(\widetilde{x}) - (W\varphi)(\widetilde{x}) + (\widetilde{V}_1\psi)(\widetilde{x}) - (W_1\phi)(\widetilde{x}) \quad \text{for } \widetilde{x} \in \Omega \tag{3.39}$$

solves the Bi-Laplace partial differential equation (3.32). Note that

$$(\widetilde{V}\omega)(\widetilde{x}) := \int_\Gamma U^*(\widetilde{x},y)\omega(y)\,ds_y, \quad (\widetilde{V}_1\psi)(\widetilde{x}) := \int_\Gamma V^*(\widetilde{x},y)\psi(y)\,ds_y \quad \text{for } \widetilde{x} \in \Omega \tag{3.40}$$

are the Laplace and Bi-Laplace single layer potentials, respectively, and for $\widetilde{x} \in \Omega$,

$$(W\varphi)(\widetilde{x}) := \int_\Gamma \frac{\partial}{\partial n_y} U^*(\widetilde{x},y)\varphi(y)\,ds_y, \quad (W_1\phi)(\widetilde{x}) := \int_\Gamma \frac{\partial}{\partial n_y} V^*(\widetilde{x},y)\phi(y)\,ds_y \tag{3.41}$$

define the Laplace and Bi-Laplace double layer potentials, respectively. The assertion now follows from the system of boundary integral equations (3.38) of u, and the jump relation of the standard single and double layer potentials as in [64, Lemma 6.18], see also [59]. □

From the projection property $\mathcal{C}^2 = \mathcal{C}$ we can immediately conclude some well-known relations of all boundary integral operators which were introduced for both the Laplace and the Bi-Laplace equations, see [59, 64].

Corollary 3.1. *For all boundary integral operators there hold the relations*

$$KV = VK', \quad DK = K'D, \quad VD = \frac{1}{4}I - K^2, \quad DV = \frac{1}{4}I - K'^2 \tag{3.42}$$

and

$$K_1V - VK_1' = V_1K' - KV_1, \tag{3.43}$$
$$K_1'D - DK_1 = D_1K - K'D_1, \tag{3.44}$$
$$VD_1 + V_1D + KK_1 + K_1K = 0, \tag{3.45}$$
$$DV_1 + D_1V + K'K_1' + K_1'K' = 0. \tag{3.46}$$

To prove the ellipticity of the Schur complement boundary integral operator as defined in (3.30) we need the following result.

Lemma 3.2. *For any $\omega, \psi \in H^{-1/2}(\Gamma)$ there holds the equality*

$$\langle \widetilde{V}\omega, \widetilde{V}\psi \rangle_{L_2(\Omega)} = \langle K_1 V\omega, \psi\rangle_\Gamma - \langle V_1(\frac{1}{2}I + K')\omega, \psi\rangle_\Gamma. \tag{3.47}$$

In particular,

$$\|\widetilde{V}\psi\|^2_{L_2(\Omega)} = \langle K_1 V\psi, \psi\rangle_\Gamma - \langle V_1(\frac{1}{2}I + K')\psi, \psi\rangle_\Gamma \tag{3.48}$$

where the single layer potential $\widetilde{V}$ is defined in (3.40)*, and $\langle \cdot, \cdot \rangle_{L_2(\Omega)}$ is the standard inner product in $L_2(\Omega)$.*

Proof. For $\omega, \psi \in H^{-1/2}(\Gamma)$ the application of the Bi-Laplace single layer potential $u = \widetilde{V}_1\omega$ and $v = \widetilde{V}_1\psi$ as defined in (3.40) are solutions of the Bi-Laplace equation (3.32) whose related Cauchy data are given by

$$u(x) = (V_1\omega)(x), \quad \frac{\partial}{\partial n_x}u(x) = (K_1'\omega)(x) \quad \text{for } x \in \Gamma.$$

On the other hand, for $x \in \Omega$

$$\Delta_x u(x) = \Delta_x \int_\Gamma V^*(x,y)\omega(y)\,ds_y = \int_\Gamma U^*(x,y)\omega(y)\,ds_y = (\widetilde{V}\omega)(x),$$
$$w(x) = \Delta_x v(x) = \Delta_x \int_\Gamma V^*(x,y)\psi(y)\,ds_y = \int_\Gamma U^*(x,y)\psi(y)\,ds_y = (\widetilde{V}\psi)(x)$$

are solutions of the Laplace equation. The related Cauchy data are given by

$$w(x) = (V\psi)(x), \quad \frac{\partial}{\partial n_x}w(x) = \frac{1}{2}\psi(x) + (K'\psi)(x) \quad \text{for almost all } x \in \Gamma.$$

Now, Green's first formula (3.34) reads

$$\langle \widetilde{V}\omega, \widetilde{V}\psi\rangle_{L_2(\Omega)} = \int\limits_{\Gamma} (K_1'\omega)(y)(V\psi)(y)\, ds_y - \int\limits_{\Gamma} [\frac{1}{2}\psi(y) + (K'\psi)(y)](V_1\omega)(y)\, ds_y,$$

and then the assertion follows. □

Remark 3.1. *For the representation of the Steklov-Poincaré operator S via boundary integral operators, we may use either the non-symmetric representation*

$$S = V^{-1}(\frac{1}{2}I + K), \tag{3.49}$$

or the symmetric representation

$$S = D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K), \tag{3.50}$$

see, e.g., [62, 63, 64].

3.3 Discretization of variational inequalities

Boundary element approximations

Let

$$S_H^1(\Gamma) = span\{\varphi_i^1\}_{i=1}^M \subset H^{1/2}(\Gamma)$$

be a boundary element space of, e.g., piecewise linear and continuous basis functions φ_i^1, which is defined with respect to a globally quasi-uniform and shape regular boundary element mesh of mesh size H. For continuous functions z_1 and z_2, define the discrete convex set

$$\mathcal{U}_H := \{w_H \in S_H^1(\Gamma) \colon z_1(x_i) \le w_H(x_i) \le z_2(x_i) \quad \text{for all nodes } x_i \in \Gamma\}.$$

Then the Galerkin discretization of the variational inequality (3.6), see also (3.29), is to find $z_H \in \mathcal{U}_H$ such that

$$\langle T_\alpha z_H, w_H - z_H\rangle_\Gamma \ge \langle g, w_H - z_H\rangle_\Gamma \quad \text{for all } w_H \in \mathcal{U}_H. \tag{3.51}$$

Theorem 3.1. *Let $z \in \mathcal{U}_{ad}$ and $z_H \in \mathcal{U}_H$ be the unique solutions of the variational inequalities* (3.6) *and* (3.51)*, respectively. Then there hold the error estimates*

$$\|z - z_H\|_{H^{1/2}(\Gamma)} \le cH^{s-\frac{1}{2}}\|z\|_{H^s(\Gamma)} \tag{3.52}$$

and

$$\|z - z_H\|_{L_2(\Gamma)} \le cH^s\|z\|_{H^s(\Gamma)}, \tag{3.53}$$

when assuming $z, z_1, z_2 \in H^s(\Gamma)$ for some $s \in [\frac{1}{2}, 2]$, and $T_\alpha z - g \in L_\infty(\Gamma) \cap H^{s-1}(\Gamma)$.

Proof. From the $H^{1/2}(\Gamma)$-ellipticity of T_α, we obtain for all $w_H \in \mathcal{U}_H$, by using the variational inequality (3.51) and $\lambda := T_\alpha z - g \in H^{-1/2}(\Gamma)$,

$$\begin{aligned} c_1^{T_\alpha} \|z - z_H\|^2_{H^{1/2}(\Gamma)} &\leq \langle T_\alpha(z - z_H), z - z_H\rangle_\Gamma \\ &= \langle T_\alpha(z - z_H), z - w_H\rangle_\Gamma + \langle T_\alpha(z - z_H), w_H - z_H\rangle_\Gamma \\ &= \langle T_\alpha(z - z_H), z - w_H\rangle_\Gamma + \langle \lambda, w_H - z_H\rangle_\Gamma + \langle g - T_\alpha z_H, w_H - z_H\rangle_\Gamma \\ &\leq c_2^{T_\alpha} \|z - z_H\|_{H^{1/2}(\Gamma)} \|z - w_H\|_{H^{1/2}(\Gamma)} + \langle \lambda, w_H - z_H\rangle_\Gamma. \end{aligned}$$

In particular for the piecewise linear interpolation $w_H = I_H z$ we conclude, by using the interpolation error estimate,

$$\begin{aligned} c_1^{T_\alpha} \|z - z_H\|^2_{H^{1/2}(\Gamma)} &\leq c_2^{T_\alpha} \|z - z_H\|_{H^{1/2}(\Gamma)} \|z - I_H z\|_{H^{1/2}(\Gamma)} + \langle \lambda, I_H z - z_H\rangle_\Gamma \\ &\leq c_2^{T_\alpha} c_I H^{s-\frac{1}{2}} \|z - z_H\|_{H^{1/2}(\Gamma)} \|z\|_{H^s(\Gamma)} + \langle \lambda, I_H z - z_H\rangle_\Gamma. \end{aligned}$$

Let

$$z_{1,H} := I_H z_1 \in S_H^1(\Gamma), \quad z_{2,H} := I_H z_2 \in S_H^1(\Gamma)$$

be the piecewise linear interpolations of the constraints z_1 and z_2, respectively. Then, for all $w_H \in \mathcal{U}_H$ we have

$$z_{1,H}(x_i) \leq w_H(x_i) \leq z_{2,H}(x_i) \quad \text{for all nodes } x_i,$$

and therefore, for the solution $z_H \in \mathcal{U}_H$ of (3.51),

$$z_{1,H}(x) \leq z_H(x) \leq z_{2,H}(x) \quad \text{for all } x \in \Gamma.$$

Let

$$\mathcal{A}_1 := \{x \in \Gamma : z(x) = z_1(x)\}, \quad \mathcal{A}_2 := \{x \in \Gamma : z(x) = z_2(x)\}$$

be the active sets. Due to $\lambda \geq 0$ on $\mathcal{A}_1$ and $\lambda \leq 0$ on $\mathcal{A}_2$ in the sense of $H^{-1/2}(\Gamma)$, see (3.12), we conclude

$$\int_{\mathcal{A}_1} \lambda(x)[z_{1,H}(x) - z_H(x)]\, ds_x \leq 0, \quad \int_{\mathcal{A}_2} \lambda(x)[z_{2,H}(x) - z_H(x)]\, ds_x \leq 0,$$

and therefore, by using $\lambda(x) = 0$ on $\mathcal{I} := \Gamma \setminus (\mathcal{A}_1 \cup \mathcal{A}_2)$,

$$\begin{aligned} \langle \lambda, I_H z - z_H\rangle_\Gamma &= \int_{\mathcal{A}_1} \lambda(x)[I_H z(x) - z_H(x)]\, ds_x + \int_{\mathcal{A}_2} \lambda(x)[I_H z(x) - z_H(x)]\, ds_x \\ &\leq \int_{\mathcal{A}_1} \lambda(x)[I_H z(x) - z_{1,H}(x)]\, ds_x + \int_{\mathcal{A}_2} \lambda(x)[I_H z(x) - z_{2,H}(x)]\, ds_x. \end{aligned}$$

Since $\lambda(x) = 0$ on $\mathcal{I}$, it remains to consider only those boundary elements τ_ℓ which include both the active and the inactive set. By using some estimates for the piecewise linear interpolation on τ_ℓ, we can conclude

$$\langle \lambda, I_H z - z_H \rangle_\Gamma \leq c \|\lambda\|_{L_\infty(\Gamma)} H^3.$$

Hence,

$$c_1^{T_\alpha} \|z - z_H\|^2_{H^{1/2}(\Gamma)} \leq c_2^{T_\alpha} c_I H^{s-\frac{1}{2}} \|z - z_H\|_{H^{1/2}(\Gamma)} \|z\|_{H^s(\Gamma)} + c\|\lambda\|_{L_\infty(\Gamma)} H^3,$$

and the inequality (3.52) follows. The error estimate (3.53) follows from the Aubin-Nitsche trick for variational inequalities, see [65]. □

Approximate variational inequality

The error estimates (3.52) and (3.53) seem to be optimal. However, the composed boundary integral operator T_α and the right hand side g as defined in (3.30), (3.31) do not allow a direct boundary element discretization in general. Hence, instead of (3.51) we need to consider a perturbed variational inequality to find $\widetilde{z}_H \in \mathcal{U}_H$ such that

$$\langle \widetilde{T}_\alpha \widetilde{z}_H, w_H - \widetilde{z}_H \rangle_\Gamma \geq \langle \widetilde{g}, w_H - \widetilde{z}_H \rangle_\Gamma \quad \text{for all } w_H \in \mathcal{U}_H, \tag{3.54}$$

where $\widetilde{T}_\alpha$ and $\widetilde{g}$ are appropriate approximations of T_α and g, respectively. The following theorem, see [51], presents an abstract consistency result, which will later be used to analyse the boundary element approximations.

Theorem 3.2. *Let z be the unique solution of the variational inequality* (3.6) *and $\widetilde{T}_\alpha : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ be a bounded and $S^1_H(\Gamma)$-elliptic approximation of T_α satisfying*

$$\langle \widetilde{T}_\alpha z_H, z_H \rangle_\Gamma \geq c_1^{\widetilde{T}_\alpha} \|z_H\|^2_{H^{1/2}(\Gamma)} \quad \textit{for all } z_H \in S^1_H(\Gamma)$$

and

$$\|\widetilde{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \leq c_2^{\widetilde{T}_\alpha} \|z\|_{H^{1/2}(\Gamma)} \quad \textit{for all } z \in H^{1/2}(\Gamma).$$

Let $\widetilde{g} \in H^{-1/2}(\Gamma)$ be some approximation of g. For the unique solution, $\widetilde{z}_H \in \mathcal{U}_H$, of the perturbed variational inequality (3.54) *there holds the error estimate*

$$\|z - \widetilde{z}_H\|_{H^{1/2}(\Gamma)} \leq c_1 \|z - z_H\|_{H^{1/2}(\Gamma)} + c_2 \|(T_\alpha - \widetilde{T}_\alpha) z\|_{H^{-1/2}(\Gamma)} + c_3 \|g - \widetilde{g}\|_{H^{-1/2}(\Gamma)}, \tag{3.55}$$

where $z_H \in \mathcal{U}_H$ is the unique solution of the discrete variational inequality (3.51).

Proof. The unique solvability of the discrete variational inequality (3.54) follows from the $S_H^1(\Gamma)$-ellipticity of $\widetilde{T}_\alpha$. From this we further obtain

$$\begin{aligned} c_1^{\widetilde{T}_\alpha}\|z_H-\widetilde{z}_H\|^2_{H^{1/2}(\Gamma)} &\le \langle \widetilde{T}_\alpha(z_H-\widetilde{z}_H), z_H-\widetilde{z}_H\rangle_\Gamma \\ &\le \langle \widetilde{T}_\alpha z_H, z_H-\widetilde{z}_H\rangle_\Gamma + \langle \widetilde{g}-g, \widetilde{z}_H-z_H\rangle_\Gamma + \langle T_\alpha z_H, \widetilde{z}_H-z_H\rangle_\Gamma \\ &\le \left(\|(\widetilde{T}_\alpha-T_\alpha)z_H\|_{H^{-1/2}(\Gamma)} + \|g-\widetilde{g}\|_{H^{-1/2}(\Gamma)}\right)\|z_H-\widetilde{z}_H\|_{H^{1/2}(\Gamma)}. \end{aligned}$$

Therefore

$$\|z_H-\widetilde{z}_H\|_{H^{1/2}(\Gamma)} \le \frac{1}{c_1^{\widetilde{T}_\alpha}}\left(\|(\widetilde{T}_\alpha-T_\alpha)z_H\|_{H^{-1/2}(\Gamma)} + \|g-\widetilde{g}\|_{H^{-1/2}(\Gamma)}\right).$$

Moreover, by using the triangle inequality and the boundedness of T_α and $\widetilde{T}_\alpha$ we have

$$\begin{aligned} \|(\widetilde{T}_\alpha-T_\alpha)z_H\|_{H^{-1/2}(\Gamma)} &\le \|(T_\alpha-\widetilde{T}_\alpha)z\|_{H^{-1/2}(\Gamma)} + \|(\widetilde{T}_\alpha-T_\alpha)(z-z_H)\|_{H^{-1/2}(\Gamma)} \\ &\le \|(T_\alpha-\widetilde{T}_\alpha)z\|_{H^{-1/2}(\Gamma)} + (c_2^{\widetilde{T}_\alpha}+c_2^{T_\alpha})\|z-z_H\|_{H^{1/2}(\Gamma)}. \end{aligned}$$

The assertion now follows from the triangle inequality. □

3.4 Non-symmetric boundary integral formulation

Based on the mapping properties of the standard Laplace and Bi-Laplace boundary integral operators as given in the previous section, we are now able to state the mapping properties of the boundary integral operator T_α as defined in (3.30), see also the properties of T_α as introduced in (3.8). Then we discuss the Galerkin discretization of (3.29). The stability and error estimates are given with an additional condition on the mesh size.

Theorem 3.3. *The composed boundary integral operator*

$$T_\alpha = \alpha S + V^{-1}K_1 - V^{-1}V_1V^{-1}(\frac{1}{2}I+K) : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$$

is self-adjoint, bounded and $H^{1/2}(\Gamma)$-elliptic, i.e.,

$$\langle T_\alpha z, z\rangle_\Gamma \ge c_1^{T_\alpha}\|z\|^2_{H^{1/2}(\Gamma)} \quad \text{for all } z \in H^{1/2}(\Gamma).$$

Proof. The mapping properties of $T_\alpha : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ follow from the boundedness of all used boundary integral operators [31, 43, 64]. In addition, we also used the compact embedding of $H^{3/2}(\Gamma)$ in $H^{1/2}(\Gamma)$.

For the self-adjointness of T_α, we consider for $z,w \in H^{1/2}(\Gamma)$

$$\begin{aligned}\langle T_\alpha z, w\rangle_\Gamma &= \langle \alpha S z, w\rangle_\Gamma + \langle V^{-1}K_1 z, w\rangle_\Gamma - \frac{1}{2}\langle V^{-1}V_1V^{-1}z, w\rangle_\Gamma - \langle V^{-1}V_1V^{-1}Kz, w\rangle_\Gamma \\ &= \langle z, \alpha S w\rangle_\Gamma + \langle z, K_1'V^{-1}w\rangle_\Gamma - \frac{1}{2}\langle z, V^{-1}V_1V^{-1}w\rangle_\Gamma - \langle z, K'V^{-1}V_1V^{-1}w\rangle_\Gamma \\ &= \langle z, \alpha S w\rangle_\Gamma - \frac{1}{2}\langle z, V^{-1}V_1V^{-1}w\rangle_\Gamma + \langle z, [K_1'V^{-1} - K'V^{-1}V_1V^{-1}]w\rangle_\Gamma.\end{aligned}$$

By using (3.42) and (3.43) we have

$$\begin{aligned}K_1'V^{-1} - K'V^{-1}V_1V^{-1} &= K_1'V^{-1} - V^{-1}KV_1V^{-1} = V^{-1}[VK_1' - KV_1]V^{-1} \\ &= V^{-1}[K_1V - V_1K']V^{-1} = V^{-1}K_1 - V^{-1}V_1K'V^{-1} \\ &= V^{-1}K_1 - V^{-1}V_1V^{-1}K.\end{aligned}$$

Hence we get

$$\begin{aligned}\langle T_\alpha z, w\rangle_\Gamma &= \langle z, \alpha S w\rangle_\Gamma - \frac{1}{2}\langle z, V^{-1}V_1V^{-1}w\rangle_\Gamma + \langle z, [V^{-1}K_1 - V^{-1}V_1V^{-1}K]w\rangle_\Gamma \\ &= \langle z, [\alpha S + V^{-1}K_1 - V^{-1}V_1V^{-1}(\frac{1}{2}I + K)]w\rangle_\Gamma = \langle z, T_\alpha w\rangle_\Gamma,\end{aligned}$$

i.e., T_α is self-adjoint.

Moreover, for $z \in H^{1/2}(\Gamma)$, by using (3.42) and by Lemma 3.2, $\psi = V^{-1}z$, we have

$$\begin{aligned}\langle T_\alpha z, z\rangle_\Gamma &= \alpha\langle Sz, z\rangle_\Gamma + \langle V^{-1}K_1 z, z\rangle_\Gamma - \langle V^{-1}V_1V^{-1}(\frac{1}{2}I + K)z, z\rangle_\Gamma \\ &= \alpha\langle Sz, z\rangle_\Gamma + \langle K_1VV^{-1}z, V^{-1}z\rangle_\Gamma - \langle V_1(\frac{1}{2}I + K')V^{-1}z, V^{-1}z\rangle_\Gamma \\ &= \alpha\langle Sz, z\rangle_\Gamma + \langle K_1V\psi, \psi\rangle_\Gamma - \langle V_1(\frac{1}{2}I + K')\psi, \psi\rangle_\Gamma \\ &= \alpha\langle Sz, z\rangle_\Gamma + \|\widetilde{V}\psi\|^2_{L_2(\Omega)}.\end{aligned}$$

The Steklov-Poincaré operator S defines a semi-norm in $H^{1/2}(\Gamma)$. However, for $z \equiv 1$ we obtain

$$\langle T_\alpha 1, 1\rangle_\Gamma = \|\widetilde{V}\psi\|^2_{L_2(\Omega)} = \|\widetilde{V}(V^{-1}1)\|^2_{L_2(\Omega)} > 0.$$

Therefore, the operator T_α defines an equivalent norm in $H^{1/2}(\Gamma)$, the $H^{1/2}(\Gamma)$-ellipticity of T_α follows. □

In what follows we introduce computable boundary element approximations $\widetilde{T}_\alpha$ and $\widetilde{g}$ of T_α and g as defined in (3.30), (3.31), respectively. We use also an appropriate approximation

of the non-symmetric representation (3.49) for S as well, see [62].
For an arbitrary but fixed $z \in H^{1/2}(\Gamma)$, the application of $T_\alpha z$ reads

$$T_\alpha z = \alpha S z + V^{-1} K_1 z - V^{-1} V_1 V^{-1} (\frac{1}{2} I + K) z = \alpha \omega_z - q_z,$$

where $q_z, \omega_z \in H^{-1/2}(\Gamma)$ are the unique solutions of the boundary integral equations

$$V q_z = V_1 \omega_z - K_1 z, \quad V \omega_z = (\frac{1}{2} I + K) z.$$

For a Galerkin approximation of the above boundary integral equations, let

$$S_h^0(\Gamma) = span\{\varphi_k^0\}_{k=1}^N \subset H^{-1/2}(\Gamma)$$

be another boundary element space of, e.g., piecewise constant basis functions φ_k^0, which is defined with respect to a second globally quasi-uniform and shape regular boundary element mesh of mesh size h. We define $\widetilde{q}_{z,h} \in S_h^0(\Gamma)$ as the unique solution of the Galerkin formulation

$$\langle V \widetilde{q}_{z,h}, \theta_h \rangle_\Gamma = \langle V_1 \omega_{z,h} - K_1 z, \theta_h \rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma), \tag{3.56}$$

where $\omega_{z,h} \in S_h^0(\Gamma)$ solves

$$\langle V \omega_{z,h}, \theta_h \rangle_\Gamma = \langle (\frac{1}{2} I + K) z, \theta_h \rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma). \tag{3.57}$$

Hence we can define an approximation $\widetilde{T}_\alpha$ of the operator T_α by

$$\widetilde{T}_\alpha z := \alpha \omega_{z,h} - \widetilde{q}_{z,h}. \tag{3.58}$$

Lemma 3.3. *The approximate operator $\widetilde{T}_\alpha : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ as defined in* (3.58) *is bounded, i.e.,*

$$\|\widetilde{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \le c_2^{\widetilde{T}_\alpha} \|z\|_{H^{1/2}(\Gamma)} \quad \text{for all } z \in H^{1/2}(\Gamma),$$

and there holds the error estimate

$$\|T_\alpha z - \widetilde{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \le \frac{c_2^V}{c_1^V} \inf_{\theta_h \in S_h^0(\Gamma)} \|q_z - \theta_h\|_{H^{-1/2}(\Gamma)} + \frac{c_2^{V_1}}{c_1^V} \|\omega_z - \omega_{z,h}\|_{H^{-3/2}(\Gamma)} + \alpha \|\omega_z - \omega_{z,h}\|_{H^{-1/2}(\Gamma)}. \tag{3.59}$$

Proof. The boundedness of the operator $\widetilde{T}_\alpha$ follows from the mapping properties of all boundary integral operators involved. Indeed, by choosing a test function $\theta_h = \omega_{z,h}$ in (3.57), we obtain, by $H^{-1/2}(\Gamma)$-ellipticity of V and the boundedness of K,

$$c_1^V \|\omega_{z,h}\|_{H^{-1/2}(\Gamma)}^2 \le \langle V \omega_{z,h}, \omega_{z,h} \rangle_\Gamma = \langle (\frac{1}{2} I + K) z, \omega_{z,h} \rangle_\Gamma \le \|(\frac{1}{2} I + K) z\|_{H^{1/2}(\Gamma)} \|\omega_{z,h}\|_{H^{-1/2}(\Gamma)} \le c_2^K \|z\|_{H^{1/2}(\Gamma)} \|\omega_{z,h}\|_{H^{-1/2}(\Gamma)}.$$

This implies

$$\|\omega_{z,h}\|_{H^{-1/2}(\Gamma)} \leq \frac{c_2^K}{c_1^V}\|z\|_{H^{1/2}(\Gamma)}.$$

Similarly, from (3.56) we have

$$\|\widetilde{q}_{z,h}\|_{H^{-1/2}(\Gamma)} \leq \frac{c_2^{V_1}}{c_1^V}\|\omega_{z,h}\|_{H^{-1/2}(\Gamma)} + \frac{c_2^{K_1}}{c_1^V}\|z\|_{H^{1/2}(\Gamma)} \leq c\|z\|_{H^{1/2}(\Gamma)}.$$

Hence, by the triangle inequality we conclude from (3.58),

$$\|\widetilde{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \leq c_2^{\widetilde{T}_\alpha}\|z\|_{H^{1/2}(\Gamma)}.$$

Moreover, for an arbitrary chosen but fixed $z \in H^{1/2}(\Gamma)$ we have, by definition,

$$T_\alpha z = \alpha\omega_z - q_z, \quad q_z = V^{-1}[V_1\omega_z - K_1 z], \quad \omega_z = V^{-1}(\frac{1}{2}I + K)z,$$

and therefore, by using (3.58),

$$T_\alpha z - \widetilde{T}_\alpha z = \alpha(\omega_z - \omega_{z,h}) - (q_z - \widetilde{q}_{z,h}).$$

Let us further define $q_{z,h} \in S_h^0(\Gamma)$ as the unique solution of the variational problem

$$\langle V q_{z,h}, \theta_h\rangle_\Gamma = \langle V_1\omega_z - K_1 z, \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma).$$

We then obtain the perturbed Galerkin orthogonality

$$\langle V(q_{z,h} - \widetilde{q}_{z,h}), \theta_h\rangle_\Gamma = \langle V_1(\omega_z - \omega_{z,h}), \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma).$$

From this we conclude

$$\|q_{z,h} - \widetilde{q}_{z,h}\|_{H^{-1/2}(\Gamma)} \leq \frac{1}{c_1^V}\|V_1(\omega_z - \omega_{z,h})\|_{H^{1/2}(\Gamma)} \leq \frac{c_2^{V_1}}{c_1^V}\|\omega_z - \omega_{z,h}\|_{H^{-3/2}(\Gamma)}.$$

The error estimate (3.59) now follows from the triangle inequality, and by applying Cea's lemma. □

By using the approximation property of the trial space $S_h^0(\Gamma)$ and the Aubin-Nitsche trick, it results in a corollary when assuming some regularity of q_z and ω_z, respectively. For the approximation properties of the trial space $S_h^0(\Gamma)$ (and $S_H^1(\Gamma)$ hereinafter), see e.g., [64, Section 10].

Corollary 3.2. *Assume $q_z, \omega_z \in H^s_{pw}(\Gamma)$ for some $s \in [0,1]$. Then there holds the error estimate*

$$\|T_\alpha z - \widetilde{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \leq c\,h^{s+\frac{1}{2}}\left(\|q_z\|_{H^s_{pw}(\Gamma)} + \|\omega_z\|_{H^s_{pw}(\Gamma)}\right). \tag{3.60}$$

Analogously we may define a boundary element approximation of the right hand side g as defined in (3.31)

$$g = V^{-1}N_0\overline{u} + V^{-1}M_0 f - V^{-1}V_1V^{-1}N_0 f.$$

In particular, $g \in H^{-1/2}(\Gamma)$ is the unique solution of the variational problem

$$\langle Vg, \theta\rangle_\Gamma = \langle N_0\overline{u} + M_0 f, \theta\rangle_\Gamma - \langle V_1\omega_f, \theta\rangle_\Gamma \quad \text{for all } \theta \in H^{-1/2}(\Gamma),$$

where $\omega_f = V^{-1}N_0 f$ solves the variational problem

$$\langle V\omega_f, \theta\rangle_\Gamma = \langle N_0 f, \theta\rangle_\Gamma \quad \text{for all } \theta \in H^{-1/2}(\Gamma).$$

Hence we can define a boundary element approximation $\widetilde{g}_h \in S_h^0(\Gamma)$ as the unique solution of the Galerkin variational problem

$$\langle V\widetilde{g}_h, \theta_h\rangle_\Gamma = \langle N_0\overline{u} + M_0 f, \theta_h\rangle_\Gamma - \langle V_1\omega_{f,h}, \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma), \tag{3.61}$$

where $\omega_{f,h} \in S_h^0(\Gamma)$ solves the variational problem

$$\langle V\omega_{f,h}, \theta_h\rangle_\Gamma = \langle N_0 f, \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma). \tag{3.62}$$

Lemma 3.4. *Let $\widetilde{g}_h$ be the boundary element approximation as defined in* (3.61) *of the right hand side g. Then there holds the error estimate*

$$\|g - \widetilde{g}_h\|_{H^{-1/2}(\Gamma)} \le \frac{c_2^V}{c_1^V} \inf_{\theta_h \in S_h^0(\Gamma)} \|g - \theta_h\|_{H^{-1/2}(\Gamma)} + \frac{c_2^{V_1}}{c_1^V} \|\omega_f - \omega_{f,h}\|_{H^{-3/2}(\Gamma)}. \tag{3.63}$$

Proof. Let $g_h \in S_h^0(\Gamma)$ be the unique solution of the variational problem

$$\langle Vg_h, \theta_h\rangle_\Gamma = \langle N_0\overline{u} + M_0 f, \theta_h\rangle_\Gamma - \langle V_1\omega_f, \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma).$$

By applying Cea's lemma, we first obtain

$$\|g - g_h\|_{H^{-1/2}(\Gamma)} \le \frac{c_2^V}{c_1^V} \inf_{\theta_h \in S_h^0(\Gamma)} \|g - \theta_h\|_{H^{-1/2}(\Gamma)}.$$

Moreover, the perturbed Galerkin orthogonality

$$\langle V(g_h - \widetilde{g}_h), \theta_h\rangle_\Gamma = \langle V_1(\omega_{f,h} - \omega_f), \theta_h\rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma)$$

follows. From this we further conclude

$$\|g_h - \widetilde{g}_h\|_{H^{-1/2}(\Gamma)} \le \frac{1}{c_1^V} \|V_1(\omega_f - \omega_{f,h})\|_{H^{1/2}(\Gamma)} \le \frac{c_2^{V_1}}{c_1^V} \|\omega_f - \omega_{f,h}\|_{H^{-3/2}(\Gamma)}.$$

The assertion now follows from the triangle inequality. □

By using the approximation property of the trial space $S_h^0(\Gamma)$ and the Aubin-Nitsche trick, from (3.63) we can conclude an error estimate when assuming some regularity of g and ω_f, respectively.

Corollary 3.3. *Assume $g, \omega_f \in H^s_{pw}(\Gamma)$ for some $s \in [0,1]$. Then there holds the error estimate*

$$\|g - \widetilde{g}_h\|_{H^{-1/2}(\Gamma)} \le c_1\, h^{s+\frac{1}{2}} \|g\|_{H^s_{pw}(\Gamma)} + c_2\, h^{s+\frac{3}{2}} \|\omega_f\|_{H^s_{pw}(\Gamma)}. \tag{3.64}$$

Approximate variational inequality

By using the approximations (3.58) and (3.61), the Galerkin boundary element approximation of the variational inequality (3.29) now reads to find $\widetilde{z}_H \in \mathcal{U}_H$ such that

$$\langle \widetilde{T}_\alpha \widetilde{z}_H - \widetilde{g}_h, w_H - \widetilde{z}_H \rangle_\Gamma = \langle \alpha \omega_{\widetilde{z}_H,h} - \widetilde{q}_{\widetilde{z}_H,h} - \widetilde{g}_h, w_H - \widetilde{z}_H \rangle_\Gamma \ge 0 \quad \text{for all } w_H \in \mathcal{U}_H, \tag{3.65}$$

where $q_h := \alpha \omega_{\widetilde{z}_H,h} - \widetilde{q}_{\widetilde{z}_H,h} - \widetilde{g}_h \in S_h^0(\Gamma)$ is the unique solution of the Galerkin formulation

$$\langle V q_h, \theta_h \rangle_\Gamma = \alpha \langle (\frac{1}{2} I + K) \widetilde{z}_H, \theta_h \rangle_\Gamma + \langle K_1 \widetilde{z}_H - V_1 \omega_{\widetilde{z}_H,h}, \theta_h \rangle_\Gamma - \langle N_0 \overline{u} + M_0 f, \theta_h \rangle_\Gamma, \tag{3.66}$$

for all $\theta_h \in S_h^0(\Gamma)$, and $\omega_{\widetilde{z}_H,h} \in S_h^0(\Gamma)$ solves

$$\langle V \omega_{\widetilde{z}_H,h}, \theta_h \rangle_\Gamma = \langle (\frac{1}{2} I + K) \widetilde{z}_H, \theta_h \rangle_\Gamma - \langle N_0 f, \theta_h \rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma). \tag{3.67}$$

The Galerkin formulation (3.66) is equivalent to a linear system

$$V_h \underline{q} = \alpha (\frac{1}{2} M_h + K_h) \underline{\widetilde{z}} + K_{1,h} \underline{\widetilde{z}} - V_{1,h} \underline{\omega} - \underline{f}_1, \tag{3.68}$$

and (3.67) is equivalent to

$$V_h \underline{\omega} = (\frac{1}{2} M_h + K_h) \underline{\widetilde{z}} - \underline{f}_2, \tag{3.69}$$

where

$$V_h[\ell,k] = \langle V \varphi_k^0, \varphi_\ell^0 \rangle_\Gamma, \qquad K_h[\ell,i] = \langle K \varphi_i^1, \varphi_\ell^0 \rangle_\Gamma,$$
$$V_{1,h}[\ell,k] = \langle V_1 \varphi_k^0, \varphi_\ell^0 \rangle_\Gamma, \qquad K_{1,h}[\ell,i] = \langle K_1 \varphi_i^1, \varphi_\ell^0 \rangle_\Gamma,$$
$$M_h[\ell,i] = \langle \varphi_i^1, \varphi_\ell^0 \rangle_\Gamma,$$

and

$$f_1[\ell] = \langle N_0 \overline{u} + M_0 f, \varphi_\ell^0 \rangle_\Gamma, \quad f_2[\ell] = \langle N_0 f, \varphi_\ell^0 \rangle_\Gamma$$

for $k, \ell = 1, \ldots, N$ and $i = 1, \ldots, M$.

Since the Laplace single layer potential V is $H^{-1/2}(\Gamma)$-elliptic and self-adjoint, the Galerkin matrix V_h is symmetric and positive definite and therefore invertible. Hence we can solve $\underline{\omega}$ and $\underline{q}$ from (3.69) and (3.68) to obtain

$$\underline{\omega} = V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{\widetilde{z}} - V_h^{-1}\underline{f}_2$$

and

$$\underline{q} = \alpha V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{\widetilde{z}} + V_h^{-1}K_{1,h}\underline{\widetilde{z}} - V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{\widetilde{z}} + V_h^{-1}V_{1,h}V_h^{-1}\underline{f}_2 - V_h^{-1}\underline{f}_1.$$

Therefore, the matrix representation of the variational inequality (3.65) is given by a discrete variational inequality

$$(M_h^\top \underline{q}, \underline{w} - \underline{\widetilde{z}}) \geq 0 \quad \text{for all } \underline{w} \in \mathbb{R}^M \leftrightarrow w_H \in \mathcal{U}_H,$$

or equivalent to

$$(\widetilde{T}_{\alpha,H}\underline{\widetilde{z}} - \underline{\widetilde{g}}, \underline{w} - \underline{\widetilde{z}}) \geq 0 \quad \text{for all } \underline{w} \in \mathbb{R}^M \leftrightarrow w_H \in \mathcal{U}_H, \tag{3.70}$$

where

$$\widetilde{T}_{\alpha,H} := \alpha M_h^\top V_h^{-1}(\frac{1}{2}M_h + K_h) + M_h^\top V_h^{-1}K_{1,h} - M_h^\top V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h) \tag{3.71}$$

defines a non-symmetric Galerkin boundary element approximation of the self-adjoint boundary integral operator T_α as defined in (3.30). Moreover,

$$\underline{\widetilde{g}} := M_h^\top V_h^{-1}\left(\underline{f}_1 - V_{1,h}V_h^{-1}\underline{f}_2\right)$$

is the boundary element approximation of g as defined in (3.31).

Theorem 3.4 (see [52]). *The approximate Schur complement $\widetilde{T}_{\alpha,H}$ as defined in* (3.71) *is positive definite, i.e.,*

$$(\widetilde{T}_{\alpha,H}\underline{z}, \underline{z}) \geq \frac{1}{2}c_1^{T_\alpha}\|z_H\|^2_{H^{1/2}(\Gamma)} \quad \text{for all } \underline{z} \in \mathbb{R}^M \leftrightarrow z_H \in S_H^1(\Gamma),$$

if $h \leq c_0 H$ is sufficiently small.

Proof. For an arbitrary chosen but fixed $\underline{z} \in \mathbb{R}^M$ let $z_H \in S_H^1(\Gamma)$ be the associated boundary element function. Then we have

$$\begin{aligned}(\widetilde{T}_{\alpha,H}\underline{z}, \underline{z}) &= \langle \widetilde{T}_\alpha z_H, z_H\rangle_\Gamma = \langle T_\alpha z_H, z_H\rangle_\Gamma - \langle (T_\alpha - \widetilde{T}_\alpha)z_H, z_H\rangle_\Gamma \\ &\geq c_1^{T_\alpha}\|z_H\|^2_{H^{1/2}(\Gamma)} - \|(T_\alpha - \widetilde{T}_\alpha)z_H\|_{H^{-1/2}(\Gamma)}\|z_H\|_{H^{1/2}(\Gamma)}.\end{aligned}$$

Since $z_H \in S_H^1(\Gamma)$ is a continuous function, we have $z_H \in H^1(\Gamma)$. Hence we find, see [14]

$$\omega_{z_H} = V^{-1}(\frac{1}{2}I + K)z_H \in L_2(\Gamma), \quad q_{z_H} = V^{-1}[V_1\omega_{z_H} - K_1 z_H] \in L_2(\Gamma).$$

Therefore we can apply the error estimate (3.60) for $s = 0$ to obtain

$$\|T_\alpha z_H - \widetilde{T}_\alpha z_H\|_{H^{-1/2}(\Gamma)} \le c\, h^{\frac{1}{2}} \left(\|q_{z_H}\|_{L_2(\Gamma)} + \|\omega_{z_H}\|_{L_2(\Gamma)}\right) \le c_1\, h^{\frac{1}{2}} \|z_H\|_{H^1(\Gamma)}.$$

Now, by applying the inverse inequality for $S_H^1(\Gamma)$,

$$\|z_H\|_{H^1(\Gamma)} \le c_I H^{-\frac{1}{2}} \|z_H\|_{H^{1/2}(\Gamma)},$$

we obtain

$$\|(T_\alpha - \widetilde{T}_\alpha) z_H\|_{H^{-1/2}(\Gamma)} \le c_1 c_I \left(\frac{h}{H}\right)^{\frac{1}{2}} \|z_H\|_{H^{1/2}(\Gamma)}.$$

Hence we get

$$(\widetilde{T}_{\alpha,H}\underline{z}, \underline{z}) \ge \left[c_1^{T_\alpha} - c_1 c_I \left(\frac{h}{H}\right)^{\frac{1}{2}}\right] \|z_H\|^2_{H^{1/2}(\Gamma)} \ge \frac{1}{2} c_1^{T_\alpha} \|z_H\|^2_{H^{1/2}(\Gamma)},$$

if

$$c_1 c_I \left(\frac{h}{H}\right)^{\frac{1}{2}} \le \frac{1}{2} c_1^{T_\alpha}$$

is satisfied. □

The above Theorem 3.4 ensures the unique solvability of the discrete variational inequality (3.70) as well as of the perturbed variational inequality (3.65). Moreover, we can apply Theorem 3.2 to derive an error estimate for the approximate solution $\widetilde{z}_H$ of the perturbed variational inequality (3.65), as follows.

When combining the error estimate (3.55) with the error estimates (3.52), (3.60) and (3.64), we obtain the error estimate

$$\|z - \widetilde{z}_H\|_{H^{1/2}(\Gamma)} \le c_1 H^{s+\frac{1}{2}} \|z\|_{H^{s+1}(\Gamma)} + c_2 h^{s+\frac{1}{2}} \left(\|q_z\|_{H^s_{pw}(\Gamma)} + \|\omega_z\|_{H^s_{pw}(\Gamma)}\right) + c_3 h^{s+\frac{1}{2}} \|g\|_{H^s_{pw}(\Gamma)} + c_4 h^{s+\frac{3}{2}} \|\omega_f\|_{H^s_{pw}(\Gamma)}$$

when assuming $z \in H^{s+1}(\Gamma)$ and $q_z, \omega_z, g, \omega_f \in H^s_{pw}(\Gamma)$ for some $s \in [0,1]$. For $h \le c_0 H$ sufficiently small, we finally obtain the error in the energy norm

$$\|z - \widetilde{z}_H\|_{H^{1/2}(\Gamma)} \le c(z, \overline{u}, f)\, H^{s+\frac{1}{2}}. \tag{3.72}$$

Moreover, by applying the Aubin-Nitsche trick [64] we are also able to derive an error estimate in $L_2(\Gamma)$, i.e.,

$$\|z-\widetilde{z}_H\|_{L_2(\Gamma)} \leq c(z,\overline{u},f)\,H^{s+1}. \tag{3.73}$$

In the case of a non-constrained minimization problem, instead of the discrete variational inequality (3.70) we have to solve the linear system

$$\widetilde{T}_{\alpha,H}\underline{\widetilde{z}} = \underline{\widetilde{g}},$$

which can be written as

$$\begin{pmatrix} -V_{1,h} & V_h & K_{1,h} \\ V_h & & -(\frac{1}{2}M_h+K_h) \\ \alpha M_h^\top & -M_h^\top & \end{pmatrix} \begin{pmatrix} \underline{w} \\ \underline{\widetilde{q}} \\ \underline{\widetilde{z}} \end{pmatrix} = \begin{pmatrix} \underline{f}_1 - V_{1,h}V_h^{-1}\underline{f}_2 \\ \underline{0} \\ \underline{0} \end{pmatrix}. \tag{3.74}$$

Remark 3.2. *For the approximation ω_h of the flux ω of the primal Dirichlet boundary value problem, the same order of an error estimate in $H^{-1/2}(\Gamma)$-norm can be obtained as in* (3.72)*, see [64], i.e.,*

$$\|\omega-\omega_h\|_{H^{-1/2}(\Gamma)} \leq c(z,\omega,\overline{u},f)\,H^{s+\frac{1}{2}}. \tag{3.75}$$

By applying standard arguments, we get also an error estimate in $L_2(\Gamma)$,

$$\|\omega-\omega_h\|_{L_2(\Gamma)} \leq c(z,\omega,\overline{u},f)\,H^{s}. \tag{3.76}$$

Remark 3.3. *The error estimates* (3.72) *and* (3.73) *provide optimal convergence rates when approximating the control z by using piecewise linear basis functions. However, we have to assume $h \leq c_0 H$ to ensure the unique solvability of the perturbed variational inequality* (3.65)*, where the constant c_0 is in general unknown. Moreover, the matrix $\widetilde{T}_{\alpha,H}$ as given in* (3.71) *defines a non-symmetric approximation of the self-adjoint operator T_α. Hence we are interested in deriving a symmetric boundary element method which is stable without any additional constraints in the choice of the boundary element trial spaces.*

3.5 Symmetric boundary integral formulation

As in the previous section, to determine the unknown Neumann datum $q \in H^{-1/2}(\Gamma)$ of the adjoint Dirichlet boundary value problem (3.9), we used the first boundary integral equation (3.25). In what follows, we will use in addition a second boundary integral equation, the so-called hypersingular boundary integral equation for the adjoint problem to obtain an alternative representation for q. In particular, when computing the normal derivative of the representation formula (3.24), this gives

$$q(x) = (\frac{1}{2}I+K')q(x) - (D_1 z)(x) - (K_1'\omega)(x) - (N_1\overline{u})(x) - (M_1 f)(x) \quad \text{for } x \in \Gamma, \tag{3.77}$$

where we introduce the Newton potentials for $x \in \Gamma$

$$(N_1\overline{u})(x) = \lim_{\Omega \ni \widetilde{x} \to x \in \Gamma} n_x.\nabla_{\widetilde{x}} \int_\Omega U^*(\widetilde{x},y)\overline{u}(y)\,dy$$

and

$$(M_1 f)(x) = \lim_{\Omega \ni \widetilde{x} \to x \in \Gamma} n_x.\nabla_{\widetilde{x}} \int_\Omega V^*(\widetilde{x},y) f(y)\,dy.$$

Furthermore, by using (3.19), (3.28) we obtain

$$\begin{aligned} q = {} & (\tfrac{1}{2}I + K')V^{-1}V_1V^{-1}(\tfrac{1}{2}I + K)z - (\tfrac{1}{2}I + K')V^{-1}K_1 z - K_1'V^{-1}(\tfrac{1}{2}I + K)z - D_1 z \\ & + (\tfrac{1}{2}I + K')V^{-1}N_0\overline{u} - N_1\overline{u} + (\tfrac{1}{2}I + K')V^{-1}[M_0 - V_1V^{-1}N_0]f + K_1'V^{-1}N_0 f - M_1 f. \end{aligned} \tag{3.78}$$

Therefore, instead of (3.10), we have to solve the variational inequality

$$\langle T_\alpha z - g, w - z\rangle_\Gamma \geq 0, \tag{3.79}$$

where we obtain an alternative representations of T_α as defined in (3.30),

$$T_\alpha = \alpha S + D_1 + K_1'V^{-1}(\tfrac{1}{2}I + K) + (\tfrac{1}{2}I + K')V^{-1}K_1 - (\tfrac{1}{2}I + K')V^{-1}V_1V^{-1}(\tfrac{1}{2}I + K) \tag{3.80}$$

and of g as defined in (3.31),

$$g = (\tfrac{1}{2}I + K')V^{-1}N_0\overline{u} - N_1\overline{u} + (\tfrac{1}{2}I + K')V^{-1}[M_0 - V_1V^{-1}N_0]f + K_1'V^{-1}N_0 f - M_1 f. \tag{3.81}$$

Theorem 3.5. *The composed boundary integral operator T_α as defined in* (3.80) *is self-adjoint, bounded, i.e., $T_\alpha : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$, and $H^{1/2}(\Gamma)$-elliptic, i.e.,*

$$\langle T_\alpha z, z\rangle_\Gamma \geq c_1^{T_\alpha} \|z\|^2_{H^{1/2}(\Gamma)} \quad \textit{for all } z \in H^{1/2}(\Gamma).$$

Proof. While the self-adjointness of T_α in the symmetric representation (3.80) is obvious, the boundedness and ellipticity estimates follow as in the proof of Theorem 3.3. In particular, the operators T_α in the symmetric representation (3.80) and in the non-symmetric representation (3.30) coincide. Indeed, by using (3.42) and (3.43) we obtain

$$\begin{aligned}
T_\alpha &= \alpha S + D_1 + K_1' V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1 - (\frac{1}{2}I + K')V^{-1}V_1V^{-1}(\frac{1}{2}I + K) \\
&= \alpha S + D_1 + \left[K_1' - (\frac{1}{2}I + K')V^{-1}V_1\right] V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1 \\
&= \alpha S + D_1 + V^{-1}\left[VK_1' - KV_1 - \frac{1}{2}V_1\right] V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1 \\
&= \alpha S + D_1 + V^{-1}\left[K_1V - V_1K' - \frac{1}{2}V_1\right] V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1 \\
&= \alpha S + D_1 + V^{-1}K_1(\frac{1}{2}I + K) - V^{-1}V_1(\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1.
\end{aligned}$$

Due to the representation of the Laplace Steklov-Poincaré operator, see, e.g., [64],

$$S = V^{-1}(\frac{1}{2}I + K) = D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K),$$

we have by using (3.42) and (3.45),

$$\begin{aligned}
T_\alpha &= \alpha S + D_1 + V^{-1}K_1(\frac{1}{2}I + K) - V^{-1}V_1\left[V^{-1}(\frac{1}{2}I + K) - D\right] + V^{-1}(\frac{1}{2}I + K)K_1 \\
&= \alpha S + V^{-1}\left[VD_1 + V_1D + K_1(\frac{1}{2}I + K) - V_1V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K)K_1\right] \\
&= \alpha S + V^{-1}\left[K_1 - V_1V^{-1}(\frac{1}{2}I + K)\right],
\end{aligned}$$

and we finally obtain the non-symmetric representation (3.30). □

Again we conclude the unique solvability of the variational inequality (3.79). By comparing the representation of the right hand side g as in (3.31) with (3.81), it results in the following corollary.

Corollary 3.4. *For any $\overline{u}, f \in L_2(\Omega)$ there hold the equalities*

$$N_1\overline{u} = (-\frac{1}{2}I + K')V^{-1}N_0\overline{u} \tag{3.82}$$

and

$$M_1f = (-\frac{1}{2}I + K')V^{-1}M_0f - (-\frac{1}{2}I + K')V^{-1}V_1V^{-1}N_0f + K_1'V^{-1}N_0f. \tag{3.83}$$

Remark 3.4. *To obtain a symmetric discretization of the operator T_α, in what follows, we shall use the symmetric representation of the Steklov-Poincaré S as given in* (3.50).

Galerkin boundary element formulation

For the Galerkin discretization of the variational inequality (3.79) we now define appropriate approximations of the symmetric representation T_α and of the right hand side g in (3.81) as well, see [52]. First, let us recall the boundary element spaces of piecewise constant and piecewise linear basis functions

$$S_h^0(\Gamma) = span\{\varphi_k^0\}_{k=1}^N \subset H^{-1/2}(\Gamma), \quad S_H^1(\Gamma) = span\{\varphi_i^1\}_{i=1}^M \subset H^{1/2}(\Gamma),$$

which are defined with respect to some admissible boundary element meshes of mesh size h and H, respectively. For the symmetric representations of T_α, S and for $z \in H^{1/2}(\Gamma)$, the application of $T_\alpha z$ reads

$$T_\alpha z = \alpha D z + \alpha(\frac{1}{2}I + K')\omega_z + D_1 z + K_1'\omega_z - (\frac{1}{2}I + K')q_z,$$

where $q_z, \omega_z \in H^{-1/2}(\Gamma)$ are the unique solutions of the boundary integral equations

$$V q_z = V_1 \omega_z - K_1 z, \quad V\omega_z = (\frac{1}{2}I + K)z.$$

As for the non-symmetric representation of T_α we can define approximate Galerkin solutions $\omega_{z,h}, \widetilde{q}_{z,h} \in S_h^0(\Gamma)$ and then we can define the approximation

$$\widehat{T}_\alpha z := \alpha D z + \alpha(\frac{1}{2}I + K')\omega_{z,h} + D_1 z + K_1'\omega_{z,h} - (\frac{1}{2}I + K')\widetilde{q}_{z,h}. \tag{3.84}$$

Lemma 3.5. *The approximate operator* $\widehat{T}_\alpha : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ *as defined in* (3.84) *is bounded, i.e.,*

$$\|\widehat{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \le c_2^{\widehat{T}_\alpha} \|z\|_{H^{1/2}(\Gamma)} \quad \textit{for all } z \in H^{1/2}(\Gamma),$$

and there holds the error estimate

$$\|T_\alpha z - \widehat{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \le c_1 \inf_{\theta_h \in S_h^0(\Gamma)} \|q_z - \theta_h\|_{H^{-1/2}(\Gamma)} + c_2 \|\omega_z - \omega_{z,h}\|_{H^{-1/2}(\Gamma)}. \tag{3.85}$$

Proof. The proof follows as for the boundary element approximation of the non-symmetric formulation, see Lemma 3.3. □

By using the approximation property of the trial space $S_h^0(\Gamma)$ and the Aubin-Nitsche trick, we conclude an error estimate from (3.85) when assuming some regularity of q_z and ω_z.

Corollary 3.5. *Assume* $q_z, \omega_z \in H_{pw}^s(\Gamma)$ *for some* $s \in [0,1]$. *Then there holds the error estimate*

$$\|T_\alpha z - \widehat{T}_\alpha z\|_{H^{-1/2}(\Gamma)} \le c\, h^{s+\frac{1}{2}} \left(\|q_z\|_{H_{pw}^s(\Gamma)} + \|\omega_z\|_{H_{pw}^s(\Gamma)} \right). \tag{3.86}$$

Similarly, we can rewrite g which was defined in (3.81), as

$$g = K_1' \omega_f + (\frac{1}{2}I + K')q_{\overline{u},f} - N_1\overline{u} - M_1 f,$$

where $q_{\overline{u},f} \in H^{-1/2}(\Gamma)$ is the unique solution of the boundary integral equation

$$(V q_{\overline{u},f})(x) = (N_0\overline{u})(x) + (M_0 f)(x) - (V_1 \omega_f)(x) \quad \text{for } x \in \Gamma,$$

and $\omega_f \in H^{-1/2}(\Gamma)$ solves

$$(V\omega_f)(x) = (N_0 f)(x) \quad \text{for } x \in \Gamma.$$

We then can define approximate Galerkin solutions $\widehat{q}_h, \omega_{f,h} \in S_h^0(\Gamma)$, and therefore, we can introduce the approximation

$$\widehat{g} := K_1' \omega_{f,h} + (\frac{1}{2}I + K')\widehat{q}_h - N_1\overline{u} - M_1 f. \tag{3.87}$$

As in (3.64) we obtain the error estimate

$$\|g - \widehat{g}\|_{H^{-1/2}(\Gamma)} \leq c_1 h^{s+\frac{1}{2}} \|q_{\overline{u},f}\|_{H^s_{pw}(\Gamma)} + c_2 h^{s+\frac{3}{2}} \|\omega_f\|_{H^s_{pw}(\Gamma)} \tag{3.88}$$

when assuming $q_{\overline{u},f}, \omega_f \in H^s_{pw}(\Gamma)$ for some $s \in [0,1]$.

Approximate variational inequality

By using the approximations (3.84) and (3.87) we now have to solve the approximate variational inequality to find $\widehat{z} \in \mathcal{U}_{ad}$ such that

$$\langle \widehat{T}_\alpha \widehat{z} - \widehat{g}, w - \widehat{z} \rangle_\Gamma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{3.89}$$

which corresponds to a discrete version

$$(\widehat{T}_{\alpha,H}\underline{\widehat{z}} - \underline{\widehat{g}}, \underline{w} - \underline{\widehat{z}}) \geq 0 \quad \text{for all } \underline{w} \in \mathbb{R}^M \leftrightarrow w_H \in \mathcal{U}_H. \tag{3.90}$$

Here,

$$\begin{aligned} \widehat{T}_{\alpha,H} := \alpha S_H + D_{1,H} - (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h) \\ + K_{1,h}^\top V_h^{-1}(\frac{1}{2}M_h + K_h) + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}K_{1,h} \end{aligned} \tag{3.91}$$

and

$$S_H = D_H + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\frac{1}{2}M_h + K_h) \tag{3.92}$$

are the symmetric Galerkin boundary element approximations of the self-adjoint operators T_α and S, respectively. Moreover,

$$\underline{\widehat{g}} = K_{1,h}^\top V_h^{-1} \underline{f}_2 + (\frac{1}{2}M_h^\top + K_h^\top) V_h^{-1} [\underline{f}_1 - V_{1,h} V_h^{-1} \underline{f}_2] - \underline{f}_3 \tag{3.93}$$

is the related boundary element approximation of g as defined in (3.81). Note that, in addition to those entries of the linear system (3.74) we use

$$D_H[i,j] = \langle D\varphi_j^1, \varphi_i^1 \rangle_\Gamma, \quad D_{1,H}[j,i] = \langle D_1 \varphi_i^1, \varphi_j^1 \rangle_\Gamma, \quad f_3[j] = \langle N_1 \overline{u} + M_1 f, \varphi_j^1 \rangle_\Gamma,$$

for $i,j = 1,...,M$.

The computation of the Galerkin matrix $D_{1,H}$ of the Bi-Laplace hypersingular boundary integral operator D_1 can be reduced to the computation of the Galerkin matrices of the Bi-Laplace and Laplace singular layer potentials V_1 and V. In particular, we can derive the following lemma in the two dimensional case.

Lemma 3.6. *Let ∂_τ denote the derivative with respect to the arc length on Γ. Let n denote the exterior normal vector. Then*

$$\langle D_1 z, w \rangle_\Gamma = -\langle V_1(\partial_\tau z), \partial_\tau w \rangle_\Gamma + \sum_{i=1}^{2} \langle V(z n_i), w n_i \rangle_\Gamma \quad \textit{for all } z, w \in H^{1/2}(\Gamma). \tag{3.94}$$

Proof. We adopt the proof from the paper by Costabel [15, Theorem 6.1].
Let $x,y \in \Gamma$, $x \neq y$. Let n_x, n_y and τ_x, τ_y denote the normal and tangent vectors at x and y, respectively. Here τ can be obtained from n by a counterclockwise rotation by a right angle. For any 2×2 matrix M with trace $\mathrm{tr}(M)$ we have

$$n_x^\top M n_y + \tau_y^\top M \tau_x = \mathrm{tr}(M)(n_x n_y).$$

Taking for M the second derivatives of the Bi-Laplacian fundamental solution $V^*(x,y)$,

$$M = \begin{pmatrix} \frac{\partial^2}{\partial x_1 \partial y_1} V^*(x,y) & \frac{\partial^2}{\partial x_1 \partial y_1} V^*(x,y) \\ \frac{\partial^2}{\partial x_1 \partial y_1} V^*(x,y) & \frac{\partial^2}{\partial x_1 \partial y_1} V^*(x,y) \end{pmatrix},$$

we obtain

$$\begin{aligned} \partial_{n_x} \partial_{n_y} V^*(x,y) &= -\partial_{\tau_x} \partial_{\tau_y} V^*(x,y) + \mathrm{tr}(M)(n_x n_y) \\ &= -\partial_{\tau_x} \partial_{\tau_y} V^*(x,y) - U^*(x,y)(n_x n_y). \end{aligned} \tag{3.95}$$

We now multiply (3.95) by $w(x)z(y)$, integrate over $\Gamma \times \Gamma$ and observe that on Γ we may use integration by parts for ∂_τ,

$$\langle z, \partial_\tau w \rangle_\Gamma = -\langle \partial_\tau z, w \rangle_\Gamma \quad \text{for all } z, w \in H^{1/2}(\Gamma),$$

and then the assertion follows. □

Remark 3.5. *To implement the right hand side $\underline{f}_3$ we may approximate the Newton potentials $N_1\overline{u}$ and $M_1 f$ by using the representation formulae* (3.82), (3.83) *as we did for the right hand side g in the non-symmetric formulation. In particular, we can define*

$$\widehat{\underline{f}}_3 = (-\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}\underline{f}_1 - (-\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}V_{1,h}V_h^{-1}\underline{f}_2 + K_{1,h}^\top V_h^{-1}\underline{f}_2,$$

i.e.,

$$\widehat{\underline{g}} \approx M_h^\top V_h^{-1}\left(\underline{f}_1 - V_{1,h}V_h^{-1}\underline{f}_2\right) = \widetilde{\underline{g}}.$$

Lemma 3.7. *The symmetric matrix*

$$\widehat{T}_H := \widehat{T}_{\alpha,H} - \alpha S_H - D_{1,H} = K_{1,h}^\top V_h^{-1}(\frac{1}{2}M_h + K_h) + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}K_{1,h}$$
$$- (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h)$$

is positive semi-definite, i.e.,

$$(\widehat{T}_H\underline{z}, \underline{z}) \geq 0 \quad \textit{for all } \underline{z} \in \mathbb{R}^M.$$

Proof. We consider the generalized eigenvalue problem

$$\widehat{T}_H\underline{z} = \lambda\left[\widetilde{S}_H + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\frac{1}{2}M_h + K_h)\right]\underline{z}, \tag{3.96}$$

where the stabilized discrete Steklov-Poincaré operator

$$\widetilde{S}_H = D_H + \underline{a}\,\underline{a}^\top + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\frac{1}{2}M_h + K_h)$$

is symmetric and positive definite. Note that the vector $\underline{a}$ is given by

$$a[i] = \int_\Gamma \varphi_i^1(x)\,ds_x \quad \text{for } i = 1, \ldots, M.$$

Since the eigenvalue problem (3.96) can be written as

$$\left((\tfrac{1}{2}M_h^\top + K_h^\top)V_h^{-1} \quad I\right)\begin{pmatrix} -V_{1,h} & K_{1,h} \\ K_{1,h}^\top & \end{pmatrix}\begin{pmatrix} V_h^{-1}(\tfrac{1}{2}M_h + K_h) \\ I \end{pmatrix}\underline{z}$$
$$= \lambda\left((\tfrac{1}{2}M_h^\top + K_h^\top)V_h^{-1} \quad I\right)\begin{pmatrix} V_h & \\ & \widetilde{S}_H \end{pmatrix}\begin{pmatrix} V_h^{-1}(\tfrac{1}{2}M_h + K_h) \\ I \end{pmatrix}\underline{z},$$

it is sufficient to consider the generalized eigenvalue problem

$$\begin{pmatrix} -V_{1,h} & K_{1,h} \\ K_{1,h}^\top & \end{pmatrix}\begin{pmatrix} \underline{\theta} \\ \underline{z} \end{pmatrix} = \lambda\begin{pmatrix} V_h\underline{\theta} \\ \widetilde{S}_H\underline{z} \end{pmatrix}, \tag{3.97}$$

where

$$\underline{\theta} = V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{z}.$$

From (3.97) we conclude

$$\begin{aligned}(K_{1,h}\underline{z},\underline{\theta}) - (V_{1,h}\underline{\theta},\underline{\theta}) &= \lambda(V_h\underline{\theta},\underline{\theta}),\\ (K_{1,h}^\top\underline{\theta},\underline{z}) &= \lambda(\widetilde{S}_H\underline{z},\underline{z}),\end{aligned}$$

and by taking the difference we obtain

$$(V_{1,h}\underline{\theta},\underline{\theta}) = \lambda\left[(\widetilde{S}_H\underline{z},\underline{z}) - (V_h\underline{\theta},\underline{\theta})\right] = \lambda\left((D_H + \underline{a}\,\underline{a}^\top)\underline{z},\underline{z}\right).$$

Since the Galerkin matrix $V_{1,h}$ is positive semi-definite, it follows that $\lambda \geq 0$, which implies the assertion. □

As a corollary of Lemma 3.7, we find the positive definiteness of the symmetric Schur complement matrix $\widehat{T}_{\alpha,H}$ as defined in (3.91).

Corollary 3.6. *The Schur complement matrix $\widehat{T}_{\alpha,H}$ as defined in* (3.91) *is positive definite, i.e.,*

$$(\widehat{T}_{\alpha,H}\underline{z},\underline{z}) \geq \alpha(S_H\underline{z},\underline{z}) + (D_{1,H}\underline{z},\underline{z}) \geq \langle(\alpha D + D_1)z_H, z_H\rangle_\Gamma \geq c\|z_H\|^2_{H^{1/2}(\Gamma)}$$

for all $\underline{z} \in \mathbb{R}^M \leftrightarrow z_H \in S_H^1(\Gamma)$, since $\alpha D + D_1$ implies an equivalent norm in $H^{1/2}(\Gamma)$.

Remark 3.6. *The symmetric Schur complement matrix $\widehat{T}_{\alpha,H}$ is positive definite for any choice of conformal boundary element spaces $S_H^1(\Gamma) \subset H^{1/2}(\Gamma)$ and $S_h^0(\Gamma) \subset H^{-1/2}(\Gamma)$. In particular we may use the same boundary element mesh with mesh size $h = H$. From a theoretical point of view, this is not possible in general when using the non-symmetric approximation $\widetilde{T}_{\alpha,H}$.*

Hence we can ensure the unique solvability of the discrete variational inequality (3.90). As in (3.55), when combining the approximation property of the ansatz space $S_H^1(\Gamma)$ with the error estimates (3.86) and (3.88), we can derive an error estimate for the approximate solution $\widehat{z}_H$ of the variational inequality (3.89), see also [52].

Theorem 3.6. *Let z and $\widehat{z}_H$ be the unique solutions of the variational inequalities* (3.79) *and* (3.90)*, respectively. Then there holds the error estimate*

$$\begin{aligned}\|z - \widehat{z}_H\|_{H^{1/2}(\Gamma)} \leq c_1 H^{s+\frac{1}{2}}\|z\|_{H^{s+1}(\Gamma)} + c_2 h^{s+\frac{1}{2}}\left(\|q_z\|_{H^s_{pw}(\Gamma)} + \|\omega_z\|_{H^s_{pw}(\Gamma)}\right)\\ + c_3 h^{s+\frac{1}{2}}\|q_{\bar{u},f}\|_{H^s_{pw}(\Gamma)} + c_4 h^{s+\frac{3}{2}}\|\omega_f\|_{H^s_{pw}(\Gamma)} \quad (3.98)\end{aligned}$$

when assuming $z \in H^{s+1}(\Gamma)$ *and* $q_z, \omega_z, q_{\overline{u},f}, \omega_f \in H^s_{pw}(\Gamma)$ *for some* $s \in [0,1]$. *In particular, for* $h = H$ *we have the error estimate*

$$\|z - \widehat{z}_H\|_{H^{1/2}(\Gamma)} \leq c(z,\overline{u},f)\, H^{s+\frac{1}{2}}.$$

Moreover, we are also able to derive the error estimate in $L_2(\Gamma)$*, i.e.,*

$$\|z - \widehat{z}_H\|_{L_2(\Gamma)} \leq c(z,\overline{u},f)\, H^{s+1}, \tag{3.99}$$

when applying the Aubin-Nitsche trick.

In the case of a non-constrained minimization problem, instead of the discrete variational inequality (3.90) we have to solve the linear system

$$\widehat{T}_{\alpha,H}\underline{\widehat{z}} = \underline{\widehat{g}},$$

which can be written as

$$\begin{pmatrix} -V_{1,h} & V_h & K_{1,h} \\ V_h & & -(\frac{1}{2}M_h + K_h) \\ K_{1,h}^\top & -(\frac{1}{2}M_h^\top + K_h^\top) & \alpha S_H + D_{1,H} \end{pmatrix} \begin{pmatrix} \underline{\omega} \\ \underline{q} \\ \underline{\widehat{z}} \end{pmatrix} = \begin{pmatrix} \underline{f}_1 \\ -\underline{f}_2 \\ -\underline{f}_3 \end{pmatrix}. \tag{3.100}$$

Moreover, by using $\underline{w} = \alpha V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{\widehat{z}}$ as given in (3.74), we obtain the linear system

$$\begin{pmatrix} -V_{1,h} & V_h & K_{1,h} & \\ V_h & & -(\frac{1}{2}M_h + K_h) & \\ K_{1,h}^\top & -(\frac{1}{2}M_h^\top + K_h^\top) & \alpha D_H + D_{1,H} & (\frac{1}{2}M_h^\top + K_h^\top) \\ & & (\frac{1}{2}M_h + K_h) & -\frac{1}{\alpha}V_h \end{pmatrix} \begin{pmatrix} \underline{\omega} \\ \underline{q} \\ \underline{\widehat{z}} \\ \underline{w} \end{pmatrix} = \begin{pmatrix} \underline{f}_1 \\ -\underline{f}_2 \\ -\underline{f}_3 \\ \underline{0} \end{pmatrix}. \tag{3.101}$$

3.6 Semi-smooth Newton methods

In this section, we study semi-smooth Newton methods to solve the discrete variational inequalities (3.70), (3.90). For the ease of presentation we consider the symmetric formulation only, i.e., we have to seek $\underline{z} \in \mathbb{R}^M \leftrightarrow z_H \in \mathcal{U}_H$ such that

$$(\widehat{T}_{\alpha,H}\,\underline{z}, \underline{w} - \underline{z}) \geq (\underline{\widehat{g}}, \underline{w} - \underline{z}) \quad \text{for all } \underline{w} \in \mathbb{R}^M \leftrightarrow w_H \in \mathcal{U}_H, \tag{3.102}$$

where we use the Galerkin boundary element approximations of the operator T_α and the right hand side g as in (3.91), (3.93). For more details on semi-smooth Newton methods, see, e.g., [24, 32, 33, 35, 61].

Semi-smooth Newton methods and regularization

By setting $\underline{\lambda} := \widehat{T}_{\alpha,H}\,\underline{z} - \underline{\widehat{g}}$ we arrive at

$$\begin{cases} \langle \widehat{T}_\alpha z_H, w_H\rangle_\Gamma - \langle \lambda_H, w_H\rangle_\Gamma = \langle \widehat{g}, w_H\rangle_\Gamma \quad \text{for all } w_H \in S^1_H(\Gamma), \\ \langle \lambda_H, w_H - z_H\rangle_\Gamma \geq 0 \quad \text{for all } w_H \in \mathcal{U}_H. \end{cases} \tag{3.103}$$

Semi-smooth Newton algorithm with regularization

(i). Choose $\overline{\lambda}$, $\sigma > 0$, z^0_H and set $k = 0$.

(ii). Set

$$\mathcal{A}^1_{k+1} = \{i \in \mathbb{N} : 1 \leq i \leq M,\, (\overline{\lambda} + \sigma(z^k_H - z_1))(x_i) < 0\},$$
$$\mathcal{A}^2_{k+1} = \{i \in \mathbb{N} : 1 \leq i \leq M,\, (\overline{\lambda} + \sigma(z^k_H - z_2))(x_i) > 0\}.$$

(iii). If $k \geq 1$, $\mathcal{A}^1_{k+1} = \mathcal{A}^1_k$ and $\mathcal{A}^2_{k+1} = \mathcal{A}^2_k$ stop, else

(iv). Solve for $z^{k+1}_H \in S^1_H(\Gamma)$:

$$\langle \widehat{T}_\alpha z^{k+1}_H, w_H\rangle_\Gamma + \langle (\overline{\lambda} + \sigma(z^{k+1}_H - z_2))\chi_{\mathcal{A}^2_{k+1}}, w_H\rangle_\Gamma + \langle (\overline{\lambda} + \sigma(z^{k+1}_H - z_1))\chi_{\mathcal{A}^1_{k+1}}, w_H\rangle_\Gamma = \langle \widehat{g}, w_H\rangle_\Gamma \tag{3.104}$$

for all $w_H \in S^1_H(\Gamma)$. Set $k := k+1$ and go to Step (ii).

Note that in step (iv) we obtain the associated linear system of (3.104)

$$\widehat{T}_{\alpha,H}\underline{z}^{k+1} + \sigma(M^1_H + M^2_H)\underline{z}^{k+1} = \underline{\widehat{g}} + \underline{f}_0 \tag{3.105}$$

where

$$M^1_H[j,i] = \langle \varphi^1_i \chi_{\mathcal{A}^1_{k+1}}, \varphi^1_j\rangle_\Gamma, \quad M^2_H[j,i] = \langle \varphi^1_i \chi_{\mathcal{A}^2_{k+1}}, \varphi^1_j\rangle_\Gamma \quad \text{for } i,j = 1,\ldots,M,$$

and

$$f_0[j] = \langle (\sigma z_1 - \overline{\lambda})\chi_{\mathcal{A}^1_{k+1}}, \varphi^1_j\rangle_\Gamma + \langle (\sigma z_2 - \overline{\lambda})\chi_{\mathcal{A}^2_{k+1}}, \varphi^1_j\rangle_\Gamma \quad \text{for } j = 1,\ldots,M.$$

Remark 3.7. *The mass matrices M^1_H and M^2_H are symmetric and positive semi-definite. Hence the conjugate gradient method can be applied to solve the linear system* (3.105).

3.7 Numerical experiments

We present in this section some numerical results for the Dirichlet boundary control problems in two-dimension $d = 2$. We test some numerical examples as given in the papers [11, 19, 42]. For the boundary element discretization we introduce a uniform triangulation of the boundary $\Gamma = \partial\Omega$ on several levels L by 2^{L+2} nodes. The boundary element discretization is done by using the trial space $S_h^0(\Gamma)$ of piecewise constant basis functions and $S_H^1(\Gamma)$ of piecewise linear and continuous functions. We use the same boundary element mesh in the symmetric formulation to approximate the control z by a piecewise linear approximation, and piecewise constant approximations for the fluxes ω and q. In the case of the non-symmetric formulation, we consider one additional level of refinement to define the trial space $S_h^0(\Gamma)$, i.e., $h/H = 1/2$. Note that in this case we can not ensure the $S_H^1(\Gamma)$-ellipticity of the non-symmetric boundary element approximation. However, the numerical examples show stability. It is not stable if we use the same mesh as in the symmetric formulation.

Since the analytic solutions are unknown in these examples, we use the approximate solutions on the finest level ($L = 9$) as reference solutions. For the following examples, we use the norm as defined in (2.7) to compute the errors in $H^{1/2}(\Gamma)$ norm.

Numerical example 1
In our first numerical example we consider the Dirichlet boundary control problem (3.1) for circle $\Omega = B_{0.4}(0)$ with regular data as given in [19]. We set $\alpha = 1$,

$$\begin{aligned} u(r,\phi) &= \frac{125}{8} r^3 \max(0, \cos^3\phi), \\ \overline{u}(r,\phi) &= \frac{25}{8}(35r^2\cos^2\phi + 30r^2 - 12r)\cos\phi + u(r,\phi) \quad \text{and} \\ f(r,\phi) &= -\frac{375}{4} r \max(0, \cos\phi). \end{aligned}$$

For a $L_2(\Gamma)$-control, i.e., instead of the Steklov-Poincaré operator S we choose an identity operator in (3.1), it is easy to check that $z(0.4,\phi) = u|_\Gamma = \max(0,\cos^3\phi)$ is the solution of the minimization problem where $[z_1, z_2] = [0, 1]$ and the associated adjoint variable is given by $p(r,\phi) = \frac{25}{8} r^3 (5r - 2)\cos^3\phi$.

We present the errors in the $L_2(\Gamma)$ norm of the boundary element approximations for the non-constrained minimization problem and the estimated order of convergence (eoc) of the non-symmetric formulation and of the symmmetric formulation in Table 3.1.

In this example, the data are smooth. Hence we can expect an optimal order of convergence, i.e., second order convergence for the control z, and linear convergence for the flux ω, see the error estimates (3.73), (3.76) for the non-symmetric boundary element approximation and the error estimate (3.99) for the symmetric boundary element approximation ($s = 1$).

L	Non-symmetric BEM (3.74)				Symmetric BEM (3.100)			
	$\|\widetilde{z}_{h_L} - \widetilde{z}_{h_9}\|_{L_2(\Gamma)}$		$\|\omega_{h_L} - \omega_{h_{10}}\|_{L_2(\Gamma)}$		$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$		$\|\omega_{h_L} - \omega_{h_9}\|_{L_2(\Gamma)}$	
	error	eoc	error	eoc	error	eoc	error	eoc
2	3.0938e-3	-	4.2361e-1	-	3.4359e-3	-	3.9355e-1	-
3	7.1975e-4	2.104	2.0095e-1	1.076	8.1293e-4	2.079	1.9543e-1	1.009
4	1.7553e-4	2.036	9.8235e-2	1.032	2.0464e-4	1.990	9.7464e-2	1.004
5	4.3428e-5	2.015	4.8796e-2	1.009	5.4279e-5	1.915	4.8632e-2	1.003
6	1.0834e-5	2.003	2.4324e-2	1.004	1.5316e-5	1.825	2.4169e-2	1.009
7	2.7031e-6	2.003	1.2085e-2	1.009	4.1463e-6	1.889	1.1793e-2	1.035
8	6.5553e-7	2.044	5.8965e-3	1.035	1.1821e-6	1.810	5.2738e-3	1.161
expected		2.000		1.000		2.000		1.000

Table 3.1: Comparison of non-symmetric and symmetric BEM.

For the box-constrained minimization problem we use semi-smooth Newton method with regularization to solve the variational inequality. We present here the symmetric formulation only. The obtained results are given in Table 3.2 where $[z_1, z_2] = [0, 1]$. The data in the semi-smooth Newton algorithm are chosen as

$$\overline{\lambda} = 0, \quad \sigma = 10^4, \quad z^0 = 0. \tag{3.106}$$

With these data, the algorithm stops after less than 20 steps, see the last column in Table 3.2. Note that at level $L = 9$ to compute the reference solutions, we need $k = 17$ iterations.

L	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{H^{1/2}(\Gamma)}$	eoc	$\|\omega_{h_L} - \omega_{h_9}\|_{L_2(\Gamma)}$	eoc	#it(k)
2	8.4004e-3	-	6.6399e-2	-	0.3970350	-	10
3	1.5959e-3	2.396	2.0421e-2	1.701	0.1960640	1.018	12
4	3.4967e-4	2.190	7.7228e-3	1.403	0.0982184	0.997	13
5	8.0322e-5	2.122	2.8896e-3	1.418	0.0496215	0.985	16
6	1.6539e-5	2.279	7.9336e-4	1.865	0.0248726	0.996	14
7	4.9567e-6	1.738	3.2703e-4	1.279	0.0122548	1.021	15
8	1.9666e-6	1.334	1.4044e-4	1.219	0.0054306	1.174	15
expected		2.000		1.500		1.000	

Table 3.2: The results of semi-smooth Newton algorithm of the symmetric formulation.

Note that the parameter σ plays the role of a penalty parameter and it should be chosen large enough. As stated in [35], for some choice of σ, the semi-smooth Newton method may lead to cycling of the iterates unless the initialization is already close to the solution. For $\sigma = 1$, the method converges for all initializations.

Figure 3.1 shows the optimal solutions of the unconstrained (left) and of the constrained (right) problems. In Figure 3.2 we also plot the optimal states of the Dirichlet boundary control problem when using the hypersingular boundary integral operator D to realize an equivalent norm in $H^{1/2}(\Gamma)$ and when using $L_2(\Gamma)$ setting where $[z_1, z_2] = [0, 1]$, see [19].

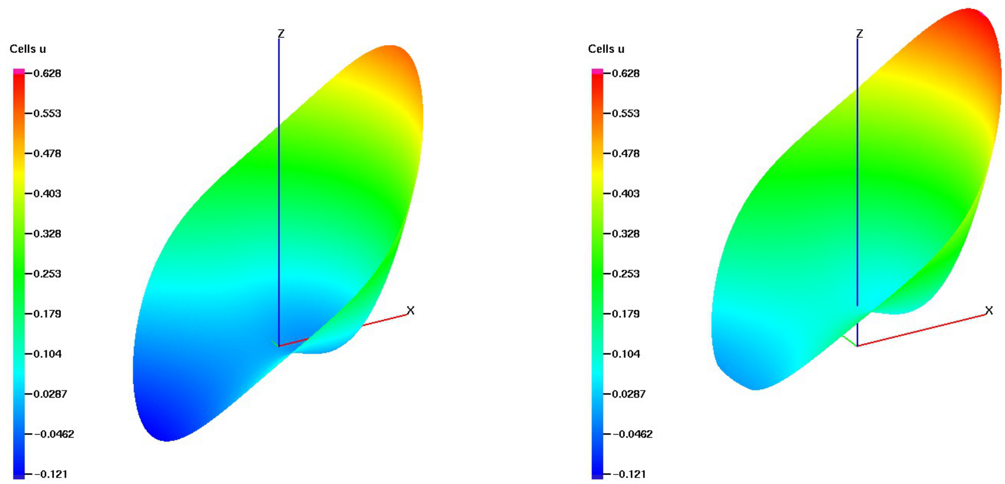

Figure 3.1: Comparison of the unconstrained (left) and of the constrained (right) optimal solutions.

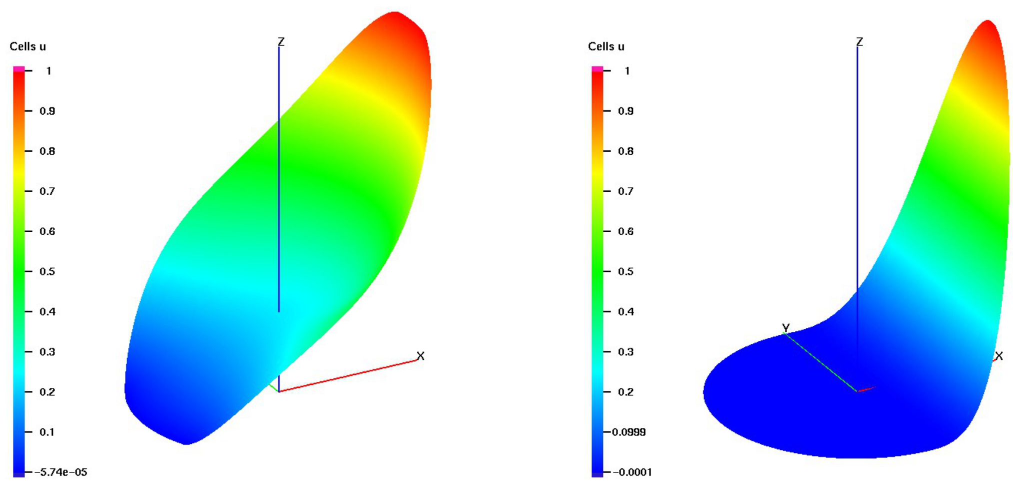

Figure 3.2: Optimal solution u_h when using the operator D and using L_2 setting.

Numerical example 2
We now consider the example as in [11], see also [52] with less regularity on the data for the domain $\Omega = (0, \frac{1}{2})^2 \subset \mathbb{R}^2$. The data are chosen as

$$\overline{u}(x) = (x_1^2 + x_2^2)^{-\frac{1}{3}}, \quad f(x) = 0, \quad \alpha = 1.$$

For these data, we have $\overline{u} \in H^s(\Omega)$ for $s < \frac{2}{3}$ which implies $p \in H^{2+s}(\Omega)$, and $\frac{\partial}{\partial n} p \in H^{1/2+s}(\Gamma)$. Hence, for the non-constrained problem we have $z \in H^{3/2+s}(\Gamma)$. The obtained results without control constraints are given in Table 3.3 and Table 3.4 which are in reasonable agreement with the theoretical results. For comparison, we also give the error of the related finite element solution, see [51]. From the numerical results we conclude that all three different approaches behave almost similar.

L	Non-symmetric BEM		Symmetric BEM		FEM	
	$\|\widetilde{z}_{h_L} - \widetilde{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|z_{h_L} - z_{h_9}\|_{L_2(\Gamma)}$	eoc
2	5.9100e-4	-	7.6323e-3	-	1.23e-3	-
3	1.6410e-4	1.848	1.8559e-3	2.040	3.47e-4	1.83
4	4.9258e-5	1.736	4.3695e-4	2.086	9.48e-5	1.87
5	1.4683e-5	1.746	1.0229e-4	2.095	2.57e-5	1.88
6	4.2760e-6	1.780	2.4016e-5	2.091	6.96e-6	1.88
7	1.2134e-6	1.817	5.4261e-6	2.146	1.87e-6	1.89
8	3.3324e-7	1.864	9.7897e-7	2.471	4.54e-7	2.04

Table 3.3: Comparison of BEM/FEM errors of the Dirichlet control.

L	Non-symmetric BEM				Symmetric BEM			
	$\|\widetilde{z}_{h_L} - \widetilde{z}_{h_9}\|_{H^{1/2}(\Gamma)}$		$\|\omega_{h_L} - \omega_{h_{10}}\|_{L_2(\Gamma)}$		$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{H^{1/2}(\Gamma)}$		$\|\omega_{h_L} - \omega_{h_9}\|_{L_2(\Gamma)}$	
	error	eoc	error	eoc	error	eoc	error	eoc
2	1.0219e-2	-	5.3718e-2	-	3.1105e-2	-	3.0001e-2	-
3	4.0384e-3	1.339	2.4044e-2	1.159	1.0776e-2	1.529	1.8082e-2	0.730
4	1.6773e-3	1.268	1.2363e-2	0.959	4.1282e-3	1.384	1.1066e-2	0.708
5	7.0266e-4	1.255	7.4291e-3	0.735	1.6163e-3	1.353	7.1354e-3	0.633
6	2.9118e-4	1.271	4.7058e-3	0.659	6.3445e-4	1.349	4.5821e-3	0.639
7	1.1788e-4	1.305	2.9591e-3	0.669	2.4108e-4	1.396	2.8209e-3	0.699
8	4.5061e-5	1.387	1.7928e-3	0.723	8.1265e-5	1.569	1.4952e-3	0.916

Table 3.4: Comparison of non-symmetric and symmetric BEM.

In Table 3.5 we also present numerical results for the constraint $z \le 2.23$. Then, in Figure 3.3 we give a comparison of the unconstrained and constrained solutions.

L	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{H^{1/2}(\Gamma)}$	eoc	$\|\omega_{h_L} - \omega_{h_9}\|_{L_2(\Gamma)}$	eoc	#it(k)
2	1.0951e-2	-	4.0474e-2	-	5.1150e-2	-	5
3	2.5157e-3	2.122	1.3748e-2	1.558	3.2851e-2	0.639	8
4	3.4465e-4	2.868	3.4424e-3	1.998	2.2249e-2	0.562	11
5	1.4260e-4	1.273	1.6853e-3	1.031	1.0105e-2	1.138	11
6	3.0029e-5	2.247	5.0309e-4	1.744	5.8395e-3	0.791	13
7	6.3171e-6	2.249	1.5802e-4	1.671	2.5087e-3	1.219	14
8	1.1518e-6	2.455	7.4408e-5	1.087	1.2581e-3	0.996	12

Table 3.5: The results of semi-smooth Newton algorithm of the symmetric formulation.

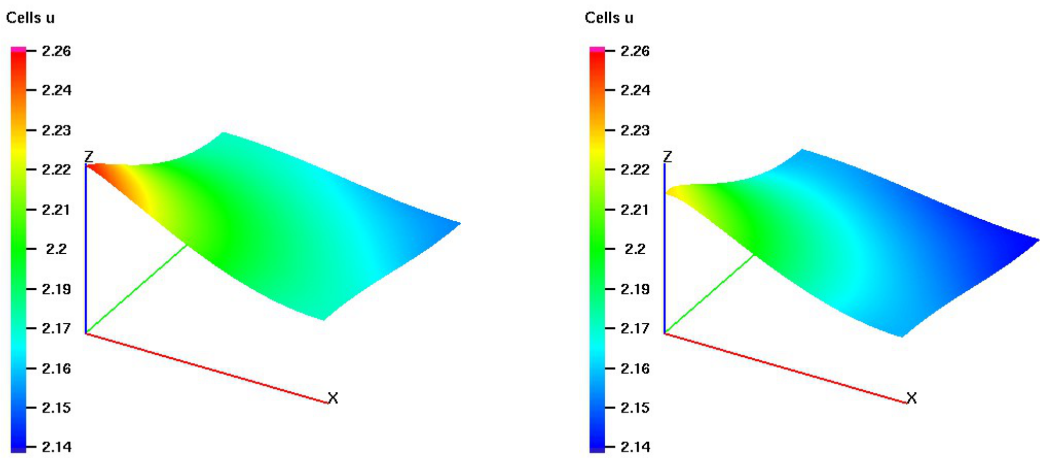

Figure 3.3: Comparison of unconstrained (left) and constrained (right) optimal solutions.

Instead of the Steklov-Poincaré operator S, one may use the so-called hypersingular boundary integral operator D to realize an equivalent norm in $H^{1/2}(\Gamma)$ as in [52]. The use of the hypersingular boundary integral operator D does not require an inversion as in (3.49), (3.50). However, it may result in a lower regularity of the control z, and therefore in a lower order of convergence. For comparison we present in Table 3.6 the numerical results for both cases and the case when considering the control in $L_2(\Gamma)$ with the same parameter $\alpha = 1$. Note, in the $L_2(\Gamma)$ control, the optimality condition reads

$$z = P_{\mathcal{U}}\xi, \quad \alpha\xi - \frac{\partial p}{\partial n} = 0, \tag{3.107}$$

where $P_{\mathcal{U}}$ denotes the pointwise projection onto $\mathcal{U}$. This approach also results in a lower regularity of the control z. In particular, for the data in example 2, we have $z \in H^{2/3}(\Gamma)$ only, see [11, 42]. Note that we can prove $z \in H^{3/2}(\Gamma)$ when considering the control in $H^{1/2}(\Gamma)$, see Proposition 3.1. Moreover, from the optimality conditions (3.107), we conclude that z is zero in all corner points due to the zero Dirichlet boundary condition of the adjoint state p. This behaviour is independent of the target function $\overline{u}$. For illustration, we plot in Figure 3.4 the states u for the $H^{1/2}(\Gamma)$ setting when using the operator D and for the $L_2(\Gamma)$ setting (without control constraint).

L	Using the operator S		Using the operator D		L_2 setting, see [42]	
	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma)}$	eoc	$\|z_{h_L} - z_{h_9}\|_{L_2(\Gamma)}$	eoc
2	7.6323e-3	-	7.7726e-3	-	4.2246e-2	-
3	1.8559e-3	2.040	1.9498e-3	1.995	2.1492e-2	0.975
4	4.3695e-4	2.086	4.8349e-4	2.012	1.1664e-2	0.882
5	1.0229e-4	2.095	1.2745e-4	1.923	6.4101e-3	0.864
6	2.4016e-5	2.091	3.8231e-5	1.737	3.5152e-3	0.867
7	5.4261e-6	2.146	1.3206e-5	1.533	1.8655e-3	0.914
8	9.7897e-7	2.471	4.6051e-6	1.520	8.9452e-4	1.060

Table 3.6: BEM for Dirichlet boundary control problems in $H^{1/2}(\Gamma)$ and $L_2(\Gamma)$.

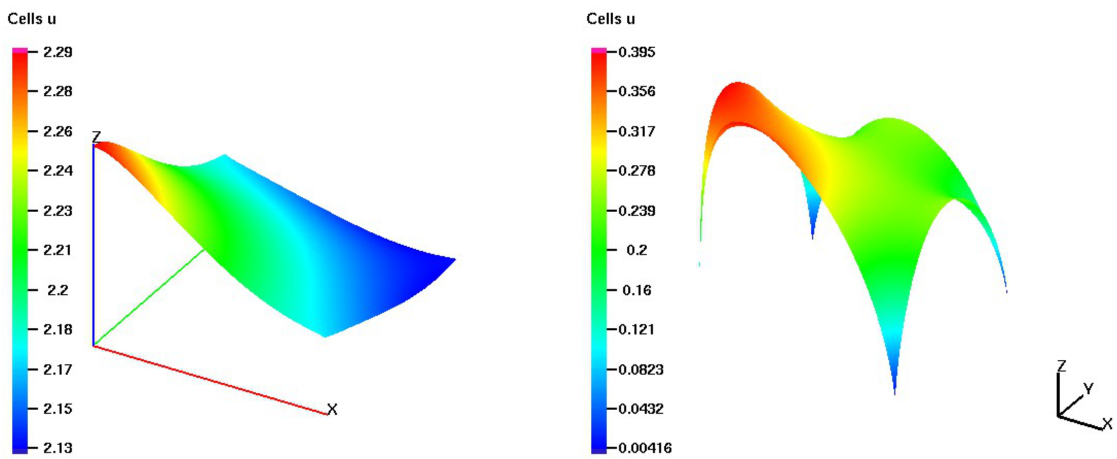

Figure 3.4: The states u for the $H^{1/2}(\Gamma)$ setting when using the opeartor D (left) and for the $L_2(\Gamma)$ setting (right).

To see the behaviour of the states u at the origin of cooridinates for smaller α, we plot in Figure 3.5 the states u of the boundary control problem (3.1)-(3.2) for $\alpha = 10^{-2}$ and $\alpha = 10^{-4}$.

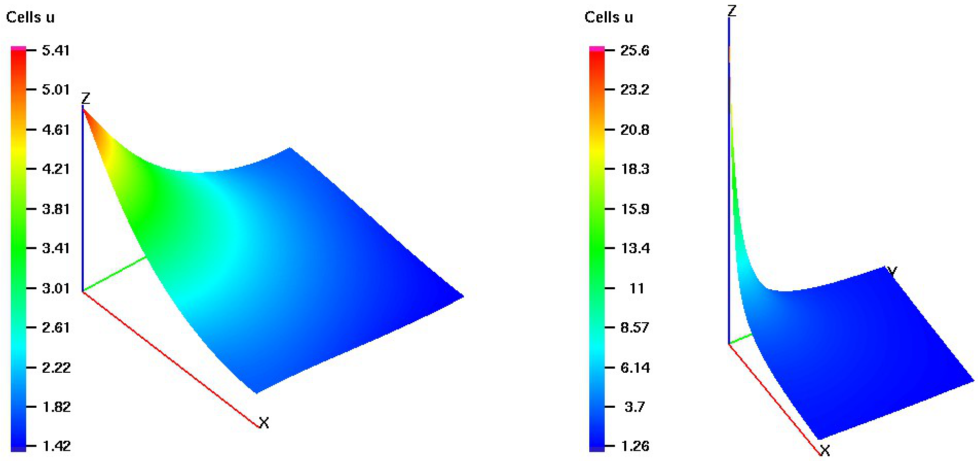

Figure 3.5: The states u for the $H^{1/2}(\Gamma)$ setting with $\alpha = 10^{-2}$ (left) and $\alpha = 10^{-4}$ (right).

The state u shows a good behaviour at the origin, whereas we obtain the zero control at all corner points when considering the control in $L_2(\Gamma)$. More precise, we present the states u for the $H^{1/2}(\Gamma)$ setting and for the $L_2(\Gamma)$ setting in Figure 3.6. Note that for this example we use different values of α to ensure comparable values for the tracking functional $\|u - \overline{u}\|_{L_2(\Omega)}$. The related controls for $x_1 \in (0, 0.5), x_2 = 0$ are given in Figure 3.7. Moreover, the behaviour of the controls near the origin is also shown in Figure 3.8.

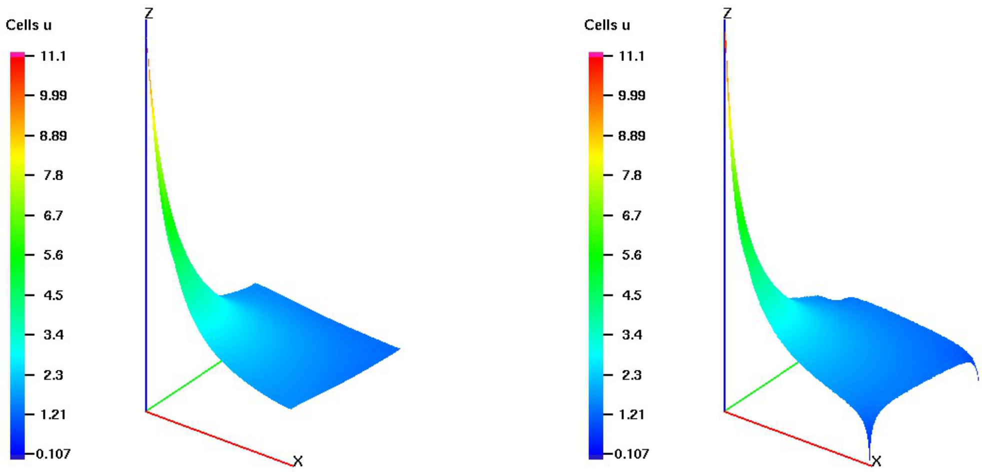

Figure 3.6: The states u for the $H^{1/2}(\Gamma)$ setting with $\alpha = 1.18 \times 10^{-3}$ (left) and for the $L_2(\Gamma)$ setting with $\alpha = 10^{-2}$ (right).

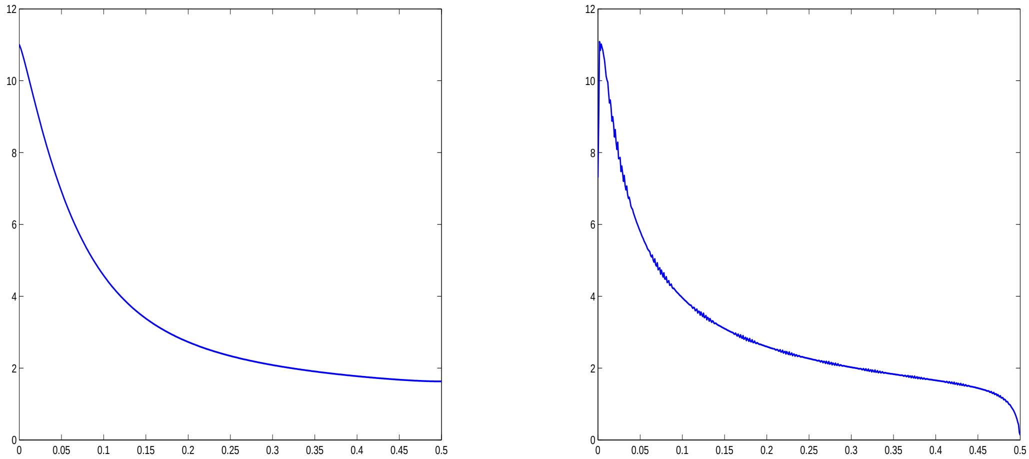

Figure 3.7: Comparison of the $H^{1/2}(\Gamma)$ setting (left) and of $L_2(\Gamma)$ setting (right) optimal controls, $x_2 = 0$.

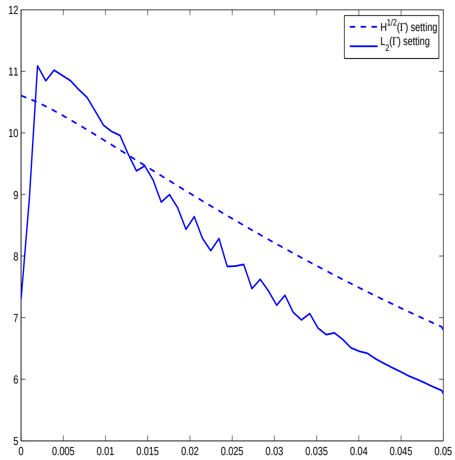

Figure 3.8: The behaviour of the optimal controls near the origin.

4 MIXED BOUNDARY CONTROL PROBLEMS

In this chapter we study a mixed boundary control problem where the control is considered in the space $H^{1/2}(\Gamma_D)$, $\Gamma_D \subset \Gamma$. One possible approach to solve mixed boundary value problems is to use the Dirichlet to Neumann map, so-called the Steklov-Poincaré operator, see [58, 62]. Then we can formulate and analyse a system of boundary integral equations for the mixed boundary control problem which is based on the idea of integration by parts as given in Chapter 3. We derive stability and error estimates of the Galerkin discretization. Some numerical examples are presented which correspond to the theoretical results.

This chapter is organized as follows. We state the model problem in Section 4.1. We also present the well-known KKT system. In Section 4.2, boundary integral equations are considered which are based on the ideas as given in Chapter 3. We formulate a system of boundary integral equations for the coupled optimality system. The Galerkin variational formulation is presented in Section 4.3. We discuss a related stability and error analysis. For illustration, we give some numerical results in Section 4.4.

4.1 Statement of the problem

Let $\Omega \subset \mathbb{R}^d, (d = 2,3)$ be a bounded Lipschitz domain. The boundary $\Gamma = \partial\Omega$ is partitioned into two nonintersecting parts $\Gamma = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, $\Gamma_D \cap \Gamma_N = \emptyset$. As a model problem, we consider the mixed boundary control problem to minimize

$$J(u,z) = \frac{1}{2}\int_\Omega [u(x) - \overline{u}(x)]^2\,dx + \frac{\alpha}{2}\langle \mathcal{S}z, z\rangle_{\Gamma_D} \quad \text{for } (u,z) \in H^1(\Omega) \times H^{1/2}(\Gamma_D) \tag{4.1}$$

subject to

$$-\Delta u(x) = f(x) \quad \text{for } x \in \Omega, \quad u(x) = z(x) \quad \text{for } x \in \Gamma_D, \quad \frac{\partial}{\partial n_x} u(x) = \psi(x) \quad \text{for } x \in \Gamma_N \tag{4.2}$$

and to pointwise control constraints

$$z \in \mathcal{U}_{ad} := \{w \in H^{1/2}(\Gamma_D) \colon z_1(x) \le w(x) \le z_2(x) \text{ for } x \in \Gamma_D\}. \tag{4.3}$$

Here $\overline{u} \in L_2(\Omega)$ is a given target; $f \in L_2(\Omega), \psi \in H^{-1/2}(\Gamma_N)$, $z_1, z_2 \in H^{1/2}(\Gamma_D)$ are given, $\alpha \in \mathbb{R}_+$ is a fixed parameter. We describe the cost by using a $H^{1/2}(\Gamma_D)$ semi-elliptic operator $\mathcal{S} : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D)$ which is specified later.

To reduce the cost functional $J(u,z)$ we introduce a linear solution operator describing the application of the constraint (4.2). Let $u_p \in H^1(\Omega)$ be a particular weak solution of the mixed boundary value problem

$$-\Delta u_p(x) = f(x) \quad \text{for } x \in \Omega, \quad u_p(x) = 0 \quad \text{for } x \in \Gamma_D, \quad \frac{\partial}{\partial n_x} u_p(x) = \psi(x) \quad \text{for } x \in \Gamma_N.$$

Let $u_z \in H^1(\Omega)$ be a weak solution of the homogeneous mixed boundary value problem

$$-\Delta u_z(x) = 0 \quad \text{for } x \in \Omega, \quad u_z(x) = z(x) \quad \text{for } x \in \Gamma_D, \quad \frac{\partial}{\partial n_x} u_z(x) = 0 \quad \text{for } x \in \Gamma_N. \tag{4.4}$$

The solution of the mixed boundary value problem (4.2) is then given by $u = u_z + u_p$. Moreover, by using Green's first formula, we have, for $z, w \in H^{1/2}(\Gamma_D)$,

$$\int_\Omega \nabla u_z(x) \nabla u_w(x)\, dx = \int_\Gamma \frac{\partial}{\partial n_x} u_z(x) u_w(x)\, ds_x = \int_{\Gamma_D} \frac{\partial}{\partial n_x} u_z(x) w(x)\, ds_x =: \langle \mathcal{S}z, w \rangle_{\Gamma_D}.$$

This is the motivation to define an operator $\mathcal{S} : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D)$ which maps the Dirichlet control z to the related Neumann datum on Γ_D. The operator $\mathcal{S}$ is self-adjoint and $H^{1/2}(\Gamma_D)$-semi elliptic. In particular, we have $\mathcal{S}1 = 0$.

The solution of the mixed boundary value problem (4.4) defines a linear map $u_z = \mathcal{H}z$, where $\mathcal{H} : H^{1/2}(\Gamma_D) \to H^1(\Omega) \subset L_2(\Omega)$. Then, by using $u = \mathcal{H}z + u_p$ we now consider the problem to find the minimizer $z \in \mathcal{U}_{ad}$ of the reduced cost functional

$$\begin{aligned}
\widetilde{J}(z) &= \frac{1}{2} \int_\Omega [(\mathcal{H}z)(x) + u_p(x) - \overline{u}(x)]^2\, dx + \frac{\alpha}{2} \langle \mathcal{S}z, z \rangle_{\Gamma_D} \\
&= \frac{1}{2} \langle \mathcal{H}z + u_p - \overline{u}, \mathcal{H}z + u_p - \overline{u} \rangle_\Omega + \frac{\alpha}{2} \langle \mathcal{S}z, z \rangle_{\Gamma_D} \\
&= \frac{1}{2} \langle \mathcal{H}^*\mathcal{H}z, z \rangle_{\Gamma_D} + \langle \mathcal{H}^*(u_p - \overline{u}), z \rangle_{\Gamma_D} + \frac{1}{2} \|u_p - \overline{u}\|^2_{L_2(\Omega)} + \frac{\alpha}{2} \langle \mathcal{S}z, z \rangle_{\Gamma_D}
\end{aligned}$$

where $\mathcal{H}^* : L_2(\Omega) \to \widetilde{H}^{-1/2}(\Gamma_D)$ is the adjoint operator of $\mathcal{H} : H^{1/2}(\Gamma_D) \to L_2(\Omega)$, i.e.,

$$\langle \mathcal{H}^* \omega, \varphi \rangle_{\Gamma_D} = \langle \omega, \mathcal{H}\varphi \rangle_\Omega \quad \text{for all } \varphi \in H^{1/2}(\Gamma_D), \omega \in L_2(\Omega).$$

Since the reduced cost functional $\widetilde{J}(\cdot)$ is convex, the minimizer $z \in \mathcal{U}_{ad}$ can be found from the variational inequality

$$\langle \alpha \mathcal{S}z + \mathcal{H}^*\mathcal{H}z - g, w - z \rangle_{\Gamma_D} \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{4.5}$$

where we define

$$g := \mathcal{H}^*(\overline{u} - u_p) \in \widetilde{H}^{-1/2}(\Gamma_D). \tag{4.6}$$

The operator

$$\mathcal{T}_\alpha := \alpha\mathcal{S} + \mathcal{H}^*\mathcal{H} : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D) \tag{4.7}$$

is bounded, self-adjoint and $H^{1/2}(\Gamma_D)$-elliptic. In particular, for $z \in H^{1/2}(\Gamma_D)$, we have

$$\langle \mathcal{T}_\alpha z, z\rangle_{\Gamma_D} = \alpha\langle \mathcal{S}z, z\rangle_{\Gamma_D} + \langle \mathcal{H}^*\mathcal{H}z, z\rangle_{\Gamma_D} = \alpha\|\nabla u_z\|^2_{L_2(\Omega)} + \|u_z\|^2_{L_2(\Omega)} \geq \min\{\alpha, 1\}\|u_z\|^2_{H^1(\Omega)}$$

and the assertion follows from the trace theorem. Hence, the elliptic variational inequality of the first kind (4.5) admits a unique solution $z \in H^{1/2}(\Gamma_D)$, see, e.g., [23, 38, 41].

The variational inequality (4.5) can be written as

$$\langle \alpha\mathcal{S}z + \mathcal{H}^*(u - \overline{u}), w - z\rangle_{\Gamma_D} \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}.$$

The application of the adjoint operator $\tau := \mathcal{H}^*(u - \overline{u})$ is characterized by the Neumann datum

$$\tau(x) = -\frac{\partial}{\partial n_x} p(x) \quad \text{for } x \in \Gamma_D,$$

where p is the unique solution of the adjoint mixed boundary value problem

$$-\Delta p(x) = u(x) - \overline{u}(x) \text{ for } x \in \Omega, \quad p(x) = 0 \text{ for } x \in \Gamma_D, \quad \frac{\partial}{\partial n_x} p(x) = 0 \text{ for } x \in \Gamma_N. \tag{4.8}$$

Hence the variational inequality (4.5) is written as

$$\langle \alpha\mathcal{S}z - \frac{\partial}{\partial n} p, w - z\rangle_{\Gamma_D} \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}. \tag{4.9}$$

The primal and the adjoint mixed boundary value problems (4.2) and (4.8) can be solved, e.g., by using the standard boundary integral equations or the Dirichlet to Neumann operator S, see e.g, [17, 58, 62, 63]. This will be discussed in the next section.

4.2 Boundary integral equations

To find the control $z \in H^{1/2}(\Gamma_D)$ we have to solve a coupled problem of the primal and the adjoint mixed boundary value problems (4.2), (4.8) and of the optimality condition (4.9). In what follows, the coupled optimality system is written in a form of boundary integral equations of the Steklov-Poincaré operator S and of some composed operator T. The well-known properties of the Dirichlet to Neumann map and of the operator T similar to the results as described in Chapter 3 induce the unique solvability of the boundary integral equation system as well as the stability of the Galerkin discretization which is presented in Section 4.3.

For the sake of convenience, let $\gamma_0\cdot$, $\gamma_1\cdot$ be the Dirichlet and the Neumann trace maps, respectively. For the primal problem, the Dirichlet to Neumann map can be written as

$$\gamma_1 u(x) = (S\gamma_0 u)(x) - (V^{-1}N_0 f)(x) \quad \text{for } x \in \Gamma, \tag{4.10}$$

see (3.19), also [63], where the boundary integral representation of the Steklov-Poincaré operator S is

$$S = V^{-1}(\frac{1}{2}I + K) = D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K). \tag{4.11}$$

We now consider the adjoint mixed boundary value problem

$$-\Delta p(x) = u(x) - \overline{u}(x) \text{ for } x \in \Omega, \quad \gamma_0 p(x) = 0 \quad \text{for } x \in \Gamma_D, \quad \gamma_1 p(x) = 0 \quad \text{for } x \in \Gamma_N.$$

We first obtain the representation formula for $\widetilde{x} \in \Omega$,

$$\begin{aligned} p(\widetilde{x}) = \int_\Gamma U^*(\widetilde{x},y)\gamma_1 p(y)\,ds_y - \int_\Gamma \frac{\partial}{\partial n_y} U^*(\widetilde{x},y)\gamma_0 p(y)\,ds_y + \int_\Gamma \frac{\partial}{\partial n_y} V^*(\widetilde{x},y)\gamma_0 u(y)\,ds_y \\ - \int_\Gamma V^*(\widetilde{x},y)\gamma_1 u(y)\,ds_y - \int_\Omega U^*(\widetilde{x},y)\overline{u}(y)\,dy - \int_\Omega V^*(\widetilde{x},y) f(y)\,dy, \end{aligned} \tag{4.12}$$

where in addition to (3.24) we have the double layer potential of the non-zero Dirichlet data $\gamma_0 p(x)$. When taking the Dirichlet and the Neumann traces, the representation formula (4.12) results in two boundary integral equations

$$\begin{cases} \gamma_0 p = V\gamma_1 p - (-\frac{1}{2}I + K)\gamma_0 p + K_1\gamma_0 u - V_1\gamma_1 u - N_0\overline{u} - M_0 f, \\ \gamma_1 p = (\frac{1}{2}I + K')\gamma_1 p + D\gamma_0 p - D_1\gamma_0 u - K_1'\gamma_1 u - N_1\overline{u} - M_1 f. \end{cases} \tag{4.13}$$

Solving $\gamma_1 p$ from the first equation of (4.13), and by inserting $\gamma_1 u$ from (4.10), (see also (3.19)), we obtain

$$\begin{aligned} \gamma_1 p = V^{-1}V_1V^{-1}(\frac{1}{2}I + K)\gamma_0 u - V^{-1}K_1\gamma_0 u + V^{-1}(\frac{1}{2}I + K)\gamma_0 p \\ + V^{-1}N_0\overline{u} - V^{-1}V_1V^{-1}N_0 f + V^{-1}M_0 f. \end{aligned} \tag{4.14}$$

When substituting $\gamma_1 u$, $\gamma_1 p$ from (4.10), (4.14) to the second equation of (4.13), this gives

$$\gamma_1 p(x) = (S\gamma_0 p)(x) - (T\gamma_0 u)(x) + \widetilde{g}(x) \quad \text{for } x \in \Gamma, \tag{4.15}$$

where the operator T is in the symmetric representation, see (3.80),

$$T = D_1 + K_1'V^{-1}(\frac{1}{2}I + K) + (\frac{1}{2}I + K')V^{-1}K_1 - (\frac{1}{2}I + K')V^{-1}V_1V^{-1}(\frac{1}{2}I + K), \tag{4.16}$$

and

$$\widetilde{g} = (\frac{1}{2}I + K')V^{-1}N_0\overline{u} - N_1\overline{u} + K_1'V^{-1}N_0 f + (\frac{1}{2}I + K')V^{-1}[M_0 - V_1V^{-1}N_0]f - M_1 f \tag{4.17}$$

as in (3.81). Moreover, we use the alternative symmetric representation of S as in (4.11).

Hence, the application of the operator S to the Dirichlet datum of the adjoint variable and of the operator T to the Dirichlet datum of the state give the Neumann datum of the adjoint variable p. Note that

$$\gamma_0 u = \gamma_0 u_z + \gamma_0 u_p, \quad \gamma_0 p \in \widetilde{H}^{1/2}(\Gamma_N), \quad \gamma_1 p \in \widetilde{H}^{-1/2}(\Gamma_D).$$

Let $\widetilde{z} \in H^{1/2}(\Gamma)$ be a fixed extension of $z \in H^{1/2}(\Gamma_D)$. Let

$$\mathsf{s}(x) := \gamma_0 u_z(x) - \widetilde{z}(x) \in \widetilde{H}^{1/2}(\Gamma_N). \tag{4.18}$$

Then the Dirichlet to Neumann map of the mixed boundary value problem (4.4) reads

$$\gamma_1 u_z(x) = (S\gamma_0 u_z)(x) = (S\mathsf{s})(x) + (S\widetilde{z})(x) \quad \text{for } x \in \Gamma.$$

This gives a boundary integral equation

$$(S\mathsf{s})(x) = -(S\widetilde{z})(x) \quad \text{for } x \in \Gamma_N. \tag{4.19}$$

Note that in the last equation we use the same notation for the operator $S : \widetilde{H}^{1/2}(\Gamma_N) \to H^{-1/2}(\Gamma_N)$. In particular, for $\mathsf{s} \in \widetilde{H}^{1/2}(\Gamma_N)$ we identify s with its zero extension $\widetilde{\mathsf{s}} \in H^{1/2}(\Gamma)$. To be more precise, we later use a subscript to indicate the pre-image and the image of the operator S.
Since the operator $S : \widetilde{H}^{1/2}(\Gamma_N) \to H^{-1/2}(\Gamma_N)$ is bounded and $\widetilde{H}^{1/2}(\Gamma_N)$-elliptic, the boundary integral equation (4.19) admits a unique solution $\mathsf{s} \in \widetilde{H}^{1/2}(\Gamma_N)$, see [63, 64]. Hence we can define an operator $\mathcal{P} : H^{1/2}(\Gamma_D) \to H^{1/2}(\Gamma)$ by

$$\mathcal{P}z := \gamma_0 u_z = \mathsf{s} + \widetilde{z}, \tag{4.20}$$

where $\mathsf{s} \in \widetilde{H}^{1/2}(\Gamma_N)$ is the unique solution of the operator equation (4.19). The function s depends on the extension $\widetilde{z}$ of z, of course. However, the sum $\mathsf{s} + \widetilde{z}$ is independent of choosing the extension $\widetilde{z}$. Indeed, let $\overline{z} \in H^{1/2}(\Gamma)$ be another extension of $z \in H^{1/2}(\Gamma_D)$ and let $\overline{\mathsf{s}} \in \widetilde{H}^{1/2}(\Gamma_N)$ be the unique solution of the variational problem

$$\langle S\overline{\mathsf{s}}, \phi\rangle_{\Gamma_N} = -\langle S\overline{z}, \phi\rangle_{\Gamma_N} \quad \text{for all } \phi \in \widetilde{H}^{1/2}(\Gamma_N).$$

Then the function

$$v := (\mathsf{s} + \widetilde{z}) - (\overline{\mathsf{s}} + \overline{z}) \in \widetilde{H}^{1/2}(\Gamma_N).$$

We obtain, by the definition of s and $\overline{\mathsf{s}}$,

$$\langle S\mathsf{s}, v\rangle_{\Gamma_N} = -\langle S\widetilde{z}, v\rangle_{\Gamma_N}, \quad \langle S\overline{\mathsf{s}}, v\rangle_{\Gamma_N} = -\langle S\overline{z}, v\rangle_{\Gamma_N}.$$

This implies

$$\langle Sv, v\rangle_{\Gamma_N} = 0.$$

Hence the assertion follows from the $\widetilde{H}^{1/2}(\Gamma_N)$-ellipticity of the operator S.

Moreover, we have

$$\|\mathcal{P}z\|_{H^{1/2}(\Gamma)} \le c_2^{\mathcal{P}} \|z\|_{H^{1/2}(\Gamma_D)}. \tag{4.21}$$

We now rewrite the boundary integral equation (4.15) in a form of a system of boundary integral equations

$$\begin{cases} (S\gamma_0 p)(x) = T(\mathcal{P}z + \gamma_0 u_p)(x) - \widetilde{g}(x) & \text{for } x \in \Gamma_N, \\ \gamma_1 p(x) = (S\gamma_0 p)(x) - T(\mathcal{P}z + \gamma_0 u_p)(x) + \widetilde{g}(x) & \text{for } x \in \Gamma_D. \end{cases} \tag{4.22}$$

Again the operator $S : \widetilde{H}^{1/2}(\Gamma_N) \to H^{-1/2}(\Gamma_N)$ is bounded and $\widetilde{H}^{1/2}(\Gamma_N)$-elliptic, we can solve $\gamma_0 p \in \widetilde{H}^{1/2}(\Gamma_N)$ from the first equation of (4.22)

$$\gamma_0 p = S_{NN}^{-1} T_N \mathcal{P}z + S_{NN}^{-1} T_N \gamma_0 u_p - S_{NN}^{-1} \widetilde{g}_N, \tag{4.23}$$

where the subscript in S_{AB} means integration over Γ_B and evaluation on Γ_A and the subscripts in T_A, etc., mean evaluation on Γ_A with $\Gamma_A, \Gamma_B \subset \Gamma$. By substituting (4.23) in the second equation of (4.22), we obtain

$$\gamma_1 p = \left(S_{DN} S_{NN}^{-1} T_N - T_D\right) \mathcal{P}z + \left(S_{DN} S_{NN}^{-1} T_N - T_D\right) \gamma_0 u_p - S_{DN} S_{NN}^{-1} \widetilde{g}_N + \widetilde{g}_D. \tag{4.24}$$

Therefore, the variational inequality (4.9) can be written as

$$\langle \mathcal{T}_\alpha z, w - z\rangle_{\Gamma_D} \ge \langle g, w - z\rangle_{\Gamma_D}, \tag{4.25}$$

where we obtain the alternative representation of $\mathcal{T}_\alpha$ as defined in (4.7),

$$\mathcal{T}_\alpha = \alpha \mathcal{S} - \left(S_{DN} S_{NN}^{-1} T_N - T_D\right) \mathcal{P} \tag{4.26}$$

and of g as defined in (4.6),

$$g = \left(S_{DN} S_{NN}^{-1} T_N - T_D\right) \gamma_0 u_p - S_{DN} S_{NN}^{-1} \widetilde{g}_N + \widetilde{g}_D. \tag{4.27}$$

Theorem 4.1. *The composed boundary integral operator $\mathcal{T}_\alpha : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D)$ as defined in* (4.26) *is self-adjoint, bounded and $H^{1/2}(\Gamma_D)$-elliptic.*

Proof. The boundedness of $\mathcal{T}_\alpha$ follows from the boundedness of all boundary integral operators involved. Moreover, let $p_z \in H^1(\Omega)$ be a particular solution of the adjoint mixed boundary value problem, i.e.,

$$-\Delta p_z(x) = u_z(x) \quad \text{for } x \in \Omega, \quad \gamma_0 p_z(x) = 0 \quad \text{for } x \in \Gamma_D, \quad \gamma_1 p_z(x) = 0 \quad \text{for } x \in \Gamma_N,$$

where $u_z \in H^1(\Omega)$ is the solution of the mixed boundary value problem (4.4). Analogously, the boundary integral equation (4.15) reads

$$\gamma_1 p_z(x) = (S\gamma_0 p_z)(x) - (T\gamma_0 u_z)(x) = (S\gamma_0 p_z)(x) - (T\mathcal{P}z)(x). \tag{4.28}$$

Therefore,

$$\begin{cases} (S\gamma_0 p_z)(x) - (T\mathcal{P}z)(x) = 0 & \text{for } x \in \Gamma_N, \\ (S\gamma_0 p_z)(x) - (T\mathcal{P}z)(x) = \gamma_1 p_z(x) & \text{for } x \in \Gamma_D. \end{cases} \tag{4.29}$$

Since the operator $S : \widetilde{H}^{1/2}(\Gamma_N) \to H^{-1/2}(\Gamma_N)$ is invertible, we can solve $\gamma_0 p_z \in \widetilde{H}^{1/2}(\Gamma_N)$ of the first boundary integral equation of (4.29). Hence, from the second boundary integral equation of (4.29), we can conclude

$$\mathcal{T}_\alpha z = \alpha \mathcal{S} z - \gamma_1 p_z \in \widetilde{H}^{-1/2}(\Gamma_D). \tag{4.30}$$

Therefore, for $z, w \in H^{1/2}(\Gamma_D)$ we have, by using Green's second formula

$$\begin{aligned} \langle \mathcal{T}_\alpha z, w \rangle_{\Gamma_D} &= \alpha \langle \mathcal{S} z, w \rangle_{\Gamma_D} - \int_{\Gamma_D} \gamma_1 p_z(x) w(x)\, ds_x \\ &= \alpha \langle \mathcal{S} z, w \rangle_{\Gamma_D} - \int_{\Gamma} \gamma_1 p_z(x) \gamma_0 u_w(x)\, ds_x \\ &= \alpha \int_{\Omega} \nabla u_z(x) \nabla u_w(x)\, dx + \int_{\Omega} u_z(x) u_w(x)\, dx, \end{aligned}$$

and the assertion follows. □

Hence we conclude the unique solvability of the variational inequality (4.25). In what follows, we consider a Galerkin boundary element discretization of the variational inequality (4.25).

4.3 Symmetric Galerkin approximation formulation

Let

$$S_h^1(\Gamma_D) := S_h^1(\Gamma) \cap H^{1/2}(\Gamma_D) = span\{\varphi_i^{1D}\}_{i=1}^{M_1}$$

be a boundary element space of piecewise linear and continuous basis functions φ_i^{1D} on Γ_D, which is defined with respect to a globally quasi-uniform and shape regular boundary element mesh of mesh size h. For continuous functions z_1 and z_2, we define the discrete convex set

$$\mathcal{U}_h := \{ w_h \in S_h^1(\Gamma_D) \colon z_1(x_i) \le w_h(x_i) \le z_2(x_i) \quad \text{for all nodes } x_i \in \overline{\Gamma}_D \} \subset H^{1/2}(\Gamma_D).$$

Then the Galerkin discretization of the variational inequality (4.25) reads to find $z_h \in \mathcal{U}_h$ such that

$$\langle \mathcal{T}_\alpha z_h, w_h - z_h \rangle_{\Gamma_D} \geq \langle g, w_h - z_h \rangle_{\Gamma_D} \quad \text{for all } w_h \in \mathcal{U}_h. \tag{4.31}$$

The operator $\mathcal{T}_\alpha$ as defined in (4.26) is bounded and $H^{1/2}(\Gamma_D)$-elliptic. The discrete variational inequality (4.31) admits a unique solution $z_h \in \mathcal{U}_h$. Moreover, we can derive the following error estimate.

Theorem 4.2. *Let $z \in \mathcal{U}_{ad}$ and $z_h \in \mathcal{U}_h$ be the unique solutions of the variational inequalities* (4.25) *and* (4.31)*, respectively. If we assume $z, z_1, z_2 \in H^s(\Gamma_D)$ and $\mathcal{T}_\alpha z - g \in \widetilde{H}^{s-1}(\Gamma_D)$ for some $s \in [\frac{1}{2}, 2]$, then there holds the error estimate*

$$\|z - z_h\|_{H^{1/2}(\Gamma_D)} \leq c\, h^{s-\frac{1}{2}} \|z\|_{H^s(\Gamma_D)}. \tag{4.32}$$

Proof. The proof is similar to the proof of Theorem 3.1 where we use the approximation property of the trial space $S_h^1(\Gamma_D)$. We skip the details. □

The error estimate (4.32) seems to be optimal. However, the composed operator $\mathcal{T}_\alpha$ as considered in the variational inequality (4.31) does not allow a practical implementation, since the inverse single layer potential V^{-1} as in the composed operators S, T is in general not given in an explicit form. Hence, instead of (4.31) we need to consider a perturbed variational inequality to seek $\widehat{z}_h \in \mathcal{U}_h$ such that

$$\langle \widehat{\mathcal{T}}_\alpha \widehat{z}_h, w_h - \widehat{z}_h \rangle_{\Gamma_D} \geq \langle \widehat{g}, w_h - \widehat{z}_h \rangle_{\Gamma_D} \quad \text{for all } w_h \in \mathcal{U}_h, \tag{4.33}$$

where $\widehat{\mathcal{T}}_\alpha$ and $\widehat{g}$ are appropriate approximations of $\mathcal{T}_\alpha$ and g, respectively. The following theorem presents an abstract consistency result, see [51]. We used a similar result as given in Theorem 3.2.

Theorem 4.3. *Let $\widehat{\mathcal{T}}_\alpha : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D)$ be a bounded and $S_h^1(\Gamma_D)$-elliptic approximation of $\mathcal{T}_\alpha$ satisfying*

$$\|\widehat{\mathcal{T}}_\alpha z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \leq c_2^{\widehat{\mathcal{T}}_\alpha} \|z\|_{H^{1/2}(\Gamma_D)} \quad \textit{for all } z \in H^{1/2}(\Gamma_D) \tag{4.34}$$

and

$$\langle \widehat{\mathcal{T}}_\alpha z_h, z_h \rangle_{\Gamma_D} \geq c_1^{\widehat{\mathcal{T}}_\alpha} \|z_h\|^2_{H^{1/2}(\Gamma_D)} \quad \textit{for all } z_h \in S_h^1(\Gamma_D).$$

Let $\widehat{g} \in \widetilde{H}^{-1/2}(\Gamma_D)$ be some approximation of g. For the unique solution $\widehat{z}_h \in \mathcal{U}_h$ of the perturbed variational inequality (4.33) *there holds the error estimate*

$$\|z - \widehat{z}_h\|_{H^{1/2}(\Gamma_D)} \leq c_1 \|z - z_h\|_{H^{1/2}(\Gamma_D)} + c_2 \|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha) z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} + c_3 \|g - \widehat{g}\|_{\widetilde{H}^{-1/2}(\Gamma_D)}, \tag{4.35}$$

where $z_h \in \mathcal{U}_h$ is the unique solution of the discrete variational inequality (4.31).

It remains to define approximations $\widehat{\mathcal{T}}_\alpha$ and $\widehat{g}$ of the operator $\mathcal{T}_\alpha$ and of the right hand side g, respectively.

Boundary element approximations of S and T

Let $w \in H^{1/2}(\Gamma)$ be a given function. By using the symmetric representations of S and T, see (4.11) and (4.16), we obtain

$$Sw = Dw + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K)w = Dw + (\frac{1}{2}I + K')\omega_w,$$
$$Tw = D_1 w + K_1' \omega_w - (\frac{1}{2}I + K')\theta_w,$$

where

$$\omega_w = V^{-1}(\frac{1}{2}I + K)w, \quad \theta_w = V^{-1}(V_1 \omega_w - K_1 w),$$

i.e., ω_w, θ_w are the unique solutions of the variational problems

$$\langle V\omega_w, \tau\rangle_\Gamma = \langle(\frac{1}{2}I + K)w, \tau\rangle_\Gamma \quad \text{for all } \tau \in H^{-1/2}(\Gamma),$$
$$\langle V\theta_w, \tau\rangle_\Gamma = \langle(V_1\omega_w - K_1 w), \tau\rangle_\Gamma \quad \text{for all } \tau \in H^{-1/2}(\Gamma).$$

Let $S_h^0(\Gamma) = span\{\varphi_k^0\}_{k=1}^N$ be the boundary element space of piecewise constant basis functions on Γ, which is defined with respect to a globally quasi-uniform and shape regular boundary element mesh of mesh size h. Then the associated Galerkin variational formulations read to find $\omega_{w,h}, \theta_{w,h} \in S_h^0(\Gamma)$ such that

$$\langle V\omega_{w,h}, \tau_h\rangle_\Gamma = \langle(\frac{1}{2}I + K)w, \tau_h\rangle_\Gamma \quad \text{for all } \tau_h \in S_h^0(\Gamma),$$
$$\langle V\theta_{w,h}, \tau_h\rangle_\Gamma = \langle(V_1\omega_{w,h} - K_1 w), \tau_h\rangle_\Gamma \quad \text{for all } \tau_h \in S_h^0(\Gamma).$$

Now we are in a position to define the approximate operators $\widehat{S}$ and $\widehat{T}$ by

$$\widehat{S}w = Dw + (\frac{1}{2}I + K')\omega_{w,h}, \tag{4.36}$$

$$\widehat{T}w = D_1 w + K_1' \omega_{w,h} - (\frac{1}{2}I + K')\theta_{w,h}. \tag{4.37}$$

Lemma 4.1. *The approximate Steklov-Poincaré operator $\widehat{S}$ as defined in* (4.36) *is bounded, i.e., $\widehat{S} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ satisfying*

$$\|\widehat{S}w\|_{H^{-1/2}(\Gamma)} \le c_2^{\widehat{S}} \|w\|_{H^{1/2}(\Gamma)} \quad \textit{for all } w \in H^{1/2}(\Gamma). \tag{4.38}$$

Moreover, $\widehat{S}$ is $\widetilde{H}^{1/2}(\Gamma_N)$-elliptic,

$$\langle \widehat{S}w, w\rangle_\Gamma \ge c_1^D \|w\|^2_{H^{1/2}(\Gamma)} \quad \textit{for all } w \in \widetilde{H}^{1/2}(\Gamma_N), \tag{4.39}$$

and satisfies the error estimate

$$\|(S-\widehat{S})w\|_{H^{-1/2}(\Gamma)} \le c \inf_{\tau_h \in S_h^0(\Gamma)} \|Sw - \tau_h\|_{H^{-1/2}(\Gamma)}. \tag{4.40}$$

Proof. The proof is similar to the proof of Lemma 3.3. In particular, the $\widetilde{H}^{1/2}(\Gamma_N)$-ellipticity of $\widehat{S}$ follows due to, see [64, Lemma 12.11],

$$\begin{aligned}
\langle \widehat{S}w, w\rangle_\Gamma &= \langle Dw, w\rangle_\Gamma + \langle (\frac{1}{2}I + K')\omega_{w,h}, w\rangle_\Gamma \\
&= \langle Dw, w\rangle_\Gamma + \langle \omega_{w,h}, (\frac{1}{2}I + K)w\rangle_\Gamma \\
&= \langle Dw, w\rangle_\Gamma + \langle V\omega_{w,h}, \omega_{w,h}\rangle_\Gamma \ge c_1^D \|w\|^2_{H^{1/2}(\Gamma)}.
\end{aligned}$$

□

Lemma 4.2. *The approximate operator $\widehat{T} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ is bounded, i.e.,*

$$\|\widehat{T}w\|_{H^{-1/2}(\Gamma)} \le c_2^{\widehat{T}} \|w\|_{H^{1/2}(\Gamma)} \quad \textit{for all } w \in H^{1/2}(\Gamma). \tag{4.41}$$

Moreover, there holds the error estimate

$$\|(T-\widehat{T})w\|_{H^{-1/2}(\Gamma)} \le c_1 \inf_{\tau_h \in S_h^0(\Gamma)} \|\theta_w - \tau_h\|_{H^{-1/2}(\Gamma)} + c_2 \|\omega_w - \omega_{w,h}\|_{H^{-3/2}(\Gamma)}. \tag{4.42}$$

Proof. The proof follows as for the boundary element approximation of the Dirichlet boundary control problems, see Lemma 3.3, [52]. □

Boundary element approximations of the operators $\mathcal{S}$ and $\mathcal{P}$

Let $z \in H^{1/2}(\Gamma_D)$ be a given function. Let $\widetilde{z} \in H^{1/2}(\Gamma)$ be a fixed extension of z satisfying

$$\|\widetilde{z}\|_{H^{1/2}(\Gamma)} \le c\,\|z\|_{H^{1/2}(\Gamma_D)} \quad \text{for some constant } c > 1. \tag{4.43}$$

By definition we have

$$(\mathcal{S}z)(x) = \gamma_1 u_z(x) \quad \text{for } x \in \Gamma_D,$$

and

$$(\mathcal{P}z)(x) = \gamma_0 u_z(x) = \mathsf{s}(x) + \widetilde{z}(x) \quad \text{for } x \in \Gamma, \quad \mathsf{s} \in \widetilde{H}^{1/2}(\Gamma_N),$$

where $u_z \in H^1(\Omega)$ is the unique solution of the mixed boundary value problem

$$-\Delta u_z(x) = 0 \quad \text{for } x \in \Omega, \quad \gamma_0 u_z(x) = z(x) \quad \text{for } x \in \Gamma_D, \quad \gamma_1 u_z(x) = 0 \quad \text{for } x \in \Gamma_N.$$

The application of the Steklov-Poincaré operator S reads

$$(S\gamma_0 u_z)(x) = \gamma_1 u_z(x) \quad \text{for } x \in \Gamma.$$

This implies

$$\begin{cases} (S\mathsf{s})(x) = -(S\widetilde{z})(x) & \text{for } x \in \Gamma_N, \\ \gamma_1 u_z(x) = (S\mathsf{s})(x) + (S\widetilde{z})(x) & \text{for } x \in \Gamma_D. \end{cases} \tag{4.44}$$

Let

$$\widetilde{S}_h^1(\Gamma_N) := S_h^1(\Gamma) \cap \widetilde{H}^{1/2}(\Gamma_N) = span\{\varphi_i^{1N}\}_{i=1}^{M_2}$$

be a boundary element space of piecewise linear and continuous basis functions φ_i^{1N} on Γ_N, which is defined with respect to a globally quasi-uniform and shape regular boundary element mesh of mesh size h. Let $\mathsf{s}_h \in \widetilde{S}_h^1(\Gamma_N)$ be the unique solution of the Galerkin variational problem

$$\langle \widehat{S}\mathsf{s}_h, \phi_h \rangle_{\Gamma_N} = -\langle \widehat{S}\widetilde{z}, \phi_h \rangle_{\Gamma_N} \quad \text{for all } \phi_h \in \widetilde{S}_h^1(\Gamma_N),$$

where $\widehat{S}$ is defined as in (4.36). Hence we can define approximations $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{P}}$ of the operators $\mathcal{S}$ and $\mathcal{P}$, respectively, by

$$(\widehat{\mathcal{S}}z)(x) := (\widehat{S}\mathsf{s}_h)(x) + (\widehat{S}\widetilde{z})(x) \quad \text{for } x \in \Gamma_D, \tag{4.45}$$

$$(\widehat{\mathcal{P}}z)(x) := \mathsf{s}_h(x) + \widetilde{z}(x) \quad \text{for } x \in \Gamma. \tag{4.46}$$

Lemma 4.3. *The approximate operators*

$$\widehat{\mathcal{S}} : H^{1/2}(\Gamma_D) \to \widetilde{H}^{-1/2}(\Gamma_D), \quad \widehat{\mathcal{P}} : H^{1/2}(\Gamma_D) \to H^{1/2}(\Gamma)$$

are bounded, i.e.,

$$\|\widehat{\mathcal{S}}z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \le c_2^{\widehat{\mathcal{S}}} \|z\|_{H^{1/2}(\Gamma_D)}, \quad \|\widehat{\mathcal{P}}z\|_{H^{1/2}(\Gamma)} \le c_2^{\widehat{\mathcal{P}}} \|z\|_{H^{1/2}(\Gamma_D)} \quad \textit{for all } z \in H^{1/2}(\Gamma_D). \tag{4.47}$$

Moreover, there hold the error estimates

$$\begin{aligned} \|(\mathcal{S}-\widehat{\mathcal{S}})z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \le c_1 \inf_{\phi_h \in \widetilde{S}_h^1(\Gamma_N)} \|\mathsf{s}-\phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2 \|(S-\widehat{S})\mathcal{P}z\|_{H^{-1/2}(\Gamma_D)} \\ + c_3 \|(S-\widehat{S})\mathsf{s}\|_{H^{-1/2}(\Gamma_N)} + c_4 \|(S-\widehat{S})\widetilde{z}\|_{H^{-1/2}(\Gamma_N)} \end{aligned} \tag{4.48}$$

and

$$\begin{aligned} \|(\mathcal{P}-\widehat{\mathcal{P}})z\|_{H^{1/2}(\Gamma)} \le c_1 \inf_{\phi_h \in \widetilde{S}_h^1(\Gamma_N)} \|\mathsf{s}-\phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2 \|(S-\widehat{S})\mathsf{s}\|_{H^{-1/2}(\Gamma_N)} \\ + c_3 \|(S-\widehat{S})\widetilde{z}\|_{H^{-1/2}(\Gamma_N)}. \end{aligned} \tag{4.49}$$

Proof. The boundedness of the operators $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{P}}$ follows from the mapping properties of all boundary integral operators involved. For an arbitrary chosen but fixed $z \in H^{1/2}(\Gamma_D)$

we have, by definition,

$$
\begin{aligned}
(\mathcal{S}-\widehat{\mathcal{S}})z &= S\mathsf{s}-\widehat{S}\mathsf{s}_h+(S-\widehat{S})\widetilde{z} \\
&= (S-\widehat{S})\mathsf{s}+\widehat{S}(\mathsf{s}-\mathsf{s}_h)+(S-\widehat{S})\widetilde{z} \\
&= (S-\widehat{S})\mathcal{P}z+\widehat{S}(\mathsf{s}-\mathsf{s}_h),
\end{aligned}
$$

and

$$(\mathcal{P}-\widehat{\mathcal{P}})z = \mathsf{s}-\mathsf{s}_h.$$

By the Strang lemma, see, e.g., [64], we obtain

$$
\begin{aligned}
\|\mathsf{s}-\mathsf{s}_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} \le c_1 \inf_{\phi_h\in\widetilde{S}_h^1(\Gamma_N)} \|\mathsf{s}-\phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2\|(S-\widehat{S})\mathsf{s}\|_{H^{-1/2}(\Gamma_N)} \\
+c_3\|(S-\widehat{S})\widetilde{z}\|_{H^{-1/2}(\Gamma_N)}.
\end{aligned}
$$

The assertion now follows from the triangle inequality. □

By using the estimates (4.21), (4.40), (4.43) and the approximation properties of the trial spaces $\widetilde{S}_h^1(\Gamma_N)$ and $S_h^0(\Gamma)$, we conclude the error estimates from (4.48), (4.49) when assuming some regularity of z.

Corollary 4.1. *Assume $z \in H^s(\Gamma_D)$ for some $s \in [\frac{1}{2},2]$. Then there hold the error estimates*

$$\|(\mathcal{S}-\widehat{\mathcal{S}})z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \le c_1 h^{s-\frac{1}{2}} \|z\|_{H^s(\Gamma_D)}, \tag{4.50}$$

$$\|(\mathcal{P}-\widehat{\mathcal{P}})z\|_{H^{1/2}(\Gamma)} \le c_2 h^{s-\frac{1}{2}} \|z\|_{H^s(\Gamma_D)}. \tag{4.51}$$

Boundary element approximation of the operator $\mathcal{T}_\alpha$
For an arbitrary but fixed $z \in H^{1/2}(\Gamma_D)$, the application of $\mathcal{T}_\alpha z$ reads as

$$(\mathcal{T}_\alpha z)(x) = \alpha(\mathcal{S}z)(x)-(Sw_z)(x)+(T\mathcal{P}z)(x) \quad \text{for } x\in\Gamma_D,$$

where $w_z \in \widetilde{H}^{1/2}(\Gamma_N)$ is the unique solution of the boundary integral equation

$$(Sw_z)(x) = (T\mathcal{P}z)(x) \quad \text{for } x\in\Gamma_N.$$

Let $w_{z,h} \in \widetilde{S}_h^1(\Gamma_N)$ be the unique solution of the Galerkin variational problem

$$\langle \widehat{S}w_{z,h},\phi_h\rangle_{\Gamma_N} = \langle \widehat{T}\widehat{\mathcal{P}}z,\phi_h\rangle_{\Gamma_N} \quad \text{for all } \phi_h\in\widetilde{S}_h^1(\Gamma_N). \tag{4.52}$$

Hence we can define an approximation $\widehat{\mathcal{T}}_\alpha$ of the operator $\mathcal{T}_\alpha$ by

$$(\widehat{\mathcal{T}}_\alpha z)(x) := \alpha(\widehat{\mathcal{S}}z)(x)-(\widehat{S}w_{z,h})(x)+(\widehat{T}\widehat{\mathcal{P}}z)(x) \quad \text{for } x\in\Gamma_D. \tag{4.53}$$

Lemma 4.4. *The approximate operator $\widehat{\mathcal{T}}_\alpha$ as defined in* (4.53) *is bounded, i.e.,*

$$\|\widehat{\mathcal{T}}_\alpha z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \le c_2^{\widehat{\mathcal{T}}_\alpha} \|z\|_{H^{1/2}(\Gamma_D)}.$$

Moreover, there holds the error estimate

$$\begin{aligned} \|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha)z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} &\le c_1 \inf_{\phi_h \in \widetilde{S}_h^1(\Gamma_N)} \|w_z - \phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + \alpha \|(\mathcal{S} - \widehat{\mathcal{S}})z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \\ &\quad + c_2\|(S - \widehat{S})w_z\|_{H^{-1/2}(\Gamma)} + c_3\|(T - \widehat{T})\mathcal{P}z\|_{H^{-1/2}(\Gamma)} + c_4\|(\mathcal{P} - \widehat{\mathcal{P}})z\|_{H^{-1/2}(\Gamma)}. \end{aligned} \tag{4.54}$$

Proof. The boundedness of the operator $\widehat{\mathcal{T}}_\alpha$ follows from the mapping properties of all boundary integral operators involved, see Lemma 4.1, 4.2 and 4.3.
For the error estimate (4.54), let $z \in H^{1/2}(\Gamma_D)$ be an arbitrary function but fixed. By definition, we have

$$(\mathcal{T}_\alpha z)(x) = \alpha(\mathcal{S}z)(x) - (Sw_z)(x) + (T\mathcal{P}z)(x) \quad \text{for } x \in \Gamma_D,$$

and by using (4.53),

$$(\widehat{\mathcal{T}}_\alpha z)(x) = \alpha(\widehat{\mathcal{S}}z)(x) - (\widehat{S}w_{z,h})(x) + (\widehat{T}\widehat{\mathcal{P}}z)(x) \quad \text{for } x \in \Gamma_D.$$

Therefore, we obtain for $x \in \Gamma_D$

$$\begin{aligned} (\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha)z(x) &= \alpha(\mathcal{S} - \widehat{\mathcal{S}})z(x) + (\widehat{S}w_{z,h})(x) - (Sw_z)(x) + (T\mathcal{P}z)(x) - (\widehat{T}\widehat{\mathcal{P}}z)(x) \\ &= \alpha(\mathcal{S} - \widehat{\mathcal{S}})z(x) + (\widehat{S} - S)w_z(x) + \widehat{S}(w_{z,h} - w_z)(x) \\ &\qquad + (T - \widehat{T})\mathcal{P}z(x) + \widehat{T}(\mathcal{P} - \widehat{\mathcal{P}})z(x). \end{aligned}$$

By using the Strang lemma and the triangle inequality, we can conclude

$$\begin{aligned} \|w_z - w_{z,h}\|_{\widetilde{H}^{1/2}(\Gamma_N)} &\le c_1 \inf_{\phi_h \in \widetilde{S}_h^1(\Gamma_N)} \|w_z - \phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2\|(S - \widehat{S})w_z\|_{H^{-1/2}(\Gamma_N)} \\ &\qquad + c_3\|(T\mathcal{P} - \widehat{T}\widehat{\mathcal{P}})z\|_{H^{-1/2}(\Gamma_N)} \\ &\le c_1 \inf_{\phi_h \in \widetilde{S}_h^1(\Gamma_N)} \|w_z - \phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2\|(S - \widehat{S})w_z\|_{H^{-1/2}(\Gamma_N)} \\ &\qquad + c_3\|(T - \widehat{T})\mathcal{P}z\|_{H^{-1/2}(\Gamma_N)} + c_3\|\widehat{T}(\mathcal{P} - \widehat{\mathcal{P}})z\|_{H^{-1/2}(\Gamma_N)}. \end{aligned}$$

The assertion now follows from the boundedness of the operators $\widehat{S}$ and $\widehat{T}$. □

By using the estimates (4.40), (4.42), (4.50), (4.51) and the approximation properties of the trial spaces $\widetilde{S}_h^1(\Gamma_N)$ and $S_h^0(\Gamma)$, we conclude an error estimate from (4.54) when assuming some regularity of $z, w_z, \theta_{\mathcal{P}z}, \omega_{\mathcal{P}z}$, respectively. Here, we recall the notations

$$\omega_{\mathcal{P}z} = V^{-1}(\frac{1}{2}I + K)\mathcal{P}z, \quad \theta_{\mathcal{P}z} = V^{-1}[V_1\omega_{\mathcal{P}z} - K_1\mathcal{P}z].$$

Corollary 4.2. *There holds the error estimate*

$$\|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha)z\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \le c_1 h^{s-\frac{1}{2}} \|w_z\|_{H^s(\Gamma_N)} + c_2 h^{s-\frac{1}{2}} \|z\|_{H^s(\Gamma_D)} + c_3 h^{\sigma+\frac{1}{2}} \|\theta_{\mathcal{P}z}\|_{H^\sigma_{pw}(\Gamma)} + c_4 h^{\sigma+\frac{1}{2}} \|\omega_{\mathcal{P}z}\|_{H^\sigma_{pw}(\Gamma)}, \quad (4.55)$$

when assuming $z \in H^s(\Gamma_D)$, $w_z \in H^s(\Gamma_N)$ *for some* $s \in [\frac{1}{2}, 2]$ *and* $\theta_{\mathcal{P}z}, \omega_{\mathcal{P}z} \in H^\sigma_{pw}(\Gamma)$ *for some* $\sigma \in [0,1]$.

Boundary element approximations of the right hand sides

Analogously we may define a boundary element approximation of the right hand side g as defined in (4.27)

$$g = \left(S_{DN} S_{NN}^{-1} T_N - T_D\right) \gamma_0 u_p - S_{DN} S_{NN}^{-1} \widetilde{g}_N + \widetilde{g}_D.$$

Let us first define boundary element approximations of $\widetilde{g}$, see (4.17), and $\gamma_0 u_p$. By using (3.82), (3.83), $\widetilde{g} \in H^{-1/2}(\Gamma)$ as in (4.17) can be read

$$\widetilde{g} = V^{-1} N_0 \overline{u} + V^{-1} M_0 f - V^{-1} V_1 V^{-1} N_0 f = V^{-1} N_0 \overline{u} + V^{-1} M_0 f - V^{-1} V_1 f_0,$$

where $f_0 := V^{-1} N_0 f$. Hence we can define an approximation $\widetilde{g}_h \in S_h^0(\Gamma)$ of $\widetilde{g}$ which is the unique solution of the Galerkin variational problem

$$\langle V \widetilde{g}_h, \theta_h \rangle_\Gamma = \langle N_0 \overline{u} + M_0 f - V_1 f_{0,h}, \theta_h \rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma), \quad (4.56)$$

where $f_{0,h} \in S_h^0(\Gamma)$ solves

$$\langle V f_{0,h}, \theta_h \rangle_\Gamma = \langle N_0 f, \theta_h \rangle_\Gamma \quad \text{for all } \theta_h \in S_h^0(\Gamma). \quad (4.57)$$

As in Corollary 3.3 we conclude the error estimates

$$\|f_0 - f_{0,h}\|_{H^{-1/2}(\Gamma)} \le c_1\, h^{\sigma+\frac{1}{2}} \|f_0\|_{H^\sigma_{pw}(\Gamma)}, \quad (4.58)$$

$$\|\widetilde{g} - \widetilde{g}_h\|_{H^{-1/2}(\Gamma)} \le c_1\, h^{\sigma+\frac{1}{2}} \|\widetilde{g}\|_{H^\sigma_{pw}(\Gamma)} + c_2\, h^{\sigma+\frac{3}{2}} \|f_0\|_{H^\sigma_{pw}(\Gamma)}, \quad (4.59)$$

when assuming $f_0, \widetilde{g} \in H^\sigma_{pw}(\Gamma)$ for some $\sigma \in [0,1]$. Note that the factor $\sigma + \frac{3}{2}$ in the last term follows from the mapping property $V_1 : H^{-3/2}(\Gamma) \to H^{3/2}(\Gamma)$ and the Aubin-Nitsche trick.

We now define a boundary element approximation of $\gamma_0 u_p$, where u_p is the unique solution of the mixed boundary value problem

$$-\Delta u_p(x) = f(x) \quad \text{for } x \in \Omega, \quad \gamma_0 u_p(x) = 0 \quad \text{for } x \in \Gamma_D, \quad \gamma_1 u_p(x) = \psi(x) \quad \text{for } x \in \Gamma_N.$$

The boundary integral equation (4.10) gives

$$(S \gamma_0 u_p)(x) = \gamma_1 u_p(x) + (V^{-1} N_0 f)(x) = \psi(x) + f_0(x) \quad \text{for } x \in \Gamma_N.$$

Hence we can define an approximation $u_{p,h} \in \widetilde{S}_h^1(\Gamma_N)$ of $\gamma_0 u_p \in \widetilde{H}^{1/2}(\Gamma_N)$ as the unique solution of the Galerkin variational problem

$$\langle \widehat{S} u_{p,h}, \phi_h \rangle_{\Gamma_N} = \langle \psi + f_{0,h}, \phi_h \rangle_{\Gamma_N} \quad \text{for all } \phi_h \in \widetilde{S}_h^1(\Gamma_N). \tag{4.60}$$

Moreover, we can derive the error estimate

$$\|\gamma_0 u_p - u_{p,h}\|_{\widetilde{H}^{1/2}(\Gamma_N)} \leq c_1\, h^{s-\frac{1}{2}} \|\gamma_0 u_p\|_{H^s(\Gamma_N)} + c_2\, h^{\sigma+\frac{1}{2}} \|f_0\|_{H^\sigma_{pw}(\Gamma)}, \tag{4.61}$$

when assuming $\gamma_0 u_p \in H^s(\Gamma_N)$ for some $s \in [\frac{1}{2}, 2]$ and $f_0 \in H^\sigma_{pw}(\Gamma)$ for some $\sigma \in [0,1]$.

Let us rewrite the right hand side g as follows

$$g(x) = (Sf_1)(x) - (T\gamma_0 u_p)(x) + \widetilde{g}(x) \quad \text{for } x \in \Gamma_D, \tag{4.62}$$

where $f_1 \in \widetilde{H}^{1/2}(\Gamma_N)$ solves

$$(Sf_1)(x) = (T\gamma_0 u_p)(x) - \widetilde{g}(x) \quad \text{for } x \in \Gamma_N.$$

Then, we define $f_{1,h} \in \widetilde{S}_h^1(\Gamma_N)$ as the unique solution of the Galerkin variational problem

$$\langle \widehat{S} f_{1,h}, \phi_h \rangle_{\Gamma_N} = \langle \widehat{T} u_{p,h}, \phi_h \rangle_{\Gamma_N} - \langle \widetilde{g}_h, \phi_h \rangle_{\Gamma_N} \quad \text{for all } \phi_h \in \widetilde{S}_h^1(\Gamma_N). \tag{4.63}$$

By using the Strang lemma, we conclude the error estimate

$$\begin{aligned} \|f_1 - f_{1,h}\|_{\widetilde{H}^{1/2}(\Gamma_N)} \leq{}& c_1 \inf_{\phi_h \in \widetilde{H}_h^1(\Gamma_N)} \|f_1 - \phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2 \|(S - \widehat{S}) f_1\|_{H^{-1/2}(\Gamma_N)} \\ &+ c_3 \|(T - \widehat{T})\gamma_0 u_p\|_{H^{-1/2}(\Gamma_N)} + c_4 \|\gamma_0 u_p - u_{p,h}\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_5 \|\widetilde{g} - \widetilde{g}_h\|_{H^{-1/2}(\Gamma_N)}. \end{aligned} \tag{4.64}$$

We are now in a position to define an approximation $\widehat{g} \in \widetilde{H}^{-1/2}(\Gamma_D)$ of g by

$$\widehat{g}(x) = (\widehat{S} f_{1,h})(x) - (\widehat{T} u_{p,h})(x) + \widetilde{g}_h(x) \quad \text{for } x \in \Gamma_D. \tag{4.65}$$

Lemma 4.5. *Let g and $\widehat{g}$ be defined as in* (4.62) *and* (4.65)*, respectively. Then there holds the error estimate*

$$\begin{aligned} \|g - \widehat{g}\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \leq{}& c_1 \inf_{\phi_h \in \widetilde{H}_h^1(\Gamma_N)} \|f_1 - \phi_h\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_2 \|(S - \widehat{S}) f_1\|_{H^{-1/2}(\Gamma)} \\ &+ c_3 \|(T - \widehat{T})\gamma_0 u_p\|_{H^{-1/2}(\Gamma)} + c_4 \|\gamma_0 u_p - u_{p,h}\|_{\widetilde{H}^{1/2}(\Gamma_N)} + c_5 \|\widetilde{g} - \widetilde{g}_h\|_{H^{-1/2}(\Gamma)}. \end{aligned} \tag{4.66}$$

Proof. By the definition of g and by using (4.65) we obtain for $x \in \Gamma_D$

$$\begin{aligned} g(x) - \widehat{g}(x) &= (Sf_1)(x) - (\widehat{S}f_{1,h})(x) - (T\gamma_0 u_p)(x) + (\widehat{T}u_{p,h})(x) + \widetilde{g}(x) - \widetilde{g}_h(x) \\ &= (S-\widehat{S})f_1(x) + \widehat{S}(f_1 - f_{1,h})(x) - (T-\widehat{T})\gamma_0 u_p(x) \\ &\qquad + \widehat{T}(u_{p,h} - \gamma_0 u_p)(x) + \widetilde{g}(x) - \widetilde{g}_h(x). \end{aligned}$$

The assertion then follows from the triangle inequality and the error estimate (4.64). □

When combining the error estimates (4.40), (4.42), (4.59) and (4.61) with the approximation properties of the trial spaces $\widetilde{S}_h^1(\Gamma_N)$ and $S_h^0(\Gamma)$, we conclude the following error estimate

$$\begin{aligned} \|g - \widehat{g}\|_{\widetilde{H}^{-1/2}(\Gamma_D)} \leq c_1 h^{s-\frac{1}{2}} \|f_1\|_{H^s(\Gamma)} + c_2 h^{\sigma+\frac{1}{2}} \|\theta_{\gamma_0 u_p}\|_{H^\sigma_{pw}(\Gamma)} + c_3 h^{\sigma+\frac{3}{2}} \|\omega_{\gamma_0 u_p}\|_{H^\sigma_{pw}(\Gamma)} \\ + c_4 h^{s-\frac{1}{2}} \|\gamma_0 u_p\|_{H^s(\Gamma_N)} + c_5 h^{\sigma+\frac{1}{2}} \|f_0\|_{H^\sigma_{pw}(\Gamma)} + c_6 h^{\sigma+\frac{1}{2}} \|\widetilde{g}\|_{H^\sigma_{pw}(\Gamma)}, \end{aligned} \tag{4.67}$$

when assuming $f_1 \in H^s(\Gamma)$, $\gamma_0 u_p \in H^s(\Gamma_N)$ for some $s \in [\frac{1}{2}, 2]$ and $\theta_{\gamma_0 u_p}, \omega_{\gamma_0 u_p}, f_0, \widetilde{g} \in H^\sigma_{pw}(\Gamma)$ for some $\sigma \in [0,1]$.

Approximate variational inequality

By using the approximations (4.53) and (4.65) we now consider the approximate variational inequality, see (4.33), to find $\widehat{z}_h \in \mathcal{U}_h$ such that

$$\langle \widehat{\mathcal{T}}_\alpha \widehat{z}_h, w_h - \widehat{z}_h \rangle_{\Gamma_D} \geq \langle \widehat{g}, w_h - \widehat{z}_h \rangle_{\Gamma_D} \quad \text{for all } w_h \in \mathcal{U}_h. \tag{4.68}$$

Let $\widetilde{z}_h, \widetilde{w}_h \in S_h^1(\Gamma)$ be the extensions of $\widehat{z}_h$ and w_h, respectively, satisfying

$$\widetilde{z}_h(x_i) = 0, \quad \widetilde{w}_h(x_i) = 0 \quad \text{for all points } x_i \notin \overline{\Gamma}_D.$$

Since $\widetilde{\mathcal{T}}_\alpha \widetilde{z}_h - \widehat{g} \in \widetilde{H}^{-1/2}(\Gamma_D)$, the variational inequality (4.68) is equivalent to

$$\langle \widehat{\mathcal{T}}_\alpha \widehat{z}_h, \widetilde{w}_h - \widetilde{z}_h \rangle_\Gamma \geq \langle \widehat{g}, \widetilde{w}_h - \widetilde{z}_h \rangle_\Gamma \quad \text{for all } \widetilde{w}_h \leftrightarrow w_h \in \mathcal{U}_h. \tag{4.69}$$

By using the extension $\widetilde{z}_h$ for the approximations (4.45) and (4.46), we obtain

$$\begin{aligned} (\widehat{\mathcal{S}} \widehat{z}_h)(x) &= \widehat{S}(\mathsf{s}_h + \widetilde{z}_h)(x) \quad \text{for } x \in \Gamma_D, \\ (\widehat{\mathcal{P}} \widehat{z}_h)(x) &= \mathsf{s}_h(x) + \widetilde{z}_h(x) \quad \text{for } x \in \Gamma, \end{aligned}$$

where $\mathsf{s}_h \in \widetilde{S}_h^1(\Gamma_N)$ is the unique solution of the Galerkin variational problem

$$\langle \widehat{S}\mathsf{s}_h, \phi_h \rangle_{\Gamma_N} = -\langle \widehat{S} \widetilde{z}_h, \phi_h \rangle_{\Gamma_N} \quad \text{for all } \phi_h \in \widetilde{S}_h^1(\Gamma_N). \tag{4.70}$$

Hence we conclude from (4.53), for $x \in \Gamma_D$,

$$(\widehat{\mathcal{T}}_\alpha \widehat{z}_h)(x) = \alpha \widehat{S}(\mathsf{s}_h + \widetilde{z}_h)(x) - (\widehat{S} w_{\widetilde{z}_h,h})(x) + \widehat{T}(\mathsf{s}_h + \widetilde{z}_h)(x), \tag{4.71}$$

where $w_{\widetilde{z}_h,h}$ is the unique solution of the Galerkin variational problem

$$\langle \widehat{S} w_{\widetilde{z}_h,h}, \phi_h \rangle_{\Gamma_N} = \langle \widehat{T}(\mathsf{s}_h + \widetilde{z}_h), \phi_h \rangle_{\Gamma_N} \quad \text{for all } \phi_h \in \widetilde{S}_h^1(\Gamma_N). \tag{4.72}$$

The Galerkin formulation (4.70) is equivalent to the linear system

$$S_h^{NN} \underline{\mathsf{s}} = -S_h^{ND} \underline{z}, \tag{4.73}$$

and (4.72) is equivalent to

$$S_h^{NN} \underline{w} = T_h^{NN} \underline{\mathsf{s}} + T_h^{ND} \underline{z}, \tag{4.74}$$

where the matrices S_h^{NN}, etc., are generated by the approximate operators $\widehat{S}$ and $\widehat{T}$, for example we have

$$S_h^{NN} = D_h^{NN} + (\frac{1}{2} M_h^N + K_h^N)^\top V_h^{-1} (\frac{1}{2} M_h^N + K_h^N),$$

and

$$\begin{aligned} T_h^{ND} = D_{1,h}^{ND} + K_{1,h}^{N\top} V_h^{-1} (\frac{1}{2} M_h^D + K_h^D) - (\frac{1}{2} M_h^N + K_h^N)^\top V_h^{-1} V_{1,h} V_h^{-1} (\frac{1}{2} M_h^D + K_h^D) \\ + (\frac{1}{2} M_h^N + K_h^N)^\top V_h^{-1} K_{1,h}^D. \end{aligned}$$

Here we introduce the matrix entries, for example

$$\begin{aligned} M_h^D[k,i] &= \langle \varphi_i^{1D}, \varphi_k^0 \rangle_\Gamma, & K_h^N[k,m] &= \langle K \varphi_m^{1N}, \varphi_k^0 \rangle_\Gamma, \\ V_h[k,\ell] &= \langle V \varphi_\ell^0, \varphi_k^0 \rangle_\Gamma, & D_h^{DD}[i,j] &= \langle D \varphi_j^{1D}, \varphi_i^{1D} \rangle_\Gamma, \\ D_h^{DN}[i,m] &= \langle D \varphi_m^{1N}, \varphi_i^{1D} \rangle_\Gamma, & D_{1,h}^{ND}[m,i] &= \langle D_1 \varphi_i^{1D}, \varphi_m^{1N} \rangle_\Gamma, \end{aligned}$$

for $i,j = 1,\dots,M_1;\ m = 1,\dots,M_2;\ k,\ell = 1,\dots,N.$

By using (4.71), the matrix representation of the variational inequality (4.69) is then given by the discrete variational inequality with the Euclidian inner product

$$(\alpha S_h^{DN} \underline{\mathsf{s}} + \alpha S_h^{DD} \underline{z} - S_h^{DN} \underline{w} + T_h^{DN} \underline{\mathsf{s}} + T_h^{DD} \underline{z}, \underline{\widetilde{w}} - \underline{z}) \geq (\underline{\widehat{g}}, \underline{\widetilde{w}} - \underline{z}) \quad \text{for all } \underline{\widetilde{w}} \in \mathbb{R}^{M_1} \leftrightarrow w_h \in \mathcal{U}_h$$

or

$$(\widehat{\mathcal{T}}_{\alpha,h} \underline{z}, \underline{\widetilde{w}} - \underline{z}) \geq (\underline{\widehat{g}}, \underline{\widetilde{w}} - \underline{z}) \quad \text{for all } \underline{\widetilde{w}} \in \mathbb{R}^{M_1} \leftrightarrow w_h \in \mathcal{U}_h \tag{4.75}$$

where

$$\begin{aligned} \widehat{\mathcal{T}}_{\alpha,h} = \alpha S_h^{DD} - \alpha S_h^{DN} S_h^{-NN} S_h^{ND} + S_h^{DN} S_h^{-NN} T_h^{NN} S_h^{-NN} S_h^{ND} \\ - S_h^{DN} S_h^{-NN} T_h^{ND} - T_h^{DN} S_h^{-NN} S_h^{ND} + T_h^{DD} \end{aligned} \tag{4.76}$$

defines a Galerkin boundary element approximation of the boundary integral operator $\mathcal{T}_\alpha$ as defined in (4.26). Note that the matrix S_h^{NN} is symmetric and positive definite. Hence it is invertible. Here $\underline{\widehat{g}}$ is the related vector right hand side which is specified as follows.

The Galerkin formulations (4.56) and (4.57) are equivalent to the linear systems

$$V_h\underline{\widetilde{g}} = \underline{f}^1 - V_{1,h}\underline{f}_0, \quad V_h\underline{f}_0 = \underline{f}^2,$$

where

$$f^1[\ell] = \langle N_0\overline{u} + M_0 f, \varphi_\ell^0\rangle_\Gamma, \quad f^2[\ell] = \langle N_0 f, \varphi_\ell^0\rangle_\Gamma \quad \text{for } \ell = 1,...,N.$$

The associated linear systems of the Galerkin formulations (4.60) and (4.63) read

$$S_h^{NN}\underline{u}_p = \underline{\psi} + M_h^{NN}\underline{f}_{0N},$$

and

$$S_h^{NN}\underline{f}_1 = T_h^{NN}\underline{u}_p - M_h^{NN}\underline{\widetilde{g}}_N,$$

respectively, where

$$\psi[\ell] = \langle \psi, \varphi_\ell^{1N}\rangle_\Gamma, \quad M_h^{NN}[\ell][i] = \langle \varphi_i^0, \varphi_\ell^{1N}\rangle_\Gamma, \quad \underline{f}_{0N} = \underline{f}_0|_{\Gamma_N}, \quad \underline{\widetilde{g}}_N = \underline{\widetilde{g}}|_{\Gamma_N}$$

for $\ell = 1,...,M_2$ and all indices i with respect to boundary elements $\tau_i \in \Gamma_N$.

Altogether we can compute the right hand side $\underline{\widehat{g}}$ from (4.65) by

$$\underline{\widehat{g}} = S_h^{DN}\underline{f}_1 - T_h^{DN}\underline{u}_p + M_h^{DD}\underline{\widetilde{g}}_D. \tag{4.77}$$

Lemma 4.6. *The symmetric matrix $\widehat{\mathcal{T}}_{\alpha,h}$ as defined in* (4.76) *is positive definite, i.e.,*

$$(\widehat{\mathcal{T}}_{\alpha,h}\underline{z}, \underline{z}) \geq c_1^{\widehat{\mathcal{T}}_\alpha}\|z_h\|^2_{H^{1/2}(\Gamma_D)} \quad \text{for all } \underline{z} \in \mathbb{R}^{M_1} \leftrightarrow z_h \in S_h^1(\Gamma_D). \tag{4.78}$$

Proof. For $\underline{z} \in \mathbb{R}^{M_1} \leftrightarrow z_h \in S_h^1(\Gamma_D)$, by using $\underline{\mathsf{s}} = -S_h^{-NN}S_h^{ND}\underline{z} \in \mathbb{R}^{M_2} \leftrightarrow \mathsf{s}_h \in \widetilde{S}_h^1(\Gamma_N)$ we have from (4.76),

$$\begin{aligned}(\widehat{\mathcal{T}}_{\alpha,h}\underline{z}, \underline{z}) &= \alpha(S_h^{DD}\underline{z}, \underline{z}) - \alpha(S_h^{DN}S_h^{-NN}S_h^{ND}\underline{z}, \underline{z}) + (T_h^{NN}\underline{\mathsf{s}}, \underline{\mathsf{s}}) + (T_h^{ND}\underline{z}, \underline{\mathsf{s}}) \\ &\qquad + (T_h^{DN}\underline{\mathsf{s}}, \underline{z}) + (T_h^{DD}\underline{z}, \underline{z}) \\ &= \alpha\left(\begin{pmatrix} S_h^{DD} & S_h^{DN} \\ S_h^{ND} & S_h^{NN}\end{pmatrix}\begin{pmatrix}\underline{z} \\ \underline{\mathsf{s}}\end{pmatrix}, \begin{pmatrix}\underline{z} \\ \underline{\mathsf{s}}\end{pmatrix}\right) + \left(\begin{pmatrix} T_h^{DD} & T_h^{DN} \\ T_h^{ND} & T_h^{NN}\end{pmatrix}\begin{pmatrix}\underline{z} \\ \underline{\mathsf{s}}\end{pmatrix}, \begin{pmatrix}\underline{z} \\ \underline{\mathsf{s}}\end{pmatrix}\right) \\ &= \alpha(S_h\underline{v}, \underline{v}) + (T_h\underline{v}, \underline{v}),\end{aligned}$$

where

$$S_h = D_h + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\frac{1}{2}M_h + K_h)$$

is the discrete form of the Steklov-Poincré operator and

$$T_h = D_{1,h} - (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h) + K_{1,h}^\top V_h^{-1}(\frac{1}{2}M_h + K_h) + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}K_{1,h},$$

see (3.91) and (3.92). Moreover, the vector $\underline{v}$ corresponds to an ansatz function $v_h = \widetilde{z}_h + \mathsf{s}_h$ where $\widetilde{z}_h$ is the extension of z_h as defined above.
Therefore, we conclude by using Lemma 3.7,

$$\begin{aligned}(\widehat{\mathcal{T}}_{\alpha,h}\underline{z},\underline{z}) &= \alpha(S_h\underline{v},\underline{v}) + (\widehat{T}_h\underline{v},\underline{v}) + (D_{1,h}\underline{v},\underline{v}) \\ &\geq \alpha(D_h\underline{v},\underline{v}) + (D_{1,h}\underline{v},\underline{v}) \\ &= \alpha\langle Dv_h, v_h\rangle_\Gamma + \langle D_1 v_h, v_h\rangle_\Gamma \geq c\|v_h\|^2_{H^{1/2}(\Gamma)} \geq c_1^{\widehat{\mathcal{T}}_\alpha}\|z_h\|^2_{H^{1/2}(\Gamma_D)}\end{aligned}$$

since $\alpha D + D_1$ implies an equivalent norm in $H^{1/2}(\Gamma)$, and $v_h \in S_h^1(\Gamma)$ defines an extension of $z_h \in S_h^1(\Gamma_D)$. □

Hence we can ensure unique solvability of the discrete variational inequality (4.75) by applying Theorem 4.3. Moreover, when combining the error estimate (4.35) with the error estimates (4.32), (4.55) and (4.67), we finally obtain the following error estimate.

Lemma 4.7. *Let $z \in \mathcal{U}_{ad}$ and $\widehat{z}_h \in \mathcal{U}_h$ be the unique solutions of the variational inequalities* (4.25) *and* (4.68). *Then there holds the error estimate*

$$\begin{aligned}\|z - \widehat{z}_h\|_{H^{1/2}(\Gamma_D)} \leq{}& c_1 h^{s-\frac{1}{2}}\|z\|_{H^s(\Gamma_D)} + c_2 h^{s-\frac{1}{2}}\|w_z\|_{H^s(\Gamma_N)} + c_3 h^{\sigma+\frac{1}{2}}\|\theta_{\mathcal{P}z}\|_{H^\sigma_{pw}(\Gamma)} \\ &+ c_4 h^{\sigma+\frac{1}{2}}\|\omega_{\mathcal{P}z}\|_{H^\sigma_{pw}(\Gamma)} + c_5 h^{s-\frac{1}{2}}\|f_1\|_{H^s(\Gamma)} + c_6 h^{\sigma+\frac{1}{2}}\|\theta_{\gamma_0 u_p}\|_{H^\sigma_{pw}(\Gamma)} \\ &+ c_7 h^{\sigma+\frac{3}{2}}\|\omega_{\gamma_0 u_p}\|_{H^\sigma_{pw}(\Gamma)} + c_8 h^{s-\frac{1}{2}}\|\gamma_0 u_p\|_{H^s(\Gamma_N)} \\ &+ c_9 h^{\sigma+\frac{1}{2}}\|f_0\|_{H^\sigma_{pw}(\Gamma)} + c_{10} h^{\sigma+\frac{1}{2}}\|\widetilde{g}\|_{H^\sigma_{pw}(\Gamma)},\end{aligned}$$

when assuming $z, z_1, z_2 \in H^s(\Gamma_D)$, $\mathcal{T}_\alpha z - g \in \widetilde{H}^{s-1}(\Gamma_D)$, $w_z, \gamma_0 u_p \in H^s(\Gamma_N)$, $f_1 \in H^s(\Gamma)$ for some $s \in [\frac{1}{2}, 2]$ and $\theta_{\mathcal{P}z}, \omega_{\mathcal{P}z}, \theta_{\gamma_0 u_p}, \omega_{\gamma_0 u_p}, f_0, \widetilde{g} \in H^\sigma_{pw}(\Gamma)$ for some $\sigma \in [0,1]$. In particular for $s = \sigma + 1$, $\sigma \in [0,1]$ we therefore obtain the error estimate

$$\|z - \widehat{z}_h\|_{H^{1/2}(\Gamma_D)} \leq c(z, \psi, f, \overline{u})\, h^{\sigma+\frac{1}{2}}. \tag{4.79}$$

Moreover, by applying the Aubin-Nitsche trick we are able to derive an error estimate in $L_2(\Gamma_D)$, i.e.,

$$\|z - \widehat{z}_h\|_{L_2(\Gamma_D)} \leq c(z, \psi, f, \overline{u})\, h^{\sigma+1}. \tag{4.80}$$

Remark 4.1. *As in Proposition 3.1 we can conclude that u_z as defined in* (4.4) *is the solution of the bilateral constraints Signorini boundary value problem with an additional Neumann boundary condition. Then we may expect $u_z \in H^2(\Omega)$, and therefore $z \in H^{3/2}(\Gamma_D)$ for a smooth domain, see [5]. This results in a linear order of the error in $H^{1/2}(\Gamma_D)$. In the case of a polygonal or a polyhedral domain, we may have only a reduced regularity, see, e.g., [34].*

4.4 Numerical experiments

In our numerical example we consider the mixed boundary control problem (4.1) and (4.2) for the domain $\Omega = (0, \frac{1}{2})^2 \subset \mathbb{R}^2$. The boundary $\Gamma = \partial\Omega$ consists of two parts Γ_D and Γ_N where

$$\Gamma_D = \{(x_1, 0) : 0 < x_1 < 0.5\} \cup \{(0, x_2) : 0 < x_2 < 0.5\} \subset \Gamma, \quad \Gamma_N = \Gamma \setminus \overline{\Gamma}_D.$$

Let $\alpha = 0.1$ and the data are chosen as

$$\overline{u}(x) = (x_1^2 + x_2^2)^{-\frac{1}{3}}, \quad f(x) = 0, \quad \psi(x) = \frac{\partial}{\partial n_x}\overline{u}(x)|_{\Gamma_N}.$$

For the boundary element discretization we introduce a uniform triangulation of the boundary $\Gamma = \Gamma_D \cup \Gamma_N$ on several levels where the mesh size is $h_L = 2^{-(L+1)}$. Note that the minimizer of (4.1) is not known in this example, we use the boundary element solution $\widehat{z}_h$ on the 9th level as reference solution.

In Table 4.1 we present the errors for the control z and the estimated order of convergence (eoc). Moreover, we test the numerical results for the Dirichlet data on Γ_N. These results correspond to the error estimates (4.79) and (4.80).

L	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{L_2(\Gamma_D)}$	eoc	$\|\widehat{z}_{h_L} - \widehat{z}_{h_9}\|_{H^{1/2}(\Gamma_D)}$	eoc	$\|\widehat{u}_{h_L} - \widehat{u}_{h_9}\|_{L_2(\Gamma_N)}$	eoc
2	1.8041e-2	-	2.1236e-1	-	2.6788e-2	-
3	4.8635e-3	1.891	8.2073e-2	1.372	8.4929e-3	1.657
4	1.4322e-3	1.764	3.4331e-2	1.257	2.7877e-3	1.607
5	4.5382e-4	1.658	1.4228e-2	1.271	9.3811e-4	1.571
6	1.5562e-4	1.544	5.7832e-3	1.299	3.2225e-4	1.542
7	5.4047e-5	1.526	2.2475e-3	1.364	1.1217e-4	1.522
8	1.5723e-5	1.781	7.4669e-4	1.590	3.9334e-5	1.512

Table 4.1: The results of mixed boundary control problems without control constraints.

In this example, we expect a linear order of convergence in $H^{1/2}(\Gamma_D)$ norm and 1.5 as order of convergence in $L_2(\Gamma_D)$ norm as stated in Remark 4.1. Note that the target $\overline{u}$ has a singularity at the origin.

As a second example, we consider an additional constraint $z \leq 2.6$. In Figure 4.1 we give a comparison of the unconstrained and constrained solutions, and in Figure 4.2 we plot the related controls for $x_1 \in (0, 0.5)$, $x_2 = 0$.

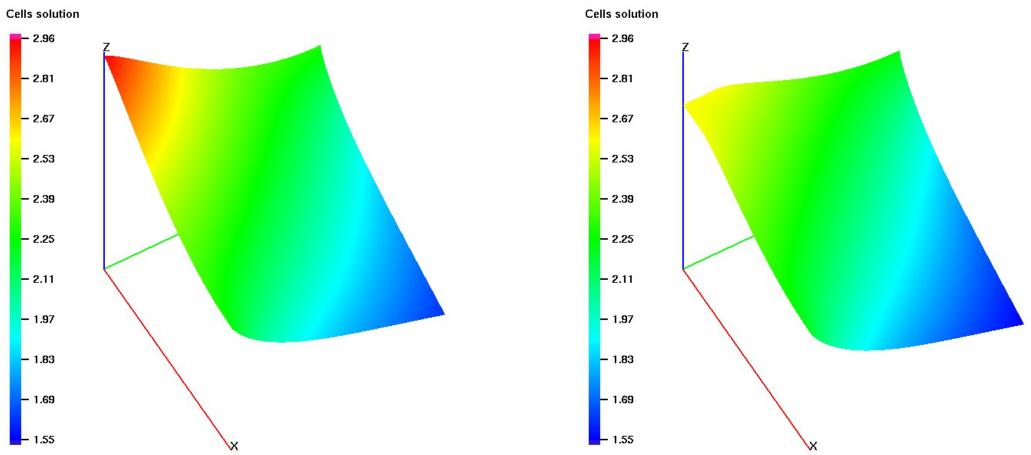

Figure 4.1: Comparison of unconstrained (left) and constrained (right) optimal solutions.

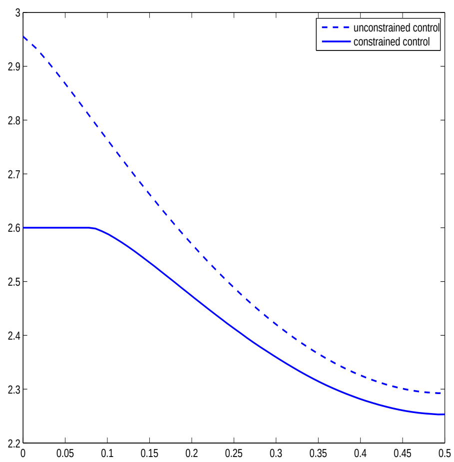

Figure 4.2: Optimal control of the unconstrained and constrained problems, $x_2 = 0$.

Moreover, we plot in Figure 4.3 the states u of the mixed boundary control problem (4.1)-(4.2) for $\alpha = 10^{-2}$ and $\alpha = 10^{-4}$. The singularity of the state at the origin appears clearly for small α, see also Figure 3.5 for the Dirichlet boundary control problem.

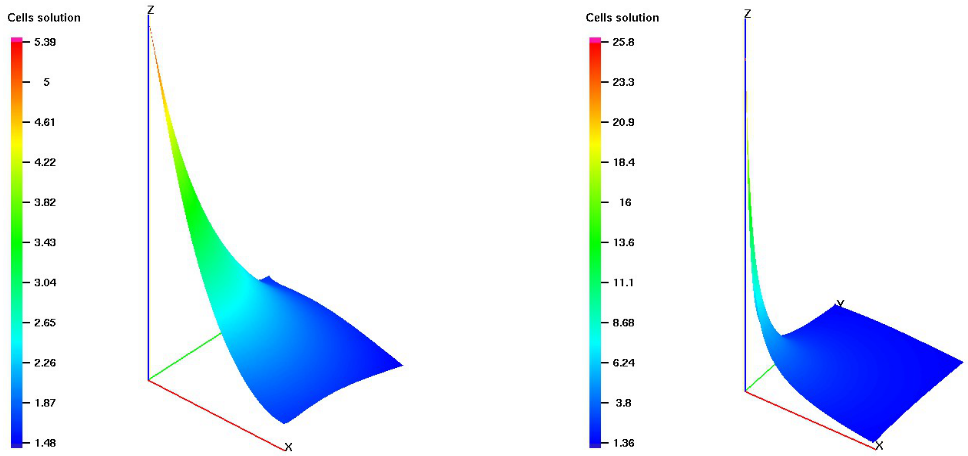

Figure 4.3: The states u with $\alpha = 10^{-2}$ (left) and $\alpha = 10^{-4}$ (right).

For comparison we consider the mixed boundary control problem (4.1)-(4.2) where the control z is in $L_2(\Gamma_D)$ with $\alpha = 0.1$. In Figure 4.4 we plot the state u for the $L_2(\Gamma_D)$ setting and the related control for $x_2 = 0$, and in Figure 4.5 we plot the related controls for $x_1 \in (0, 0.05)$, $x_2 = 0$ and for $x_1 \in (0.45, 0.5)$, $x_2 = 0$. As discussed in Section 3.7, the control is zero at all corner points.

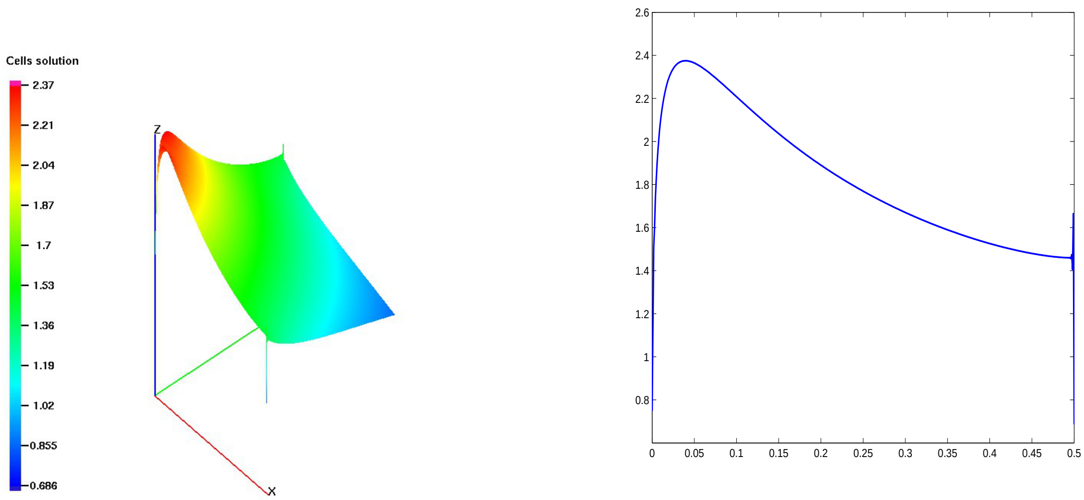

Figure 4.4: The state u for the $L_2(\Gamma_D)$ setting (left) and the related control for $x_2 = 0$ (right).

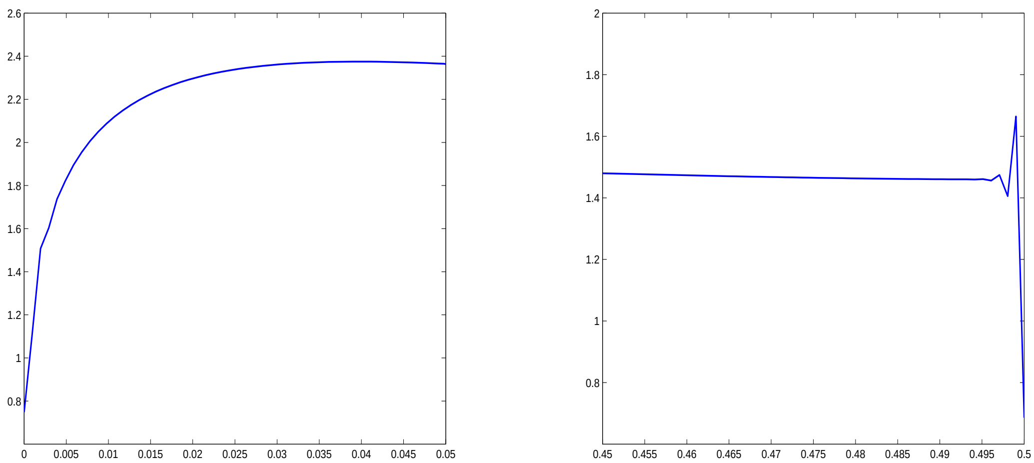

Figure 4.5: The related controls for $x_1 \in (0, 0.05)$, $x_2 = 0$ (left) and for $x_1 \in (0.45, 0.5)$, $x_2 = 0$ (right).

5 PARABOLIC BOUNDARY CONTROL PROBLEMS

The Dirichlet boundary optimal control problem governed by a linear heat equation is analysed in this chapter where the observed temperature is considered at the end time T. We propose boundary element approaches to solve the related coupled optimality system. Similar formulations of boundary integral equations as in the case of stationary boundary control problems are obtained. Again we ensure the unique solvability of the resulting variational inequalities and we derive a priori error estimates of Galerkin boundary element discretizations. This approach can be applied to the Neumann boundary control problem as well. Some numerical results are given at the end of the chapter.

In the first section a model problem is described where the control is considered in the energy space $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$. We use an equivalent norm in $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ which is induced by the hypersingular layer heat potential D, see [15] for instance. We also derive the optimality condition, i.e., the variational inequality to be solved. In Section 5.2 we discuss the boundary integral equations to solve the primal and the adjoint heat equations. For the boundary integral equations of the heat equation, see, for example [6, 15, 16, 26, 48, 60].

Since the temperature of the state at the end time T appears in a representation formula of the adjoint state as a volume density, an additional kernel which is based on the fundamental solution of the heat operator is considered. By Green's second formula, we can express the volume potential by some boundary potentials of the unknown data and some volume potentials of given densities. We end up with boundary integral equations in a symmetric formulation which is analyzed in Section 5.3. Again we discuss the stability and error estimates of a related Galerkin boundary element method. In Section 5.4, we present the main results of the application of the boundary element approach to the parabolic Neumann boundary control problem. Finally, we give some numerical results.

5.1 Parabolic Dirichlet boundary control problems

Let $\Omega \subset \mathbb{R}^d, d = 2,3$ be a bounded Lipschitz domain with boundary $\Gamma = \partial\Omega$. For a fixed real number $T > 0$, we write

$$I := (0,T), \quad Q := \Omega \times I, \quad \Sigma := \Gamma \times I.$$

To find a Dirichlet control z that minimizes the distance of the actual temperature $u(\cdot,T)$ at the end time and the desired temperature $\overline{u}$, we consider the cost functional

$$J(u,z) = \frac{1}{2}\int_\Omega [u(x,T)-\overline{u}(x)]^2\,dx + \frac{\alpha}{2}\langle Dz,z\rangle_\Sigma \tag{5.1}$$

to be minimized subject to

$$\begin{cases} \partial_t u(x,t) - \Delta u(x,t) = 0 & \text{for } (x,t)\in Q,\\ u(x,t) = z(x,t) & \text{for } (x,t)\in\Sigma,\\ u(x,0) = u_0(x) & \text{for } x\in\Omega, \end{cases} \tag{5.2}$$

and to pointwise control constraints

$$z\in\mathcal{U}_{ad} := \{w\in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)\colon z_1(x,t)\le w(x,t)\le z_2(x,t) \text{ for } (x,t)\in\Sigma\}. \tag{5.3}$$

Here $\overline{u},u_0\in L_2(\Omega)$, $\alpha\in\mathbb{R}_+$, $z_1,z_2\in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$, and the regularization term, via a norm in $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$, is defined by using the hypersingular heat boundary integral operator

$$D : H^{\frac{1}{2},\frac{1}{4}}(\Sigma)\to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma),$$

see [15]. For $z\in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ we have

$$(Dz)(x,t) := -\frac{\partial}{\partial n_x}\int_0^t\int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,t-\tau)z(y,\tau)\,ds_y\,d\tau \quad \text{for } (x,t)\in\Sigma,$$

where

$$\mathcal{E}(x,t) = \begin{cases} \dfrac{1}{(4\pi t)^{d/2}}e^{-\dfrac{|x|^2}{4t}} & \text{for } t>0,\\ 0 & \text{for } t\le 0 \end{cases} \tag{5.4}$$

is the fundamental solution of the heat equation. For the related Sobolev spaces, see Chapter 2, also [1, 15, 40].

Let v be a given function defined on $\Omega\times\mathbb{R}_+$ (or $\Gamma\times\mathbb{R}_+$) and $t_0\in\mathbb{R}_+$ be arbitrary. Define the time reversal map κ_{t_0} by

$$\kappa_{t_0}v(x,t) := v(x,t_0-t). \tag{5.5}$$

The hypersingular heat boundary integral operator D is $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$-elliptic and self-adjoint with respect to a "time-twisted" duality $\langle\cdot,\cdot\rangle := \langle\cdot,\kappa_T\cdot\rangle_\Sigma$, see [15], i.e.,

$$\langle Dz,z\rangle_\Sigma \ge c_1^D\|z\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}, \quad \langle Dz,\kappa_T w\rangle_\Sigma = \langle Dw,\kappa_T z\rangle_\Sigma \quad \text{for all } z,w\in H^{\frac{1}{2},\frac{1}{4}}(\Sigma). \tag{5.6}$$

In order to formulate the KKT system, we reduce the cost functional and obtain the optimality condition as follows, see [28, 38].

Theorem 5.1. *Let (u,z) be an optimal solution. Then there exists $p \in H_{0,}^{1,\frac{1}{2}}(Q)$ such that the following optimality system holds in the weak sense.*
Primal heat boundary value problem

$$\begin{cases} \partial_t u(x,t) - \Delta u(x,t) = 0 & \textit{for } (x,t) \in Q, \\ u(x,t) = z(x,t) & \textit{for } (x,t) \in \Sigma, \\ u(x,0) = u_0(x) & \textit{for } x \in \Omega. \end{cases}$$

Adjoint heat boundary value problem

$$\begin{cases} -\partial_t p(x,t) - \Delta p(x,t) = 0 & \textit{for } (x,t) \in Q, \\ p(x,t) = 0 & \textit{for } (x,t) \in \Sigma, \\ p(x,T) = u(x,T) - \overline{u}(x) & \textit{for } x \in \Omega. \end{cases} \tag{5.7}$$

Optimality condition

$$\langle \alpha \widetilde{D} z - \frac{\partial}{\partial n} p, w - z \rangle_\Sigma \geq 0 \quad \textit{for all } w \in \mathcal{U}_{ad}, \tag{5.8}$$

where

$$\widetilde{D} := \frac{1}{2}(D + \kappa_T D \kappa_T). \tag{5.9}$$

Proof. For a given $z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ there exists a unique solution $u_z \in H^{1,\frac{1}{2}}(Q)$ of the primal problem, see [15, 40]. Then the cost functional $J(u,z)$ can be rewritten as

$$\widetilde{J}(z) = \frac{1}{2}\|u_z(T) - \overline{u}\|^2_{L_2(\Omega)} + \frac{\alpha}{2}\langle Dz, z \rangle_\Sigma.$$

Let $h \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ be a given direction. We have

$$\begin{aligned} \widetilde{J}(z+h) - \widetilde{J}(z) &= \frac{1}{2}\|u_{z+h}(T) - \overline{u}\|^2_{L_2(\Omega)} - \frac{1}{2}\|u_z(T) - \overline{u}\|^2_{L_2(\Omega)} \\ &\qquad + \frac{\alpha}{2}\langle D(z+h), z+h \rangle_\Sigma - \frac{\alpha}{2}\langle Dz, z \rangle_\Sigma \\ &= \langle u_z(T) - \overline{u}, v(T) \rangle_{L_2(\Omega)} + \frac{1}{2}\|v(T)\|^2_{L_2(\Omega)} \\ &\qquad + \frac{\alpha}{2}\langle Dz, h \rangle_\Sigma + \frac{\alpha}{2}\langle Dh, z \rangle_\Sigma + \frac{\alpha}{2}\langle Dh, h \rangle_\Sigma \end{aligned}$$

where $u_{z+h}(x,t) = u_z(x,t) + v(x,t)$, and $v(x,t)$ is the unique solution of the problem

$$\partial_t v(x,t) - \Delta v(x,t) = 0 \quad \text{in } Q, \quad v(x,t) = h(x,t) \quad \text{on } \Sigma, \quad v(x,0) = 0 \quad \text{on } \Omega.$$

Applying Green's second formula for the pair (v,p),

$$\int_0^T\int_\Omega [p(\partial_t-\Delta)v+v(\partial_t+\Delta)p]\,dx\,dt=\int_0^T\int_\Gamma\left(\frac{\partial}{\partial n}p(x,t)v(x,t)-\frac{\partial}{\partial n}v(x,t)p(x,t)\right)ds_x\,dt$$
$$+\int_\Omega [v(x,T)p(x,T)-v(x,0)p(x,0)]\,dx$$

we get

$$\langle u_z(T)-\overline{u},v(T)\rangle_{L_2(\Omega)}+\langle\frac{\partial}{\partial n}p,h\rangle_\Sigma=0.$$

Therefore, by using the self-adjointness of the operator D, see (5.6), we obtain

$$\begin{aligned}\widetilde{J}(z+h)-\widetilde{J}(z)&=\frac{\alpha}{2}\langle Dz,h\rangle_\Sigma+\frac{\alpha}{2}\langle\kappa_T D\kappa_T z,h\rangle_\Sigma-\langle\frac{\partial}{\partial n}p,h\rangle_\Sigma+\frac{1}{2}\|v(T)\|^2_{L_2(\Omega)}+\frac{\alpha}{2}\langle Dh,h\rangle_\Sigma\\&=\langle\alpha\widetilde{D}z-\frac{\partial}{\partial n}p,h\rangle_\Sigma+o\left(\|h\|_{H^{\frac12,\frac14}(\Sigma)}\right),\end{aligned}$$

since $\|v(T)\|_{L_2(\Omega)}\le c\|h\|_{H^{\frac12,\frac14}(\Sigma)}$ and $D:H^{\frac12,\frac14}(\Sigma)\to H^{-\frac12,-\frac14}(\Sigma)$ is a bounded operator. This implies that the gradient of $\widetilde{J}(z)$ satisfies

$$\langle\nabla\widetilde{J}(z),h\rangle_\Sigma=\langle\alpha\widetilde{D}z-\frac{\partial}{\partial n}p,h\rangle_\Sigma.$$

The assertion follows, see also [28, 38]. □

In the following we will use a boundary element approach to solve the coupled problem of the primal heat equation (5.2), the adjoint heat equation (5.7) and the optimality condition (5.8).

5.2 Boundary integral equations

The boundary integral equations for the heat equation are first recalled. Some properties of the standard boundary integral layer heat operators can be found in, e.g., [15]. For the adjoint heat equation, instead of using the volume potential of the state u, we introduce some boundary potentials with a regular kernel. We also discuss some properties of these operators. The related anisotropic Sobolev spaces were introduced in Chapter 2.

The primal heat equation

Let us first start with the primal heat equation. The solution of the primal heat equation (5.2) can be written by the representation formula for $(\widetilde{x},t) \in Q$,

$$u(\widetilde{x},t) = \int_0^t \int_\Gamma \mathcal{E}(\widetilde{x}-y,t-\tau)\frac{\partial}{\partial n_y}u(y,\tau)\,ds_y\,d\tau - \int_0^t \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(\widetilde{x}-y,t-\tau)z(y,\tau)\,ds_y\,d\tau + \int_\Omega \mathcal{E}(\widetilde{x}-y,t)u_0(y)\,dy, \quad (5.10)$$

where $\mathcal{E}(x,t)$ is the fundamental solution of the heat equation as given in (5.4). By taking $\Omega \ni \widetilde{x} \to x \in \Gamma$, we obtain the first kind boundary integral equation to find $\omega(x,t) := \frac{\partial}{\partial n}u(x,t)$,

$$(V\omega)(x,t) = (\frac{1}{2}I+K)z(x,t) - (M_0u_0)(x,t) \quad \text{for } (x,t) \in \Sigma, \quad (5.11)$$

where

$$(V\omega)(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\omega(y,\tau)\,ds_y\,d\tau \quad \text{for } (x,t) \in \Sigma$$

is the single layer heat potential $V : H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ and

$$(Kz)(x,t) = \int_0^t \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,t-\tau)z(y,\tau)\,ds_y\,d\tau \quad \text{for } (x,t) \in \Sigma$$

is the double layer heat potential $K : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$, see [15]. Moreover, for $(x,t) \in \Sigma$,

$$(M_0u_0)(x,t) = \int_\Omega \mathcal{E}(x-y,t)u_0(y)\,dy$$

is the related Newton potential. As stated in [15], the single layer heat potential V is $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$-elliptic, i.e.,

$$\langle V\omega,\omega\rangle_\Sigma \geq c_1^V \|\omega\|^2_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \quad \text{for all } \omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma).$$

Then the boundary integral equation (5.11) is solvable for a given Dirichlet datum z,

$$\omega = V^{-1}(\frac{1}{2}I+K)z - V^{-1}M_0u_0. \quad (5.12)$$

The adjoint heat equation

We now consider the adjoint heat equation (5.7). The time reversal of the adjoint state variable, $\kappa_T p$ solves the heat equation, i.e.,

$$\begin{cases} \partial_t(\kappa_T p)(x,t) - \Delta(\kappa_T p)(x,t) = 0 & \text{for } (x,t) \in Q, \\ (\kappa_T p)(x,t) = 0 & \text{for } (x,t) \in \Sigma, \\ (\kappa_T p)(x,0) = u(x,T) - \overline{u}(x) & \text{for } x \in \Omega. \end{cases}$$

Then we have the representation formula for $(\widetilde{x},t) \in Q$,

$$(\kappa_T p)(\widetilde{x},t) = \int_0^t \int_\Gamma \mathcal{E}(\widetilde{x}-y,t-\tau) \frac{\partial}{\partial n_y} \kappa_T p(y,\tau)\, ds_y\, d\tau + \int_\Omega \mathcal{E}(\widetilde{x}-y,t)(\kappa_T p)(y,0)\, dy. \tag{5.13}$$

This gives the first kind boundary integral equation

$$(V(\kappa_T q))(x,t) = (M_0\overline{u})(x,t) - (M_0 u(\cdot,T))(x,t) \quad \text{for } (x,t) \in \Sigma \tag{5.14}$$

to determine the unknown Neumann datum $q(x,t) = \dfrac{\partial}{\partial n_x} p(x,t)$ for $(x,t) \in \Sigma$.

In (5.14) the unknown state $u(\cdot,T)$ at the end time T appears in the Newton potential. As discussed in Chapter 3 we will modify the representation formula (5.13). The crucial idea is to use an auxiliary function

$$G(x,t,\tau) = \left(\frac{t}{T+t-\tau}\right)^{d/2} e^{\frac{T-\tau}{T+t-\tau}\frac{|x|^2}{4t}} \quad \text{for } x \in \Omega;\ t,\tau \in (0,T) \tag{5.15}$$

which satisfies

$$\mathcal{E}(\widetilde{x}-y,t)G(\widetilde{x}-y,t,\tau) = \mathcal{E}(\widetilde{x}-y,T+t-\tau).$$

We first write the Newton potential in the representation formula (5.13) as

$$(\widetilde{M}_0 u(\cdot,T))(\widetilde{x},t) = \int_\Omega \mathcal{E}(\widetilde{x}-y,t)u(y,T)\, dy \quad \text{for } (\widetilde{x},t) \in Q. \tag{5.16}$$

By $\lim\limits_{\tau\to T^-} G(\widetilde{x}-y,t,\tau) = 1$ for all $t \in (0,T)$, $y \in \Omega$ we have

$$\begin{aligned} u(y,T) &= u(y,T)G(\widetilde{x}-y,t,T) - u(y,0)G(\widetilde{x}-y,t,0) + u_0(y)G(\widetilde{x}-y,t,0) \\ &= \int_0^T \partial_\tau[u(y,\tau)G(\widetilde{x}-y,t,\tau)]\, d\tau + u_0(y)G(\widetilde{x}-y,t,0) \\ &= \int_0^T \partial_\tau G(\widetilde{x}-y,t,\tau)u(y,\tau)\, d\tau + \int_0^T G(\widetilde{x}-y,t,\tau)\partial_\tau u(y,\tau)\, d\tau + u_0(y)G(\widetilde{x}-y,t,0). \end{aligned}$$

Hence for $\partial_\tau u(y,\tau) = \Delta_y u(y,\tau)$ we can rewrite the Newton potential in (5.16)

$$(\widetilde{M}_0 u(\cdot,T))(\widetilde{x},t) = \int_0^T \int_\Omega \mathcal{E}(\widetilde{x}-y,t)\partial_\tau G(\widetilde{x}-y,t,\tau)u(y,\tau)\,dy\,d\tau$$
$$+ \int_0^T \int_\Omega \mathcal{E}(\widetilde{x}-y,t)G(\widetilde{x}-y,t,\tau)\Delta_y u(y,\tau)\,dy\,d\tau + \int_\Omega \mathcal{E}(\widetilde{x}-y,t)G(\widetilde{x}-y,t,0)u_0(y)\,dy.$$

It is easy to check that

$$\Delta_y[\mathcal{E}(\widetilde{x}-y,t)G(\widetilde{x}-y,t,\tau)] = \Delta_y \mathcal{E}(\widetilde{x}-y,T+t-\tau) = -\mathcal{E}(\widetilde{x}-y,t)\partial_\tau G(\widetilde{x}-y,t,\tau),$$

and by definition, we have

$$\mathcal{E}(\widetilde{x}-y,t)G(\widetilde{x}-y,t,\tau) = \mathcal{E}(\widetilde{x}-y,T+t-\tau).$$

Together with Green's second formula we finally obtain

$$(\widetilde{M}_0 u(\cdot,T))(\widetilde{x},t) = \int_0^T \int_\Omega [\mathcal{E}(\widetilde{x}-y,T+t-\tau)\Delta_y u(y,\tau) - u(y,\tau)\Delta_y \mathcal{E}(\widetilde{x}-y,T+t-\tau)]\,dy\,d\tau$$
$$+ \int_\Omega \mathcal{E}(\widetilde{x}-y,T+t)u_0(y)\,dy$$
$$= \int_0^T \int_\Gamma \left[\mathcal{E}(\widetilde{x}-y,T+t-\tau)\frac{\partial}{\partial n_y}u(y,\tau) - u(y,\tau)\frac{\partial}{\partial n_y}\mathcal{E}(\widetilde{x}-y,T+t-\tau)\right] ds_y\,d\tau$$
$$+ \int_\Omega \mathcal{E}(\widetilde{x}-y,T+t)u_0(y)\,dy$$

and this gives the modified representation formula for the adjoint variable for $(\widetilde{x},t) \in Q$,

$$\kappa_T p(\widetilde{x},t) = \int_0^t \int_\Gamma \mathcal{E}(\widetilde{x}-y,t-\tau)\frac{\partial}{\partial n_y}\kappa_T p(y,\tau)\,ds_y\,d\tau - \int_\Omega \mathcal{E}(\widetilde{x}-y,t)\overline{u}(y)\,dy$$
$$+ \int_0^T \int_\Gamma \left[\mathcal{E}(\widetilde{x}-y,T+t-\tau)\frac{\partial}{\partial n_y}u(y,\tau) - u(y,\tau)\frac{\partial}{\partial n_y}\mathcal{E}(\widetilde{x}-y,T+t-\tau)\right] ds_y\,d\tau$$
$$+ \int_\Omega \mathcal{E}(\widetilde{x}-y,T+t)u_0(y)\,dy. \quad (5.17)$$

Taking the limit $\Omega \ni \widetilde{x} \to x \in \Gamma$ without jump relations, we obtain a boundary integral equation

$$0 = (V(\kappa_T q))(x,t) + (V_1\omega)(x,t) - (K_1 z)(x,t) - (M_0\overline{u})(x,t) + (M_{10}u_0)(x,t) \qquad (5.18)$$

for $(x,t) \in \Sigma$ where

$$(V_1\omega)(x,t) = \int_0^T \int_\Gamma \mathcal{E}(x-y, T+t-\tau)\omega(y,\tau)\, ds_y\, d\tau \quad \text{for } (x,t) \in \Sigma, \qquad (5.19)$$

$$(K_1 z)(x,t) = \int_0^T \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y, T+t-\tau) z(y,\tau)\, ds_y\, d\tau \quad \text{for } (x,t) \in \Sigma \qquad (5.20)$$

are the bi-single and the bi-double layer heat potentials. Moreover, we introduce a new volume potential

$$(M_{10}u_0)(x,t) = \int_\Omega \mathcal{E}(x-y, T+t) u_0(y) dy \quad \text{for } (x,t) \in \Sigma.$$

Inserting (5.12) into the boundary integral equation (5.18), this gives

$$V(\kappa_T q) = K_1 z - V_1 V^{-1}(\frac{1}{2}I + K)z + V_1 V^{-1} M_0 u_0 + M_0\overline{u} - M_{10}u_0,$$

and hence

$$\kappa_T q = V^{-1}K_1 z - V^{-1}V_1V^{-1}(\frac{1}{2}I+K)z + V^{-1}V_1V^{-1}M_0u_0 + V^{-1}M_0\overline{u} - V^{-1}M_{10}u_0. \quad (5.21)$$

Now the optimality condition (5.8) can be rewritten as a variational inequality to find $z \in \mathcal{U}_{ad}$, such that

$$\langle \mathcal{T}_\alpha z - g, w - z\rangle_\Sigma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \qquad (5.22)$$

where

$$\mathcal{T}_\alpha := \alpha\widetilde{D} - \kappa_T V^{-1}K_1 + \kappa_T V^{-1}V_1V^{-1}(\frac{1}{2}I + K) \qquad (5.23)$$

and

$$g := \kappa_T V^{-1}M_0\overline{u} + \kappa_T\left(V^{-1}V_1V^{-1}M_0 - V^{-1}M_{10}\right)u_0. \qquad (5.24)$$

Mapping properties

To investigate the properties of the composed boundary integral operator $\mathcal{T}_\alpha$ as defined in (5.23), let us summarize some properties of the bi-layer heat potentials V_1, K_1 which are similar to the properties of the Bi-Laplace layer potentials as given in Chapter 3.

Once again, for $t \in (0,T)$ let $\gamma_0 \cdot (\cdot,t)$, $\gamma_1 \cdot (\cdot,t)$ be the Dirichlet and the Neumann trace maps, respectively.

Lemma 5.1. *For $\omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, there holds*

$$\langle (\frac{1}{2}I + K')\omega, \kappa_T V_1 \omega \rangle_\Sigma - \langle \kappa_T K_1' \omega, V\omega \rangle_\Sigma = \|(\widetilde{V}\omega)(\cdot,T)\|^2_{L_2(\Omega)} \tag{5.25}$$

where

$$(\widetilde{V}\omega)(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\omega(y,\tau)\,ds_y\,d\tau \quad \textit{for } (x,t) \in Q,$$

and

$$(K'\omega)(x,t) = \int_0^t \int_\Gamma \frac{\partial}{\partial n_x}\mathcal{E}(x-y,t-\tau)\omega(y,\tau)\,ds_y\,d\tau \quad \textit{for } (x,t) \in \Sigma, \tag{5.26}$$

$$(K_1'\omega)(x,t) = \int_0^T \int_\Gamma \frac{\partial}{\partial n_x}\mathcal{E}(x-y,T+t-\tau)\omega(y,\tau)\,ds_y\,d\tau \quad \textit{for } (x,t) \in \Sigma. \tag{5.27}$$

The operators K', K_1' are the adjoint of the operators K, K_1 with respect to the "time-twisted" duality, respectively, i.e.,

$$\langle \kappa_T \omega, Kz \rangle_\Sigma = \langle \kappa_T z, K'\omega \rangle_\Sigma, \quad \langle \kappa_T \omega, K_1 z \rangle_\Sigma = \langle \kappa_T z, K_1'\omega \rangle_\Sigma. \tag{5.28}$$

Proof. Consider the following functions for $(x,t) \in Q$

$$u(x,t) = (\widetilde{V}\omega)(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\omega(y,\tau)\,ds_y\,d\tau,$$

$$v(x,t) = \int_0^T \int_\Gamma \mathcal{E}(x-y,2T-t-\tau)\omega(y,\tau)\,ds_y\,d\tau.$$

The functions u and v solve the heat equation and the adjoint heat equation, respectively,

$$\partial_t u(x,t) - \Delta u(x,t) = 0, \quad -\partial_t v(x,t) - \Delta v(x,t) = 0 \quad \text{for } (x,t) \in Q,$$

and there hold

$$u(x,T) = v(x,T), \quad u(x,0) = 0.$$

The application of the trace maps gives

$$\gamma_0 u(x,t) = (V\omega)(x,t), \qquad \gamma_1 u(x,t) = (\frac{1}{2}I + K')\omega(x,t),$$

$$\gamma_0 v(x,t) = \kappa_T (V_1\omega)(x,t), \qquad \gamma_1 v(x,t) = \kappa_T (K_1'\omega)(x,t).$$

The assertion now follows from Green's second formula

$$\int_0^T\int_\Omega [v(\partial_t-\Delta)u+u(\partial_t+\Delta)v]\,dx\,dt=\int_0^T\int_\Gamma[\gamma_1 v(x,t)\gamma_0 u(x,t)-\gamma_1 u(x,t)\gamma_0 v(x,t)]\,ds_x\,dt$$
$$+\int_\Omega[u(x,T)v(x,T)-u(x,0)v(x,0)]\,dx.$$

□

As in the case of the Bi-Laplace operator, see Corollary 3.1, we can state the following properties.

Lemma 5.2. *For the boundary integral operators, there hold*

$$KV=VK',\quad DK=K'D,\quad VD=\frac{1}{4}I-K^2,\quad DV=\frac{1}{4}I-K'^2, \tag{5.29}$$

$$V^{-1}(\frac{1}{2}I+K)=D+(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K), \tag{5.30}$$

and

$$VK_1'+V_1K'=K_1V+KV_1, \tag{5.31}$$

$$DK_1-D_1K=K_1'D-K'D_1, \tag{5.32}$$

$$V_1D-VD_1+KK_1+K_1K=0, \tag{5.33}$$

$$DV_1-D_1V+K'K_1'+K_1'K'=0, \tag{5.34}$$

where D_1 is the normal derivative of the bi-double layer heat potential K_1,

$$(D_1z)(x,t)=\frac{\partial}{\partial n_x}\int_0^T\int_\Gamma\frac{\partial}{\partial n_y}\mathcal{E}(x-y,T+t-\tau)z(y,\tau)\,ds_y\,d\tau,\quad (x,t)\in\Sigma. \tag{5.35}$$

Proof. The relations of (5.29) for the layer heat potentials are well known, see [15]. The relation of (5.30) is an alternative representation of the so-called Dirichlet to Neumann operator, see Corollary 3.1 for similar properties of the Laplace boundary integral operators. Indeed, by (5.29) we have

$$\begin{aligned}D+(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K) &= V^{-1}(\frac{1}{4}I-K^2)+(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K)\\ &= V^{-1}(\frac{1}{2}I-K)(\frac{1}{2}I+K)+(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K)\\ &= (\frac{1}{2}V^{-1}-K'V^{-1})(\frac{1}{2}I+K)+(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K)\\ &= V^{-1}(\frac{1}{2}I+K).\end{aligned}$$

Moreover, for the relations (5.31)-(5.34) let $\omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, $\varphi \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ be arbitrary. We then define functions for $(x,t) \in Q$,

$$u(x,t) = \int_0^T \int_\Gamma \mathcal{E}(x-y,T+t-\tau)\omega(y,\tau)\,ds_y\,d\tau + \int_0^T \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,T+t-\tau)\varphi(y,\tau)\,ds_y\,d\tau,$$

$$v(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\omega(y,\tau)\,ds_y\,d\tau + \int_0^t \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,t-\tau)\varphi(y,\tau)\,ds_y\,d\tau.$$

These functions solve the heat equation. Their related boundary and initial conditions are given by

$$\gamma_0 u = V_1\omega + K_1\varphi, \qquad \gamma_1 u = K_1'\omega + D_1\varphi, \qquad u(x,0) = v(x,T),$$

$$\gamma_0 v = V\omega + (-\frac{1}{2}I + K)\varphi, \qquad \gamma_1 v = (\frac{1}{2}I + K')\omega - D\varphi, \qquad v(x,0) = 0.$$

Moreover, by $u(x,0) = v(x,T)$ we can also represent the function $u(x,t)$ for $(x,t) \in Q$, by

$$u(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\gamma_1 u(y,\tau)\,ds_y\,d\tau - \int_0^t \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,t-\tau)\gamma_0 u(y,\tau)\,ds_y\,d\tau + \int_\Omega \mathcal{E}(x-y,t)v(y,T)\,dy.$$

Again, we modify the volume potential as in (5.16) to obtain the representation formula

$$u(x,t) = \int_0^t \int_\Gamma \mathcal{E}(x-y,t-\tau)\gamma_1 u(y,\tau)\,ds_y\,d\tau - \int_0^t \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,t-\tau)\gamma_0 u(y,\tau)\,ds_y\,d\tau$$
$$+ \int_0^T \int_\Gamma \mathcal{E}(x-y,T+t-\tau)\gamma_1 v(y,\tau)\,ds_y\,d\tau - \int_0^T \int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y,T+t-\tau)\gamma_0 v(y,\tau)\,ds_y\,d\tau.$$

This gives the following traces

$$\begin{pmatrix} \gamma_0 u \\ \gamma_1 u \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V & -K_1 & V_1 \\ D & \frac{1}{2}I + K' & -D_1 & K_1' \end{pmatrix} \begin{pmatrix} \gamma_0 u \\ \gamma_1 u \\ \gamma_0 v \\ \gamma_1 v \end{pmatrix}.$$

By inserting the traces of the functions u and v, we obtain

$$V_1\omega + K_1\varphi = (\frac{1}{2}I - K)[V_1\omega + K_1\varphi] + V[K_1'\omega + D_1\varphi]$$
$$- K_1[V\omega + (-\frac{1}{2}I + K)\varphi] + V_1[(\frac{1}{2}I + K')\omega - D\varphi],$$

and

$$K_1'\omega + D_1\varphi = D[V_1\omega + K_1\varphi] + (\frac{1}{2}I + K')[K_1'\omega + D_1\varphi]$$
$$- D_1[V\omega + (-\frac{1}{2}I + K)\varphi] + K_1'[(\frac{1}{2}I + K')\omega - D\varphi],$$

for all $\omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, $\varphi \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ which imply

$$V_1 = (\frac{1}{2}I - K)V_1 + VK_1' - K_1V + V_1(\frac{1}{2}I + K'),$$
$$K_1 = (\frac{1}{2}I - K)K_1 + VD_1 + K_1(\frac{1}{2}I - K) - V_1D,$$
$$K_1' = DV_1 + (\frac{1}{2}I + K')K_1' - D_1V + K_1'(\frac{1}{2}I + K'),$$
$$D_1 = DK_1 + (\frac{1}{2}I + K')D_1 + D_1(\frac{1}{2}I - K) - K_1'D,$$

and the assertion follows. □

Note that V, D, V_1, D_1 are self-adjoint operators with respect to the "time-twisted" duality, see (5.6) for D, and hence the operator $\widetilde{D}$ is self-adjoint with respect to the inner product $\langle\cdot,\cdot\rangle_\Sigma$, i.e.,

$$\langle V\omega, \kappa_T\theta\rangle_\Sigma = \langle V\theta, \kappa_T\omega\rangle_\Sigma, \qquad \langle V_1\omega, \kappa_T\theta\rangle_\Sigma = \langle V_1\theta, \kappa_T\omega\rangle_\Sigma, \tag{5.36}$$
$$\langle D_1\varphi, \kappa_T w\rangle_\Sigma = \langle D_1 w, \kappa_T\varphi\rangle_\Sigma, \qquad \langle \widetilde{D}\varphi, w\rangle_\Sigma = \langle \widetilde{D}w, \varphi\rangle_\Sigma, \tag{5.37}$$

for all $\omega, \theta \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, $\varphi, w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$.

Lemma 5.3. *For the operator*

$$A := \begin{pmatrix} V_1 & -K_1 \\ -K_1' & D_1 \end{pmatrix},$$

there holds for $\omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, $\varphi \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$,

$$\langle A\begin{pmatrix}\omega\\ \varphi\end{pmatrix}, \kappa_T\begin{pmatrix}\omega\\ \varphi\end{pmatrix}\rangle_\Sigma = \langle V_1\omega, \kappa_T\omega\rangle_\Sigma - \langle K_1\varphi, \kappa_T\omega\rangle_\Sigma - \langle K_1'\omega, \kappa_T\varphi\rangle_\Sigma + \langle D_1\varphi, \kappa_T\varphi\rangle_\Sigma \geq 0.$$

Proof. For $\omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$, $\varphi \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$, we define functions in $Q \cup Q_R^c$

$$u(x,t) = \int_0^T\int_\Gamma \mathcal{E}(x-y, T+t-\tau)\omega(y,\tau)\,ds_y\,d\tau - \int_0^T\int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y, T+t-\tau)\varphi(y,\tau)\,ds_y\,d\tau,$$

$$v(x,t) = \int_0^t\int_\Gamma \mathcal{E}(x-y, t-\tau)\omega(y,\tau)\,ds_y\,d\tau - \int_0^t\int_\Gamma \frac{\partial}{\partial n_y}\mathcal{E}(x-y, t-\tau)\varphi(y,\tau)\,ds_y\,d\tau.$$

Here, we define a complementary domain

$$\Omega_R^c := B_R \setminus \overline{\Omega} \quad \text{and} \quad Q_R^c := \Omega_R^c \times I,$$

where $B_R := \{x \in \mathbb{R}^d : |x| < R\}$ is a sufficiently large ball containing Γ, see [15].
The functions u, v solve the heat equation in $Q \cup Q_R^c$. The related boundary traces of u are given by

$$\gamma_0 u = V_1 \omega - K_1 \varphi, \quad \gamma_1 u = K_1' \omega - D_1 \varphi.$$

For the function v, there hold the jump relations across Σ,

$$[\gamma_0 v] := \gamma_0(v|_{Q^c}) - \gamma_0(v|_Q) = -\varphi, \quad [\gamma_1 v] := \gamma_1(v|_{Q^c}) - \gamma_1(v|_Q) = -\omega.$$

The above equations allow us to write the bilinear form in terms of the traces of u and v,

$$\begin{aligned}
\langle A \begin{pmatrix} \omega \\ \varphi \end{pmatrix}, \kappa_T \begin{pmatrix} \omega \\ \varphi \end{pmatrix} \rangle_\Sigma &= \langle \begin{pmatrix} \gamma_0 u \\ -\gamma_1 u \end{pmatrix}, \kappa_T \begin{pmatrix} -[\gamma_1 v] \\ -[\gamma_0 v] \end{pmatrix} \rangle_\Sigma \\
&= \langle \gamma_0 u, \kappa_T \gamma_1(v|_Q) \rangle_\Sigma - \langle \gamma_0 u, \kappa_T \gamma_1(v|_{Q^c}) \rangle_\Sigma \\
&\qquad + \langle \gamma_1 u, \kappa_T \gamma_0(v|_{Q^c}) \rangle_\Sigma - \langle \gamma_1 u, \kappa_T \gamma_0(v|_Q) \rangle_\Sigma \\
&= \langle \gamma_0(u|_Q), \kappa_T \gamma_1(v|_Q) \rangle_\Sigma - \langle \gamma_1(u|_Q), \kappa_T \gamma_0(v|_Q) \rangle_\Sigma \\
&\qquad + \langle \gamma_1(u|_{Q^c}), \kappa_T \gamma_0(v|_{Q^c}) \rangle_\Sigma - \langle \gamma_0(u|_{Q^c}), \kappa_T \gamma_1(v|_{Q^c}) \rangle_\Sigma.
\end{aligned}$$

The application of Green's second formula to the solutions u, v of the heat equation in Q and Q_R^c gives

$$\langle \gamma_0(u|_Q), \kappa_T \gamma_1(v|_Q) \rangle_\Sigma - \langle \gamma_1(u|_Q), \kappa_T \gamma_0(v|_Q) \rangle_\Sigma = \int_\Omega u(x,0) v(x,T)\, dx = \int_\Omega [u(x,0)]^2\, dx,$$

$$\begin{aligned}
\langle \gamma_1(u|_{Q^c}), \kappa_T \gamma_0(v|_{Q^c}) \rangle_\Sigma - \langle \gamma_0(u|_{Q^c}), \kappa_T \gamma_1(v|_{Q^c}) \rangle_\Sigma &= \int_{\Omega_R^c} [u(x,0)]^2\, dx - \langle \gamma_1 v, \kappa_T \gamma_0 u \rangle_{\partial B_R \times I} \\
&\qquad + \langle \gamma_1 u, \kappa_T \gamma_0 v \rangle_{\partial B_R \times I}.
\end{aligned}$$

Thus we obtain

$$\langle A \begin{pmatrix} \omega \\ \varphi \end{pmatrix}, \kappa_T \begin{pmatrix} \omega \\ \varphi \end{pmatrix} \rangle_\Sigma = \int_{\Omega \cup \Omega_R^c} [u(x,0)]^2\, dx - \int_{\partial B_R \times I} \kappa_T u \partial_r v\, ds_x\, dt + \int_{\partial B_R \times I} \kappa_T v \partial_r u\, ds_x\, dt.$$

We will show that the last two terms tend to zero as $R \to \infty$. To do this, let us consider the function v first. Let us choose $0 < R_0 < R$ such that $\overline{\Omega} \subset B_{R_0}$. By the representation formula for the solution v of the heat equation, it follows that outside $Q_{R_0}^c$, in particular for $|x| > R_0$, the function v coincides with

$$v_0(x,t) := \int_0^t \int_{\partial B_{R_0}} \mathcal{E}(x-y, t-\tau) \omega_0(y,\tau)\, ds_y\, d\tau - \int_0^t \int_{\partial B_{R_0}} \frac{\partial}{\partial n_y} \mathcal{E}(x-y, t-\tau) \varphi_0(y,\tau)\, ds_y\, d\tau,$$

where the single and the double layer potentials are now defined for density functions on $\Sigma_{R_0} := \partial B_{R_0} \times I$,

$$\omega_0 := \partial_r v|_{\Sigma_{R_0}}, \quad \varphi_0 := v|_{\Sigma_{R_0}}.$$

The densities ω_0, φ_0, as well as the new boundary Σ_{R_0}, are smooth. We can now easily estimate v, and $\partial_r v$ on the boundary Σ_R for $R > R_0$, using the behaviour of the fundamental solution $\mathcal{E}(x,t)$. From the simple estimates

$$|\mathcal{E}(x,t)| \leq c_\mu t^{-\mu} |x|^{2\mu-d}, \quad |\nabla \mathcal{E}(x,t)| \leq c_\mu t^{-\mu} |x|^{2\mu-d-1}$$

and

$$|\frac{\partial^2}{\partial x_i \partial x_j} \mathcal{E}(x,t)| \leq c_\mu t^{-\mu} |x|^{2\mu-d-2}$$

for all $\mu \in \mathbb{R}; i, j = 1,2$, we obtain for finite T,

$$\kappa_T v = \mathcal{O}(R^{-d}), \quad \partial_r v = \mathcal{O}(R^{-d-1}), \quad \text{as} \quad |x| = R \to \infty.$$

Similarly, for $(x,t) \in \partial B_R \times I$, the kernel $\mathcal{E}(x-y, T+t-\tau)$, $(y,\tau) \in \Sigma$ is smooth. Then $\kappa_T u$ and $\partial_r u$ are bounded as $|x| = R \to \infty$. Hence

$$-\int\limits_{\partial B_R \times I} \kappa_T u \partial_r v \, ds_x \, dt + \int\limits_{\partial B_R \times I} \kappa_T v \partial_r u \, ds_x \, dt = \mathcal{O}(R^{-1}) \to 0 \quad \text{as} \quad |x| = R \to \infty.$$

Hence we finally conclude

$$\langle A \begin{pmatrix} \omega \\ \varphi \end{pmatrix}, \kappa_T \begin{pmatrix} \omega \\ \varphi \end{pmatrix} \rangle_\Sigma = \int\limits_{\mathbb{R}^d} [u(x,0)]^2 \, dx \geq 0.$$

□

Corollary 5.1. *The operators V_1 and D_1 are positive semi-definite with respect to the "time-twisted" duality $\langle \cdot, \cdot \rangle = \langle \cdot, \kappa_T \cdot \rangle_\Sigma$, i.e.,*

$$\langle V_1 \omega, \kappa_T \omega \rangle_\Sigma \geq 0, \quad \langle D_1 \varphi, \kappa_T \varphi \rangle_\Sigma \geq 0 \quad \textit{for all } \omega \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma), \varphi \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma).$$

To close this section, let us recall the mapping properties of the Newton potential $\widetilde{M}_0$ as defined in (5.16), see [48, Lemma 7.10]. For the mapping property of $\widetilde{M}_0$ in a higher order Sobolev space, see [37, chapter IV].

Lemma 5.4. *Let Ω denote any bounded, open subset in $\mathbb{R}^d$. For any $f \in L_2(\Omega)$, let*

$$(\widetilde{M}_0 f)(x,t) = \int\limits_\Omega \mathcal{E}(x-y,t) f(y) \, dy, \quad x \in \mathbb{R}^d, \quad t > 0.$$

Then there exists a positive constant $C(\Omega)$ such that

$$\|\widetilde{M}_0 f\|_{\mathcal{V}(Q)} \leq C(\Omega) \|f\|_{L_2(\Omega)}.$$

The function $\widetilde{M}_0 f$ solves the homogeneous heat equation. By [15, Lemma 2.15], the norms of $\mathcal{V}(Q)$ and $H^{1,\frac{1}{2}}(Q)$ on the subspace of functions satisfying the homogeneous heat equation are equivalent. Thus we obtain

$$\|\widetilde{M}_0 f\|_{H^{1,\frac{1}{2}}(Q)} \leq C(\Omega)\|f\|_{L_2(\Omega)}.$$

Therefore, the operator $M_0 : L_2(\Omega) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ is continuous by the trace theorem. Note that, since $\mathcal{E}(x, T+t) \in C^\infty(\mathbb{R}^d \times \mathbb{R}_+)$ for $T > 0$, the operator M_{10} is continuous on the considered Sobolev spaces.

We are now in a position to prove the properties of the boundary integral operator $\mathcal{T}_\alpha$.

Theorem 5.2. *The operator* $\mathcal{T}_\alpha : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ *as defined in* (5.23)*,*

$$\mathcal{T}_\alpha = \alpha\widetilde{D} - \kappa_T V^{-1}K_1 + \kappa_T V^{-1}V_1V^{-1}(\frac{1}{2}I + K)$$

is bounded, self-adjoint with respect to the inner product $\langle\cdot,\cdot\rangle_\Sigma$ *and* $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$*-elliptic, i.e., there exists a constant* $c_1^{\mathcal{T}_\alpha} > 0$ *such that*

$$\langle\mathcal{T}_\alpha z, z\rangle_\Sigma \geq c_1^{\mathcal{T}_\alpha}\|z\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma).$$

Proof. The proof is similar to the proof of Theorem 3.3. We skip the details. Note that, for the mapping properties of the layer heat potentials, see [15]. In particular, we have

$$V^{-1} : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma), \quad K : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma), \quad \widetilde{D} : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma).$$

Since the kernels of the bi-layer heat potentials are regular, we can also derive

$$V_1 : H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma), \quad K_1 : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma).$$

□

Hence we conclude the unique solvability of the variational inequality (5.22). However, as stated in Remark 3.3, we will obtain a non-symmetric approximation of the self-adjoint operator $\mathcal{T}_\alpha$ when using a Galerkin boundary element approximation. Moreover, we require an additional condition on the discretization to ensure the stability of the discrete variational inequality. Hence we only consider the symmetric formulation in the next section.

5.3 Symmetric boundary integral formulation

In this section, we investigate a symmetric boundary integral formulation by using a second boundary integral equation for the solution of the adjoint heat boundary value problem. We ensure unique solvability and we derive a priori error estimates for a Galerkin boundary element approximation.

In particular, when computing the normal derivative of the representation formula (5.17) of the adjoint variable, this gives

$$\kappa_T q(x,t) = (\frac{1}{2}I + K')\kappa_T q(x,t) + (K_1'\omega)(x,t) - (D_1 z)(x,t) - (M_1\overline{u})(x,t) + (M_{11}u_0)(x,t) \tag{5.38}$$

for all $(x,t) \in \Sigma$, where, in addition, we introduce the Newton potentials for $(x,t) \in \Sigma$

$$(M_1\overline{u})(x,t) = \frac{\partial}{\partial n_x}\int_\Omega \mathcal{E}(x-y,t)\overline{u}(y)\,dy, \quad (M_{11}u_0)(x,t) = \frac{\partial}{\partial n_x}\int_\Omega \mathcal{E}(x-y,T+t)u_0(y)\,dy.$$

By substituting (5.12) and (5.21) into the right hand side of (5.38) we obtain the alternative representation

$$\begin{aligned}\kappa_T q =& (\frac{1}{2}I + K')V^{-1}K_1 z - (\frac{1}{2}I + K')V^{-1}V_1V^{-1}(\frac{1}{2}I + K)z + (\frac{1}{2}I + K')V^{-1}V_1V^{-1}M_0u_0 \\ &+ (\frac{1}{2}I + K')V^{-1}M_0\overline{u} - (\frac{1}{2}I + K')V^{-1}M_{10}u_0 + K_1'V^{-1}(\frac{1}{2}I + K)z - K_1'V^{-1}M_0u_0 \\ &- D_1z - M_1\overline{u} + M_{11}u_0.\end{aligned}$$

Hence we have to solve the variational inequality to find the control $z \in \mathcal{U}_{ad}$ such that

$$\langle \mathcal{T}_\alpha z - g, w - z\rangle_\Sigma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad} \tag{5.39}$$

where

$$\begin{aligned}\mathcal{T}_\alpha = \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T K_1'V^{-1}(\frac{1}{2}I + K) - \kappa_T(\frac{1}{2}I + K')V^{-1}K_1 \\ + \kappa_T(\frac{1}{2}I + K')V^{-1}V_1V^{-1}(\frac{1}{2}I + K)\end{aligned} \tag{5.40}$$

is the alternative representation of $\mathcal{T}_\alpha$ as defined in (5.23) and

$$\begin{aligned}\kappa_T g = (\frac{1}{2}I + K')V^{-1}M_0\overline{u} - M_1\overline{u} + (\frac{1}{2}I + K')V^{-1}V_1V^{-1}M_0u_0 - (\frac{1}{2}I + K')V^{-1}M_{10}u_0 \\ - K_1'V^{-1}M_0u_0 + M_{11}u_0\end{aligned} \tag{5.41}$$

is the related right hand side.

Theorem 5.3. *The operator $\mathcal{T}_\alpha$ as given in* (5.40) *coincides with the operator as defined in* (5.23)*. In particular, $\mathcal{T}_\alpha$ is bounded, self-adjoint with respect to the inner product $\langle\cdot,\cdot\rangle_\Sigma$ and $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$-elliptic, i.e., there holds, for some $c_1^{\mathcal{T}_\alpha} > 0$,*

$$\langle \mathcal{T}_\alpha z, z\rangle_\Sigma \geq c_1^{\mathcal{T}_\alpha} \|z\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma).$$

Proof. The proof is similar to the proof of Theorem 3.5. The self-adjointness of $\mathcal{T}_\alpha$ is obvious from the symmetric representation (5.40) and (5.28), (5.36), (5.37). In particular, the operators $\mathcal{T}_\alpha$ in the symmetric representation (5.40) and in the non-symmetric representation (5.23) coincide. Indeed, by using (5.29) and (5.31) we have

$$\begin{aligned}
\mathcal{T}_\alpha &= \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T\left(K_1' - (\frac{1}{2}I + K')V^{-1}V_1\right)V^{-1}(\frac{1}{2}I+K) - \kappa_T(\frac{1}{2}I+K')V^{-1}K_1 \\
&= \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T V^{-1}\left(VK_1' - KV_1 - \frac{1}{2}V_1\right)V^{-1}(\frac{1}{2}I+K) - \kappa_T(\frac{1}{2}I+K')V^{-1}K_1 \\
&= \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T V^{-1}\left(K_1V - V_1K' - \frac{1}{2}V_1\right)V^{-1}(\frac{1}{2}I+K) - \kappa_T(\frac{1}{2}I+K')V^{-1}K_1 \\
&= \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T V^{-1}K_1(\frac{1}{2}I+K) + \kappa_T V^{-1}V_1(\frac{1}{2}I+K')V^{-1}(\frac{1}{2}I+K) \\
&\qquad - \kappa_T(\frac{1}{2}I+K')V^{-1}K_1.
\end{aligned}$$

By using (5.30), (5.29) and (5.33) we further conclude

$$\begin{aligned}
\mathcal{T}_\alpha &= \alpha\widetilde{D} + \kappa_T D_1 - \kappa_T V^{-1}K_1(\frac{1}{2}I+K) + \kappa_T V^{-1}V_1\left(V^{-1}(\frac{1}{2}I+K) - D\right) \\
&\qquad - \kappa_T(\frac{1}{2}I+K')V^{-1}K_1 \\
&= \alpha\widetilde{D} + \kappa_T V^{-1}\left(VD_1 - K_1(\frac{1}{2}I+K) + V_1V^{-1}(\frac{1}{2}I+K) - V_1D - (\frac{1}{2}I+K)K_1\right) \\
&= \alpha\widetilde{D} + \kappa_T V^{-1}\left(V_1V^{-1}(\frac{1}{2}I+K) - K_1\right) = \alpha\widetilde{D} - \kappa_T V^{-1}K_1 + \kappa_T V^{-1}V_1V^{-1}(\frac{1}{2}I+K)
\end{aligned}$$

and we obtain the non-symmetric representation (5.23).
Moreover, the ellipticity estimate can be shown directly by using Lemma 5.3. Indeed, for $z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ and $\omega = V^{-1}(\frac{1}{2}I+K)z \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ we have

$$\begin{aligned}
\langle \mathcal{T}_\alpha z, z\rangle_\Sigma &= \alpha\langle\widetilde{D}z,z\rangle_\Sigma + \langle\kappa_T D_1 z, z\rangle_\Sigma - \langle\kappa_T K_1'\omega, z\rangle_\Sigma - \langle\kappa_T(\frac{1}{2}I+K')V^{-1}K_1 z, z\rangle_\Sigma \\
&\qquad + \langle\kappa_T(\frac{1}{2}I+K')V^{-1}V_1\omega, z\rangle_\Sigma \\
&= \alpha\langle\widetilde{D}z,z\rangle_\Sigma + \langle\kappa_T D_1 z, z\rangle_\Sigma - \langle K_1'\omega, \kappa_T z\rangle_\Sigma - \langle K_1 z, \kappa_T\omega\rangle_\Sigma + \langle V_1\omega, \kappa_T\omega\rangle_\Sigma \\
&\geq \alpha\langle\widetilde{D}z,z\rangle_\Sigma \geq \alpha c_1^D \|z\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \text{(see Lemma 5.3).}
\end{aligned}$$

$\square$

Hence the variational inequality (5.39) admits a unique solution. Moreover, in consequence of the alternative representation (5.41) of the right hand side g as defined in (5.24), we obtain the following corollary.

Corollary 5.2. *For any $u_0, \overline{u} \in L_2(\Omega)$ there hold the identities*

$$M_1 \overline{u} = (-\frac{1}{2} I + K') V^{-1} M_0 \overline{u}, \tag{5.42}$$

$$M_{11} u_0 = K_1' V^{-1} M_0 u_0 + (\frac{1}{2} I - K') V^{-1} V_1 V^{-1} M_0 u_0 - (\frac{1}{2} I - K') V^{-1} M_{10} u_0. \tag{5.43}$$

Galerkin boundary element approximations

In what follows, we study the numerical solution of the variational inequality (5.39) by a Galerkin boundary element method. The ellipticity of the Schur complement boundary integral operator $\mathcal{T}_\alpha$ will imply the quasi-optimality of Galerkin approximations. Let us first introduce some finite dimensional trial spaces.

For the approximating subspaces of $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ and $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ it is customary to use tensor products of spaces of functions of the space variables and of spaces of functions of the time variable. We introduce a standard class of tensor product spaces $Q_h^{d_x,d_t}(\Sigma) = S_{h_x}^{d_x}(\Gamma) \otimes T_{h_t}^{d_t}$ which are based on polynomials of degree d_t in time and polynomials of degree d_x in space, see Section 2.2. We choose an approximation for the Neumann data ω, q which is piecewise constant both in space and in time. For continuous functions z_1 and z_2, we define the discrete convex set

$$\mathcal{U}_h := \{ w_h \in Q_h^{1,0}(\Sigma) \colon z_1(x_i,t_j) \le w_h(x_i,t_j) \le z_2(x_i,t_j) \quad \text{for all nodes } (x_i,t_j) \in \Sigma \},$$

where $Q_h^{1,0}(\Sigma)$ is a boundary element space of piecewise linear and continuous basis functions in space and piecewise constant ones in time. Then the Galerkin discretization of the variational inequality (5.39) is to seek $z_h \in \mathcal{U}_h$ such that

$$\langle \mathcal{T}_\alpha z_h, w_h - z_h \rangle_\Sigma \ge \langle g, w_h - z_h \rangle_\Sigma \quad \text{for all } w_h \in \mathcal{U}_h. \tag{5.44}$$

Theorem 5.4. *Let $z \in \mathcal{U}_{ad}$ and $z_h \in \mathcal{U}_h$ be the unique solutions of the variational inequalities* (5.39) *and* (5.44)*, respectively. Then there holds the error estimate*

$$\|z - z_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le c(h_x^{s-\frac{1}{2}} + h_t^{\frac{1}{2}(s-\frac{1}{2})}) \|z\|_{H^{s,\frac{s}{2}}(\Sigma)}, \tag{5.45}$$

when assuming $z, z_1, z_2 \in H^{s,\frac{s}{2}}(\Sigma)$ and $\mathcal{T}_\alpha z - g \in H^{s-1,\frac{s-1}{2}}(\Sigma)$ for some $s \in [\frac{1}{2}, 2]$.

Proof. The proof is similar to the proof of Theorem 3.1, see [8, 21, 49] for the general abstract theory.

Indeed, similarly to the proof of Theorem 3.1, by the assumption $\mathcal{T}_\alpha z - g \in H^{s-1,\frac{s-1}{2}}(\Sigma)$ we have

$$c_1^{\mathcal{T}_\alpha} \|z - z_h\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le \|\mathcal{T}_\alpha z - g\|_{H^{s-1,\frac{s-1}{2}}(\Sigma)} \left(\|z - w_h\|_{H^{1-s,\frac{1-s}{2}}(\Sigma)} + \|z_h - w\|_{H^{1-s,\frac{1-s}{2}}(\Sigma)} \right) + c_2^{\mathcal{T}_\alpha} \|z - z_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \|z - w_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}$$

for all $w \in \mathcal{U}_{ad}$ and $w_h \in \mathcal{U}_h$. By using the approximation properties of the trial space $Q_h^{1,0}(\Sigma)$, see (2.17) and (2.18), see also [15, 48], we can conclude

$$c_1^{\mathcal{T}_\alpha} \|z - z_h\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le c_1 \left(h_x^{s-1} + h_t^{\frac{s-1}{2}} \right) \left(h_x^s + h_t^{\frac{s}{2}} \right) \|z\|^2_{H^{s,\frac{s}{2}}(\Sigma)} + c_2 \left(h_x^{s-\frac{1}{2}} + h_t^{\frac{1}{2}(s-\frac{1}{2})} \right) \|z - z_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \|z\|_{H^{s,\frac{s}{2}}(\Sigma)}.$$

The assertion follows. □

Since the composed boundary integral operator $\mathcal{T}_\alpha$ and the right hand g as defined in (5.40), (5.41) do not allow a practical implementation in general, instead of (5.44) we consider a perturbed variational inequality to find $\widehat{z}_h \in \mathcal{U}_h$ such that

$$\langle \widehat{\mathcal{T}}_\alpha \widehat{z}_h, w_h - \widehat{z}_h \rangle_\Sigma \ge \langle \widehat{g}, w_h - \widehat{z}_h \rangle_\Sigma \quad \text{for all } w_h \in \mathcal{U}_h. \tag{5.46}$$

Theorem 5.5. *Let $\widehat{\mathcal{T}}_\alpha : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ be a bounded and $Q_h^{1,0}(\Sigma)$-elliptic approximation of $\mathcal{T}_\alpha$ satisfying*

$$\langle \widehat{\mathcal{T}}_\alpha z_h, z_h \rangle_\Sigma \ge c_1^{\widehat{\mathcal{T}}_\alpha} \|z_h\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } z_h \in Q_h^{1,0}(\Sigma)$$

and

$$\|\widehat{\mathcal{T}}_\alpha z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c_2^{\widehat{\mathcal{T}}_\alpha} \|z\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma).$$

Let $\widehat{g} \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ be some approximation of g. For the unique solution $\widehat{z}_h \in \mathcal{U}_h$ of the perturbed variational inequality (5.46) *there holds the error estimate*

$$\|z - \widehat{z}_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le c_1 \|z - z_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + c_2 \left(\|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha) z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} + \|g - \widehat{g}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \right) \tag{5.47}$$

where $z_h \in \mathcal{U}_h$ is the unique solution of the discrete variational inequality (5.44).

Proof. Since the operator $\widehat{\mathcal{T}}_\alpha$ is bounded and $Q_h^{1,0}(\Sigma)$-elliptic, the discrete variational inequality (5.46) admits a unique solution. From this we further obtain

$$\begin{aligned}
c_1^{\widehat{\mathcal{T}}_\alpha}\|z_h-\widehat{z}_h\|^2_{H^{\frac12,\frac14}(\Sigma)} &\le \langle\widehat{\mathcal{T}}_\alpha(z_h-\widehat{z}_h),z_h-\widehat{z}_h\rangle_\Sigma\\
&\le \langle\widehat{\mathcal{T}}_\alpha z_h,z_h-\widehat{z}_h\rangle_\Sigma+\langle\widehat{g},\widehat{z}_h-z_h\rangle_\Sigma+\langle\mathcal{T}_\alpha z_h,\widehat{z}_h-z_h\rangle_\Sigma-\langle g,\widehat{z}_h-z_h\rangle_\Sigma\\
&= \langle\widehat{\mathcal{T}}_\alpha z_h,z_h-\widehat{z}_h\rangle_\Sigma+\langle\widehat{g}-g,\widehat{z}_h-z_h\rangle_\Sigma+\langle\mathcal{T}_\alpha z_h,\widehat{z}_h-z_h\rangle_\Sigma\\
&\le \left(\|(\widehat{\mathcal{T}}_\alpha-\mathcal{T}_\alpha)z_h\|_{H^{-\frac12,-\frac14}(\Sigma)}+\|g-\widehat{g}\|_{H^{-\frac12,-\frac14}(\Sigma)}\right)\|z_h-\widehat{z}_h\|_{H^{\frac12,\frac14}(\Sigma)}.
\end{aligned}$$

By using the triangle inequality and the boundedness of $\mathcal{T}_\alpha$ and $\widehat{\mathcal{T}}_\alpha$ we have

$$\begin{aligned}
\|(\widehat{\mathcal{T}}_\alpha-\mathcal{T}_\alpha)z_h\|_{H^{-\frac12,-\frac14}(\Sigma)} &\le \|(\widehat{\mathcal{T}}_\alpha-\mathcal{T}_\alpha)z\|_{H^{-\frac12,-\frac14}(\Sigma)}+\|(\mathcal{T}_\alpha-\widehat{\mathcal{T}}_\alpha)(z-z_h)\|_{H^{-\frac12,-\frac14}(\Sigma)}\\
&\le \|(\widehat{\mathcal{T}}_\alpha-\mathcal{T}_\alpha)z\|_{H^{-\frac12,-\frac14}(\Sigma)}+(c_2^{\mathcal{T}_\alpha}+c_2^{\widehat{\mathcal{T}}_\alpha})\|z-z_h\|_{H^{\frac12,\frac14}(\Sigma)}.
\end{aligned}$$

The assertion now follows from the triangle inequality

$$\|z-\widehat{z}_h\|_{H^{\frac12,\frac14}(\Sigma)}\le\|z-z_h\|_{H^{\frac12,\frac14}(\Sigma)}+\|z_h-\widehat{z}_h\|_{H^{\frac12,\frac14}(\Sigma)}.$$

□

It remains to define the appropriate approximations $\widehat{\mathcal{T}}_\alpha$, $\widehat{g}$ which are based on the use of boundary element methods, see Section 3.5 for the case of an elliptic problem.

For $z\in H^{\frac12,\frac14}(\Sigma)$, the application of $\mathcal{T}_\alpha z$ reads

$$\mathcal{T}_\alpha z=\alpha\widetilde{D}z+\kappa_T D_1 z-\kappa_T K_1'\omega_z-\kappa_T(\frac12 I+K')q_z,$$

where $q_z,\omega_z\in H^{-\frac12,-\frac14}(\Sigma)$ are the unique solutions of the boundary integral equations

$$V\omega_z=(\frac12 I+K)z,\quad Vq_z=K_1z-V_1\omega_z.$$

Let $Q_h^{0,0}(\Sigma)$ be another boundary element space of piecewise constant basis functions both in space and in time. Let $q_{z,h}\in Q_h^{0,0}(\Sigma)$ be the unique solution of the Galerkin variational problem

$$\langle Vq_{z,h},\theta_h\rangle_\Sigma=\langle K_1z-V_1\omega_{z,h},\theta_h\rangle_\Sigma\quad\text{for all }\theta_h\in Q_h^{0,0}(\Sigma),$$

where $\omega_{z,h}\in Q_h^{0,0}(\Sigma)$ solves

$$\langle V\omega_{z,h},\theta_h\rangle_\Sigma=\langle(\frac12 I+K)z,\theta_h\rangle_\Sigma\quad\text{for all }\theta_h\in Q_h^{0,0}(\Sigma).$$

We are now in a position to define an approximation $\widehat{\mathcal{T}}_\alpha$ of the operator $\mathcal{T}_\alpha$ by

$$\widehat{\mathcal{T}}_\alpha z = \alpha \widetilde{D} z + \kappa_T D_1 z - \kappa_T K_1' \omega_{z,h} - \kappa_T (\frac{1}{2} I + K') q_{z,h}. \tag{5.48}$$

Lemma 5.5. *The approximate operator* $\widehat{\mathcal{T}}_\alpha : H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ *as defined in* (5.48) *is bounded, i.e.,*

$$\|\widehat{\mathcal{T}}_\alpha z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c_2^{\widehat{\mathcal{T}}_\alpha} \|z\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma),$$

and there holds the error estimate

$$\|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha) z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c_1 \inf_{\theta_h \in Q_h^{0,0}(\Sigma)} \|q_z - \theta_h\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} + c_2 \|\omega_z - \omega_{z,h}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)}, \tag{5.49}$$

where $\mathcal{T}_\alpha$ was defined in (5.40).

Proof. The boundedness of the operator $\widehat{\mathcal{T}}_\alpha$ follows from the mapping properties of all boundary integral operators involved. In particular, the Galerkin boundary element solutions $\omega_{z,h}$, $q_{z,h}$ in (5.48) satisfy

$$\|\omega_{z,h}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c_1 \|z\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}, \quad \|q_{z,h}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c_2 \|z\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}.$$

For the error estimate (5.49) let $z \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ be arbitrary but fixed. By definition, we have

$$\mathcal{T}_\alpha z = \alpha \widetilde{D} z + \kappa_T D_1 z - \kappa_T K_1' \omega_z - \kappa_T (\frac{1}{2} I + K') q_z,$$

where

$$V \omega_z = (\frac{1}{2} I + K) z, \quad V q_z = K_1 z - V_1 \omega_z.$$

By using (5.48), we then obtain

$$\mathcal{T}_\alpha z - \widehat{\mathcal{T}}_\alpha z = \kappa_T K_1' (\omega_{z,h} - \omega_z) + \kappa_T (\frac{1}{2} I + K') (q_{z,h} - q_z),$$

where $q_{z,h} \in Q_h^{0,0}(\Sigma)$ is the unique solution of the Galerkin variational problem

$$\langle V q_{z,h}, \theta_h \rangle_\Sigma = \langle K_1 z - V_1 \omega_{z,h}, \theta_h \rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma),$$

and $\omega_{z,h} \in Q_h^{0,0}(\Sigma)$ solves

$$\langle V \omega_{z,h}, \theta_h \rangle_\Sigma = \langle (\frac{1}{2} I + K) z, \theta_h \rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma).$$

Moreover we define $\widehat{q}_{z,h} \in Q_h^{0,0}(\Sigma)$ as the unique solution of the Galerkin variational problem

$$\langle V\widehat{q}_{z,h}, \theta_h \rangle_\Sigma = \langle K_1 z - V_1 \omega_z, \theta_h \rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma).$$

Then the perturbed Galerkin orthogonality

$$\langle V(q_{z,h} - \widehat{q}_{z,h}), \theta_h \rangle_\Sigma = \langle V_1(\omega_{z,h} - \omega_z), \theta_h \rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma)$$

follows. This implies the inequality

$$\|q_{z,h} - \widehat{q}_{z,h}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le \frac{1}{c_1^V} \|V_1(\omega_{z,h} - \omega_z)\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le \frac{c_2^{V_1}}{c_1^V} \|\omega_{z,h} - \omega_z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)}.$$

Therefore, by the boundedness of the operators $K', K_1' : H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ and by the triangle inequality we conclude

$$\begin{aligned}
\|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha)z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} &\le c_2^{K_1'} \|\omega_{z,h} - \omega_z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} + c_2^{K'} \|q_{z,h} - q_z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \\
&\le c_2^{K_1'} \|\omega_{z,h} - \omega_z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} + c_2^{K'} \|q_{z,h} - \widehat{q}_{z,h}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} + c_2^{K'} \|\widehat{q}_{z,h} - q_z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)}.
\end{aligned}$$

The assertion now follows by applying Cea's lemma. □

By using the approximation property of the trial space $Q_h^{0,0}(\Sigma)$, see (2.17), we conclude an error estimate from (5.49) when assuming some regularity of q_z and ω_z, respectively.

Corollary 5.3. *Assume $q_z, \omega_z \in H^{s,\frac{s}{2}}(\Sigma)$ for some $s \in [0,1]$. Then there holds the error estimate*

$$\|(\mathcal{T}_\alpha - \widehat{\mathcal{T}}_\alpha)z\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c(h_x^{\frac{1}{2}} + h_t^{\frac{1}{4}})(h_x^s + h_t^{\frac{s}{2}})(\|q_z\|_{H^{s,\frac{s}{2}}(\Sigma)} + \|\omega_z\|_{H^{s,\frac{s}{2}}(\Sigma)}). \tag{5.50}$$

The approximation of the right hand side g

Similarly, the right hand side in (5.41) can be rewritten as

$$g = \kappa_T(\frac{1}{2}I + K')q_{\bar{u},u_0} + \kappa_T K_1' \omega_{u_0} - \kappa_T M_1 \bar{u} + \kappa_T M_{11} u_0,$$

where $q_{\bar{u},u_0} \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ is the unique solution of the boundary integral equation

$$(Vq_{\bar{u},u_0})(x,t) = (M_0\bar{u})(x,t) - (M_{10}u_0)(x,t) - (V_1\omega_{u_0})(x,t) \quad \text{for } (x,t) \in \Sigma,$$

and $\omega_{u_0} \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ solves

$$(V\omega_{u_0})(x,t) = -(M_0u_0)(x,t) \quad \text{for } (x,t) \in \Sigma.$$

Hence we define approximate Galerkin solutions $\widetilde{q}_h, \widetilde{\omega}_h \in Q_h^{0,0}(\Sigma)$ of $q_{\overline{u},u_0}$ and ω_{u_0}, and then we can introduce the approximation

$$\widehat{g} = \kappa_T(\frac{1}{2}I + K')\widetilde{q}_h + \kappa_T K_1'\widetilde{\omega}_h - \kappa_T M_1\overline{u} + \kappa_T M_{11}u_0 \tag{5.51}$$

and we obtain the error estimate

$$\|g-\widehat{g}\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \le c(h_x^{\frac{1}{2}} + h_t^{\frac{1}{4}})(h_x^s + h_t^{\frac{s}{2}})(\|q_{\overline{u},u_0}\|_{H^{s,\frac{s}{2}}(\Sigma)} + \|\omega_{u_0}\|_{H^{s,\frac{s}{2}}(\Sigma)}), \tag{5.52}$$

when assuming $q_{\overline{u},u_0}, \omega_{u_0} \in H^{s,\frac{s}{2}}(\Sigma)$ for some $s \in [0,1]$.

Approximate variational inequality
By using the approximations (5.48) and (5.51), the perturbed variational inequality (5.46) reads to find $\widehat{z}_h \in \mathcal{U}_h$ such that

$$\begin{aligned}\langle \alpha\widetilde{D}\widehat{z}_h + \kappa_T D_1\widehat{z}_h - \kappa_T K_1'\omega_{\widehat{z}_h,h} - \kappa_T(\frac{1}{2}I + K')q_{\widehat{z}_h,h}, w_h - \widehat{z}_h\rangle_\Sigma \\ \ge \langle \kappa_T(\frac{1}{2}I + K')\widetilde{q}_h + \kappa_T K_1'\widetilde{\omega}_h - \kappa_T M_1\overline{u} + \kappa_T M_{11}u_0, w_h - \widehat{z}_h\rangle_\Sigma \quad \text{for all } w_h \in \mathcal{U}_h\end{aligned}$$

which can be written as

$$\langle \alpha\widetilde{D}\widehat{z}_h + \kappa_T D_1\widehat{z}_h - \kappa_T K_1'\omega_h - \kappa_T(\frac{1}{2}I + K')q_h, w_h - \widehat{z}_h\rangle_\Sigma \ge \langle \kappa_T M_{11}u_0 - \kappa_T M_1\overline{u}, w_h - \widehat{z}_h\rangle_\Sigma \tag{5.53}$$

for all $w_h \in \mathcal{U}_h$, where we introduce $q_h := q_{\widehat{z}_h,h} + \widetilde{q}_h \in Q_h^{0,0}(\Sigma)$ which is the unique solution of the Galerkin variational problem

$$\langle Vq_h, \theta_h\rangle_\Sigma = \langle K_1\widehat{z}_h - V_1\omega_h, \theta_h\rangle_\Sigma + \langle M_0\overline{u} - M_{10}u_0, \theta_h\rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma), \tag{5.54}$$

and $\omega_h := \omega_{\widehat{z}_h,h} + \widetilde{\omega}_h \in Q_h^{0,0}(\Sigma)$ which solves

$$\langle V\omega_h, \theta_h\rangle_\Sigma = \langle(\frac{1}{2}I + K)\widehat{z}_h - M_0u_0, \theta_h\rangle_\Sigma \quad \text{for all } \theta_h \in Q_h^{0,0}(\Sigma), \tag{5.55}$$

(see the corresponding boundary integral equations (5.18), (5.11)).

Let

$$\omega_h(x,t) = \sum_{k=0}^{N-1}\sum_{\ell=0}^{N_0-1}\omega_{\ell k}\varphi_\ell^0(x)\psi_k^0(t), \quad q_h(x,t) = \sum_{k=0}^{N-1}\sum_{\ell=0}^{N_0-1}q_{\ell k}\varphi_\ell^0(x)\psi_k^0(t),$$

and

$$\widehat{z}_h(x,t) = \sum_{k=0}^{N-1}\sum_{n=0}^{N_1-1}z_{nk}\varphi_n^1(x)\psi_k^0(t), \quad (x,t) \in \Sigma,$$

where N_i denotes the dimension of $S^i_{h_x}(\Gamma)$, $i = 0,1$ and N is the number of time steps. Substituting these expansions into (5.54) with the test functions $\theta_h(x,t) = \varphi^0_i(x)\kappa_T\psi^0_j(t)$ for $i = 0,1,...,N_0-1$; $j = 0,1,...,N-1$, we get

$$\sum_{k=0}^{N-1}\sum_{\ell=0}^{N_0-1}\Big(\omega_{\ell k}\langle V_1[\varphi^0_\ell(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma + q_{\ell k}\langle V[\varphi^0_\ell(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma\Big)$$
$$-\sum_{k=0}^{N-1}\sum_{n=0}^{N_1-1} z_{nk}\langle K_1[\varphi^1_n(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma = \langle M_0\bar{u} - M_{10}u_0,\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma$$

for all $i = 0,1,...,N_0-1$; $j = 0,1,...,N-1$.

Since the last equation is indexed by four integers, it requires some ordering or partitioning of the unknowns. For $0 \le k \le N-1$ we define vectors $\underline{\omega}_k$, $\underline{q}_k \in \mathbb{R}^{N_0}$ and $\underline{z}_k \in \mathbb{R}^{N_1}$ by

$$\omega_k[\ell] = \omega_{\ell k}, \quad q_k[\ell] = q_{\ell k}, \quad z_k[n] = z_{nk} \quad \text{for} \quad \ell = 0,1,...,N_0-1; n = 0,1,...,N_1-1.$$

Similarly, $\underline{f}^1_j$ denote vectors of length N_0 whose components are given by

$$f^1_j[i] = \langle M_0\bar{u} - M_{10}u_0,\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma, \quad \text{for} \quad i = 0,1,...,N_0-1; j = 0,1,...,N-1.$$

Finally, we define square matrices V^1_{jk}, $V_{jk} \in \mathbb{R}^{N_0\times N_0}$ and matrices $K^1_{jk} \in \mathbb{R}^{N_0\times N_1}$ for $0 \le k,j \le N-1$ by

$$\begin{aligned}
V^1_{jk}[i][\ell] &= \langle V_1[\varphi^0_\ell(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,\\
V_{jk}[i][\ell] &= \langle V[\varphi^0_\ell(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,\\
K^1_{jk}[i][n] &= \langle K_1[\varphi^1_n(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,
\end{aligned}$$

for $i,\ell = 0,1,...,N_0-1$; $n = 0,1,...,N_1-1$.
With these notations, the system (5.54) can be written in the form

$$\sum_{k=0}^{N-1}\Big(V^1_{jk}\underline{\omega}_k + V_{jk}\underline{q}_k - K^1_{jk}\underline{z}_k\Big) = \underline{f}^1_j, \quad \text{for} \quad j = 0,1,...,N-1. \tag{5.56}$$

In the same way, the system (5.55) reads

$$\sum_{k=0}^{N-1} V_{jk}\underline{\omega}_k - \sum_{k=0}^{N-1}\left(\frac{1}{2}M_{jk} + K_{jk}\right)\underline{z}_k = \underline{f}^2_j, \quad \text{for} \quad j = 0,1,...,N-1, \tag{5.57}$$

where the matrices $M_{jk}, K_{jk} \in \mathbb{R}^{N_0\times N_1}$ are defined by

$$\begin{aligned}
M_{jk}[i][n] &= \langle \varphi^1_n(x)\psi^0_k(t),\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,\\
K_{jk}[i][n] &= \langle K[\varphi^1_n(x)\psi^0_k(t)],\varphi^0_i(x)\kappa_T\psi^0_j(t)\rangle_\Sigma
\end{aligned}$$

and

$$f_j^2[i] = -\langle M_0 u_0, \varphi_i^0(x)\kappa_T \psi_j^0(t)\rangle_\Sigma.$$

Let us rewrite the linear systems (5.56) and (5.57) as follows. For the N^2 matrices A_{jk}, $j,k = 0,1,...,N-1$, which correspond to one of the layer heat potentials A, i.e.,

$$A_{jk}[i][\ell] = \langle A[\varphi_\ell^0(x)\psi_k^0(t)], \varphi_i^0(x)\kappa_T \psi_j^0(t)\rangle_\Sigma,$$

we denote a block matrix A_h by

$$A_h := \begin{pmatrix} A_{00} & A_{01} & \cdots & A_{0,N-1} \\ A_{10} & A_{11} & \cdots & A_{1,N-1} \\ \vdots & \vdots & \vdots & \vdots \\ A_{N-1,0} & A_{N-1,1} & \cdots & A_{N-1,N-1} \end{pmatrix}.$$

We define a vector $\underline{a}$ which is constructed from the N vectors $\underline{a}_k$ by

$$\underline{a} := \begin{pmatrix} \underline{a}_0^\top & \underline{a}_1^\top & \cdots & \underline{a}_{N-1}^\top \end{pmatrix}^\top.$$

With these notations, the inner-product of two vectors $A_h\underline{a}$ and $\underline{b}$ can be expressed by the “time-twisted” duality, i.e.,

$$(A_h\underline{a}, \underline{b}) = \langle A a_h, \kappa_T b_h\rangle_\Sigma,$$

where a_h, b_h are trial functions whose coefficients of the expansions in trial spaces correspond to the vectors $\underline{a}, \underline{b}$. Here the operator A can be one of the layer heat potentials $V, K, V_1, \ldots$. In case of the identity operator, we have a mass matrix M_h, as usual.

We now rewrite the linear systems (5.56) and (5.57) in the forms

$$V_{1,h}\underline{\omega} + V_h\underline{q} - K_{1,h}\underline{z} = \underline{f}^1 \tag{5.58}$$

and

$$V_h\underline{\omega} - (\frac{1}{2}M_h + K_h)\underline{z} = \underline{f}^2, \tag{5.59}$$

respectively.

Discrete variational inequality
Analogously, we can reformulate the perturbed variational inequality (5.53) to find $\underline{z} \in \mathbb{R}^{N_1 N} \leftrightarrow \widehat{z}_h \in \mathcal{U}_h$ such that

$$(\alpha\widetilde{D}_h\underline{z} + D_{1,h}\underline{z} - K_{1,h}^\top\underline{\omega} - (\frac{1}{2}M_h^\top + K_h^\top)\underline{q}, \underline{w} - \underline{z}) \geq (\underline{f}^3, \underline{w} - \underline{z}) \quad \text{for all } \underline{w} \in \mathbb{R}^{N_1 N} \leftrightarrow w_h \in \mathcal{U}_h \tag{5.60}$$

where $\underline{\omega}, \underline{q} \in \mathbb{R}^{N_0 N}$ are the unique solutions of the linear systems (5.59), (5.58), respectively. Here, in addition, we define the square matrices $D^1_{jk}, \widetilde{D}_{jk} \in \mathbb{R}^{N_1 \times N_1}$ and the vectors $\underline{f}^3_j \in \mathbb{R}^{N_1}$ by

$$D^1_{jk}[m][n] = \langle D_1[\varphi^1_n(x)\psi^0_k(t)], \varphi^1_m(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,$$
$$\widetilde{D}_{jk}[m][n] = \frac{1}{2}\langle D[\varphi^1_n(x)\psi^0_k(t)], \varphi^1_m(x)\psi^0_j(t)\rangle_\Sigma + \frac{1}{2}\langle D[\varphi^1_n(x)\kappa_T\psi^0_k(t)], \varphi^1_m(x)\kappa_T\psi^0_j(t)\rangle_\Sigma,$$
$$f^3_j[m] = \langle M_{11}u_0 - M_1\bar{u}, \varphi^1_m(x)\kappa_T\psi^0_j(t)\rangle_\Sigma$$

for $j,k = 0,1,...,N-1$; $m,n = 0,1,...,N_1-1$. Note that

$$(\widetilde{D}_h\underline{a}, \underline{b}) = \langle \widetilde{D}a_h, b_h\rangle_\Sigma \quad \text{for all } \underline{a}, \underline{b} \in \mathbb{R}^{N_1 N} \leftrightarrow a_h, b_h \in Q^{1,0}_h(\Sigma).$$

The Galerkin matrix V_h of the single layer heat potential V is symmetric and positive definite, hence it is invertible. We can solve $\underline{\omega}$ and $\underline{q}$ from (5.59), (5.58). Then the discrete variational inequality (5.60) is equivalent to

$$(\mathcal{T}_{\alpha,h}\underline{z}, \underline{w} - \underline{z}) \geq (\underline{g}, \underline{w} - \underline{z}) \quad \text{for all } \underline{w} \in \mathbb{R}^{N_1 N} \leftrightarrow w_h \in \mathcal{U}_h \tag{5.61}$$

where

$$\mathcal{T}_{\alpha,h} = \alpha\widetilde{D}_h + D_{1,h} - (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}K_{1,h} - K_{1,h}^\top V_h^{-1}(\frac{1}{2}M_h + K_h)$$
$$+ (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}V_{1,h}V_h^{-1}(\frac{1}{2}M_h + K_h) \tag{5.62}$$

defines a symmetric Galerkin boundary element approximation of the self-adjoint operator $\mathcal{T}_\alpha$ and

$$\underline{g} = \underline{f}^3 + K_{1,h}^\top V_h^{-1}\underline{f}^2 + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\underline{f}^1 - V_{1,h}V_h^{-1}\underline{f}^2) \tag{5.63}$$

is the related boundary element approximation of the right hand side g as defined in (5.41).

Lemma 5.6. *The symmetric matrix $\mathcal{T}_{\alpha,h}$ as defined in* (5.62) *is positive definite, i.e.,*

$$(\mathcal{T}_{\alpha,h}\underline{z}, \underline{z}) \geq \alpha c_1^D \|z_h\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \quad \textit{for all } \underline{z} \in \mathbb{R}^{N_1 N} \leftrightarrow z_h \in Q^{1,0}_h(\Sigma).$$

Proof. While the symmetry of $\mathcal{T}_{\alpha,h}$ is obvious, the positive definiteness follows by using Lemma 5.3. Indeed, by using the symmetry of V_h and with $\underline{\omega} = V_h^{-1}(\frac{1}{2}M_h + K_h)\underline{z}$, we have

$$\begin{aligned}(\mathcal{T}_{\alpha,h}\underline{z}, \underline{z}) &= \alpha(\widetilde{D}_h\underline{z}, \underline{z}) + (D_{1,h}\underline{z}, \underline{z}) - 2(K_{1,h}\underline{z}, \underline{\omega}) + (V_{1,h}\underline{\omega}, \underline{\omega}), \\ &= \alpha\langle\widetilde{D}z_h, z_h\rangle_\Sigma + \langle D_1 z_h, \kappa_T z_h\rangle_\Sigma - 2\langle K_1 z_h, \kappa_T\omega_h\rangle_\Sigma + \langle V_1\omega_h, \kappa_T\omega_h\rangle_\Sigma, \\ &\geq \alpha\langle\widetilde{D}z_h, z_h\rangle_\Sigma \geq \alpha c_1^D\|z_h\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}.\end{aligned}$$

□

Hence we conclude the unique solvability of the variational inequality (5.61) and (5.46) as well. Moreover, we can derive an error estimate for the approximate control solution $\widehat{z}_h$ by applying Theorem 5.5 and with the error estimates (5.45), (5.50) and (5.52).

Theorem 5.6. *Let z and $\widehat{z}_h$ be the unique solutions of the variational inequalities* (5.39) *and* (5.46)*, respectively. Then there holds the error estimate*

$$\|z-\widehat{z}_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le c_1(h_x^{s+\frac{1}{2}}+h_t^{\frac{1}{2}(s+\frac{1}{2})})\|z\|_{H^{s+1,\frac{s+1}{2}}(\Sigma)} + c_2(h_x^{\frac{1}{2}}+h_t^{\frac{1}{4}})(h_x^s+h_t^{\frac{s}{2}})\|q_z\|_{H^{s,\frac{s}{2}}(\Sigma)}$$
$$+c_3(h_x^{\frac{1}{2}}+h_t^{\frac{1}{4}})(h_x^s+h_t^{\frac{s}{2}})\left(\|\omega_z\|_{H^{s,\frac{s}{2}}(\Sigma)}+\|q_{\overline{u},u_0}\|_{H^{s,\frac{s}{2}}(\Sigma)}+\|\omega_{u_0}\|_{H^{s,\frac{s}{2}}(\Sigma)}\right) \quad (5.64)$$

when assuming $z \in H^{s+1,\frac{s+1}{2}}(\Sigma)$ and $q_z, \omega_z, q_{\overline{u},u_0}, \omega_{u_0} \in H^{s,\frac{s}{2}}(\Sigma)$ for some $s \in [0,1]$.

In particular, if there are constants $c_1, c_2 > 0$ such that

$$c_1 h_x^2 \le h_t \le c_2 h_x^2,$$

we obtain the estimate

$$\|z-\widehat{z}_h\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} \le c(z,\overline{u},u_0)h_x^{s+\frac{1}{2}} \quad \text{for } z \in H^{s+1,\frac{s+1}{2}}(\Sigma), s\in[0,1]. \quad (5.65)$$

In the case of a non-constrained minimization problem, instead of the discrete variational inequality (5.61) we have to solve the linear system

$$\mathcal{T}_{\alpha,h}\underline{z} = \underline{g},$$

which can be written as

$$\begin{pmatrix} V_{1,h} & V_h & -K_{1,h} \\ V_h & & -(\frac{1}{2}M_h+K_h) \\ -K_{1,h}^\top & -(\frac{1}{2}M_h^\top+K_h^\top) & D_{1,h}+\alpha\widetilde{D}_h \end{pmatrix} \begin{pmatrix} \underline{\omega} \\ \underline{q} \\ \underline{z} \end{pmatrix} = \begin{pmatrix} \underline{f}^1 \\ \underline{f}^2 \\ \underline{f}^3 \end{pmatrix}. \quad (5.66)$$

Implementation
In what follows, we discuss on the computation of the matrix entries for the Galerkin scheme. For more details, we refer to [15, 48, 60].
We consider the Galerkin matrix of the single layer heat potential

$$V_{jk}[i][\ell] = \langle V[\varphi_\ell^0(x)\psi_k^0(t)], \varphi_i^0(x)\kappa_T\psi_j^0(t)\rangle_\Sigma = \int_0^T\int_\Gamma \varphi_i^0(x)\psi_j^0(T-t)V[\varphi_\ell^0(x)\psi_k^0(t)]\,ds_x\,dt$$
$$= \int_0^T\int_\Gamma \varphi_i^0(x)\psi_j^0(T-t)\int_0^t\int_\Gamma \mathcal{E}(x-y,t-\tau)\varphi_\ell^0(y)\psi_k^0(\tau)\,ds_y\,d\tau\,ds_x\,dt.$$

By interchanging the order of integration, the entries $V_{jk}[i][\ell]$ can be written as follows

$$V_{jk}[i][\ell] = \int_\Gamma \int_\Gamma \varphi_i^0(x) a_{jk}(x,y) \varphi_\ell^0(y)\, ds_y\, ds_x,$$

where for $x,y \in \mathbb{R}^d$, $a_{jk}(x,y)$ are denoted by

$$a_{jk}(x,y) = \int_0^T \psi_j^0(T-t) \int_0^t \psi_k^0(\tau) \mathcal{E}(x-y,t-\tau)\, d\tau\, dt.$$

The basis functions $\psi_k^0(t)$ are given in (2.16) for $k = 0,1,...,N-1$,

$$\psi_k^0(t) = \begin{cases} 1 & \text{if } kh_t < t < (k+1)h_t, \\ 0 & \text{otherwise.} \end{cases}$$

Hence, with $T = Nh_t$, the time integrals

$$a_{jk}(x,y) = \int_{(N-j-1)h_t}^{(N-j)h_t} \int_{kh_t}^{(k+1)h_t} \mathcal{E}(x-y,t-\tau)\, d\tau\, dt = h_t^2 \int_0^1 \int_0^1 \mathcal{E}(x-y,h_t(\delta - t' - \tau'))\, d\tau'\, dt'$$

can be computed explicitly for $\delta := N-j-k \geq 1$, see, e.g., [15] for $d=2$ and [48] for $d=3$. Note that $a_{jk}(x,y) = 0$ for $\delta < 1$, so $V_{jk} = 0$ for $\delta < 1$. Obviously,

$$V_{j_1k_1} = V_{j_2k_2} \quad \text{if} \quad j_1 + k_1 = j_2 + k_2.$$

The symmetric matrix V_h is (block) left-upper triangular. Thus only N blocks of size $N_0 \times N$ have to be computed and stored. In particular, only one block of size $N_0 \times N$ has to be inverted in order to get V_h^{-1}.

For the Galerkin matrix of the hypersingular integral operator we can reduce the computation to weakly singular integrals in the two dimensional case, see [15].

Lemma 5.7. *For $d = 2$, let ∂_γ and ∂_t denote the derivative with respect to the arc length on Γ and the time derivative, respectively. Let n denote the exterior normal vector. Then*

$$\begin{aligned} \langle Dz,w\rangle_\Sigma &= \langle V(\partial_\gamma z), \partial_\gamma w\rangle_\Sigma + \sum_{i=1}^{2} \langle \partial_t V(zn_i), wn_i\rangle_\Sigma, \\ \langle D_1 z,w\rangle_\Sigma &= -\langle V_1(\partial_\gamma z), \partial_\gamma w\rangle_\Sigma - \sum_{i=1}^{2} \langle \partial_t V_1(zn_i), wn_i\rangle_\Sigma, \end{aligned}$$

for all $z,w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$.

Moreover, to implement the right hand side $\underline{f}^3$ we can approximate the Newton potentials $M_1\overline{u}$ and $M_{11}u_0$ by using the identities (5.42) and (5.43) as we did for the right hand side g. In particular, we can write

$$M_{11}u_0 - M_1\overline{u} = K_1'V^{-1}M_0u_0 + (\frac{1}{2}I - K')V^{-1}V_1V^{-1}M_0u_0 + (\frac{1}{2}I - K')V^{-1}[M_0\overline{u} - M_{10}u_0]$$
$$= -K_1'\omega_{u_0} + (\frac{1}{2}I - K')q_{\overline{u},u_0}$$

where $\omega_{u_0} \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ is the unique solution of the boundary integral equation

$$(V\omega_{u_0})(x,t) = -(M_0u_0)(x,t) \quad \text{for } (x,t) \in \Sigma,$$

and $q_{\overline{u},u_0}$ solves

$$(Vq_{\overline{u},u_0})(x,t) = (M_0\overline{u})(x,t) - (M_{10}u_0)(x,t) - (V_1\omega_{u_0})(x,t) \quad \text{for } (x,t) \in \Sigma.$$

Then we define an approximation $\widehat{f}^3$ as in (5.51)

$$\widehat{f}^3 = (\frac{1}{2}I - K')\widetilde{q}_h - K_1'\widetilde{\omega}_h$$

which implies

$$\widehat{\underline{f}}^3 = (\frac{1}{2}M_h^\top - K_h^\top)V_h^{-1}(\underline{f}^1 - V_{1,h}V_h^{-1}\underline{f}^2) - K_{1,h}^\top V_h^{-1}\underline{f}^2.$$

Therefore, instead of the vector $\underline{g}$ as defined in (5.63) we use an approximation

$$\begin{aligned}\widehat{\underline{g}} &= \widehat{\underline{f}}^3 + K_{1,h}^\top V_h^{-1}\underline{f}^2 + (\frac{1}{2}M_h^\top + K_h^\top)V_h^{-1}(\underline{f}^1 - V_{1,h}V_h^{-1}\underline{f}^2) \\ &= M_h^\top V_h^{-1}\left(\underline{f}^1 - V_{1,h}V_h^{-1}\underline{f}^2\right).\end{aligned}$$

Remark 5.1. *We have presented the use of a boundary element analysis for the solution of parabolic Dirichlet boundary control problem. The error estimate* (5.65) *provides the best possible order of convergence for boundary element approximation of the Dirichlet control z when considering the lowest order trial spaces. The boundary element approach can be applied to parabolic Neumann boundary control problem as well. This will be discussed in the next section.*

5.4 Parabolic Neumann boundary control problems

In this section, we apply the boundary integral equation method to a parabolic Neumann boundary control problem which is based on the idea as used for the parabolic Dirichlet boundary control problem. This approach results in a similar formulation as those in the case of a parabolic Dirichlet boundary control problem. Hence we give here the main results only.

By using the setting as for the parabolic Dirichlet boundary control problem, we consider the parabolic Neumann boundary control problem to find the control $\omega \in \mathcal{U}_{ad} \subset H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ which minimizes the functional

$$J(u,\omega) = \frac{1}{2}\int_{\Omega} [u(x,T) - \overline{u}(x)]^2\,dx + \frac{\alpha}{2}\langle V\omega,\omega\rangle_\Sigma \tag{5.67}$$

where the state u solves the initial boundary value problem

$$\begin{cases} \partial_t u(x,t) - \Delta u(x,t) = 0 & \text{for } (x,t) \in Q, \\ \dfrac{\partial}{\partial n} u(x,t) = \omega(x,t) & \text{for } (x,t) \in \Sigma, \\ u(x,0) = u_0(x) & \text{for } x \in \Omega, \end{cases} \tag{5.68}$$

and $\mathcal{U}_{ad}$ is a closed and convex subset of $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$. Here $\overline{u}, u_0 \in L_2(\Omega)$, $\alpha \in \mathbb{R}_+$.

Analogously, we obtain a variational inequality to be solved

$$\langle \alpha \widetilde{V}\omega + p, w - \omega\rangle_\Sigma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{5.69}$$

where

$$\widetilde{V} := \frac{1}{2}(V + \kappa_T V \kappa_T),$$

and the adjoint state $p(x,t)$ is the solution of the initial boundary value problem

$$\begin{cases} -\partial_t p(x,t) - \Delta p(x,t) = 0 & \text{for } (x,t) \in Q, \\ \dfrac{\partial}{\partial n} p(x,t) = 0 & \text{for } (x,t) \in \Sigma, \\ p(x,T) = u(x,T) - \overline{u}(x) & \text{for } x \in \Omega. \end{cases} \tag{5.70}$$

The variational inequality (5.69) can be written as

$$\langle \mathcal{T}_\alpha \omega - g, w - \omega\rangle_\Sigma \geq 0 \quad \text{for all } w \in \mathcal{U}_{ad}, \tag{5.71}$$

which admits a unique solution $\omega \in \mathcal{U}_{ad}$. Here the operator $\mathcal{T}_\alpha : H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ is bounded and $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$-elliptic, and $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$. By applying the idea as used for the parabolic Dirichlet boundary control problem, we can derive a representation of $\mathcal{T}_\alpha$ by the boundary integral heat layer potentials as

$$\mathcal{T}_\alpha = \alpha\widetilde{V} + \kappa_T V_1 - \kappa_T K_1 D^{-1}(\frac{1}{2}I - K') - \kappa_T(\frac{1}{2}I - K)D^{-1}K_1' + \kappa_T(\frac{1}{2}I - K)D^{-1}D_1 D^{-1}(\frac{1}{2}I - K'). \quad (5.72)$$

Since the composed operator $\mathcal{T}_\alpha$ as defined in (5.72) does not allow a practical implementation, instead of (5.71), we consider a perturbed variational inequality to find $\widehat{\omega}_h \in \mathcal{U}_h$ such that

$$\langle \widehat{\mathcal{T}}_\alpha \widehat{\omega}_h - \widehat{g}, w_h - \widehat{\omega}_h \rangle_\Sigma \geq 0 \quad \text{for all } w_h \in \mathcal{U}_h, \quad (5.73)$$

where $\widehat{\mathcal{T}}_\alpha$ and $\widehat{g}$ are appropriate approximations of $\mathcal{T}_\alpha$ and g, respectively. Moreover, we introduce a boundary element space $\mathcal{U}_h$ of $\mathcal{U}_{ad}$ which covers piecewise constant basis functions both in space and in time.

In particular, the operator $\widehat{\mathcal{T}}_\alpha : H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ is bounded and $Q_h^{0,0}(\Sigma)$-elliptic. Hence the perturbed variational inequality (5.73) admits a unique solution $\widehat{\omega}_h \in \mathcal{U}_h$. Moreover, we can derive the following error estimate.

Theorem 5.7. *Let $\omega \in \mathcal{U}_{ad}$ and $\widehat{\omega}_h \in \mathcal{U}_h$ be the unique solutions of the variational inequalities* (5.71) *and* (5.73)*, respectively. Then there holds the error estimate*

$$\|\omega - \widehat{\omega}_h\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)} \leq c(\omega, u_0, \overline{u})\, h_x^{s+\frac{1}{2}} \quad (5.74)$$

when assuming some regularity of $u_0, \overline{u}$ for which $\omega \in H^{s,\frac{s}{2}}(\Sigma)$ for some $s \in [0,1]$ and

$$c_1 h_x^2 \leq h_t \leq c_2 h_x^2 \quad \text{for some } 0 < c_1 < c_2.$$

In particular, we can expect a linear convergence for the error in $L_2(\Sigma)$ norm in the case of smooth data.

5.5 Numerical experiments

In this section we test some numerical examples where the domain Ω is a circle. For the boundary element discretization we use a uniform triangulation of the boundary $\Gamma = \partial\Omega$ on several levels by $N_0 = N_1 = 2^{L+2}$ nodes and a uniform decomposition of the interval $(0,T)$ by N time steps. We choose the trial space $Q_h^{1,0}(\Sigma)$ of piecewise linear and continuous basis functions in the space variable x, and piecewise constant ones in the time variable t to approximate the Dirichlet control z. For the fluxes ω, q, we use the trial space $Q_h^{0,0}(\Sigma)$ of piecewise constant basis functions both in space and in time.

Numerical example 1: Parabolic Dirichlet boundary control problem
As first numerical example we consider the unconstrained parabolic Dirichlet boundary control problem (5.1)-(5.2) for the domain $\Omega = B_{0.5}(O) \subset \mathbb{R}^2$ where

$$\overline{u}(x) = (x_1^2 + x_2^2)\log(x_1^2 + x_2^2) + 4x_1x_2, \quad u_0(x) = 0, \quad \alpha = 0.1, \quad T = 0.5.$$

In particular, we have to solve the linear system (5.66). Since the minimizer of (5.1) is not known, we use the boundary element solutions z_{ref}, ω_{ref} where $N_0 = N_1 = 512$, $N = 512$ as reference solutions.

In Table 5.1, we present the errors for the control z and the estimated order of convergence (eoc). The errors of the flux ω in the $L_2(\Sigma)$ norm are also given. Since the data are smooth in this case, we can expect the optimal order of convergence 1.5 for the control z in the energy space $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ which agrees with the theoretical results, see (5.65).

M	N	$\|\widehat{z}_h - z_{ref}\|_{L_2(\Sigma)}$	eoc	$\|\widehat{z}_h - z_{ref}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}$	eoc	$\|\omega_h - \omega_{ref}\|_{L_2(\Sigma)}$	eoc
32	4	0.155637	-	1.061380	-	0.733535	-
64	16	0.054384	1.517	0.562186	0.917	0.322231	1.187
128	64	0.012916	2.074	0.213010	1.400	0.185283	0.798
256	256	0.003017	2.098	0.071749	1.570	0.063744	1.539
expected			2.000		1.500		1.000

Table 5.1: The results of the unconstrained parabolic Dirichlet boundary control problem.

In Figure 5.1 we compare the final optimal solution $u(\cdot,T)$ with the target function $\overline{u}$ where the relative error is

$$\frac{\|u(\cdot,T) - \overline{u}\|_{L_2(\Omega)}}{\|\overline{u}\|_{L_2(\Omega)}} = \frac{0.034505}{0.082929} = 0.416079.$$

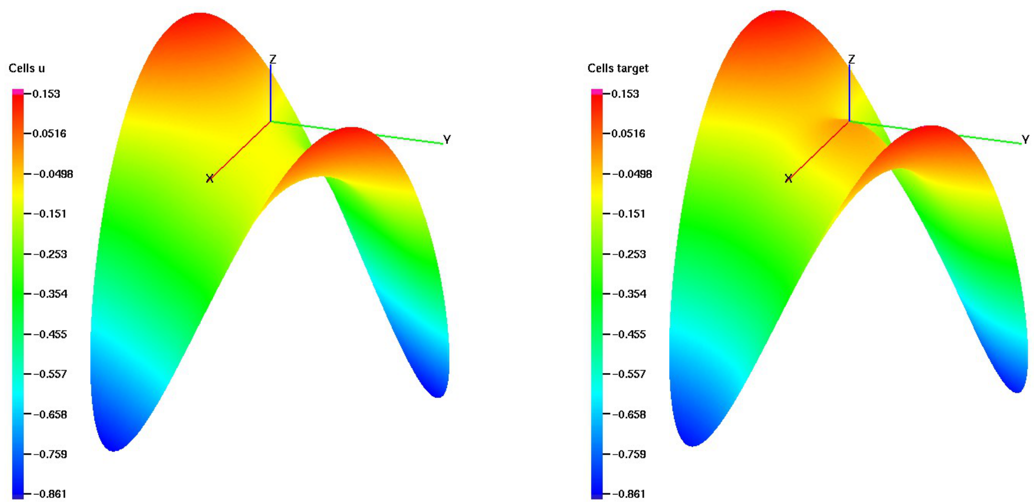

Figure 5.1: Comparison of final optimal solution (left) and target function (right).

For box constrained problem, we add the control constraint $-1 \leq z \leq 0.11$. The results are given in Table 5.2.

M	N	$\|\widehat{z}_h - z_{ref}\|_{L_2(\Sigma)}$	eoc	$\|\widehat{z}_h - z_{ref}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)}$	eoc	$\|\omega_h - \omega_{ref}\|_{L_2(\Sigma)}$	eoc
32	4	0.154249	-	1.050200	-	0.727606	-
64	16	0.054260	1.507	0.561425	0.903	0.321477	1.178
128	64	0.012887	2.074	0.212840	1.399	0.187099	0.781
256	256	0.003018	2.094	0.071736	1.569	0.064487	1.537
expected			2.000		1.500		1.000

Table 5.2: The results of the parabolic Dirichlet boundary control problem with the constraints $-1 \leq z \leq 0.11$.

Numerical example 2: Parabolic Neumann boundary control problem
In this example, we give numerical results for the unconstrained parabolic Neumann boundary control problem (5.67)-(5.68) for the domain $\Omega = B_{0.5}(O) \subset \mathbb{R}^2$. The data are the same as in numerical example 1,

$$\overline{u}(x) = (x_1^2 + x_2^2)\log(x_1^2 + x_2^2) + 4x_1x_2, \quad u_0(x) = 0, \quad \alpha = 0.1, \quad T = 0.5.$$

Here, we use the boundary element solutions ω_{ref}, z_{ref} where $N_0 = N_1 = 512$, and $N = 1024$ as reference solutions.

In Table 5.3, we present the errors for the control ω. We present also the errors of the Dirichlet data z in the $L_2(\Sigma)$ norm. These errors correspond to the estimate (5.74).

M	N	$\|\widehat{\omega}_h - \omega_{ref}\|_{L_2(\Sigma)}$	eoc	$\|z_h - z_{ref}\|_{L_2(\Sigma)}$	eoc
32	4	0.772516	-	0.169835	-
64	16	0.313851	1.299	0.057649	1.559
128	64	0.190589	0.720	0.015202	1.923
256	256	0.055004	1.793	0.003354	2.180
expected			1.000		2.000

Table 5.3: The results of the unconstrained parabolic Neumann boundary control problem.

In Figure 5.2 we compare the final optimal solution $u(\cdot,T)$ with the target function $\overline{u}$ where the relative error is

$$\frac{\|u(\cdot,T)-\overline{u}\|_{L_2(\Omega)}}{\|\overline{u}\|_{L_2(\Omega)}} = \frac{0.032212}{0.082929} = 0.388429.$$

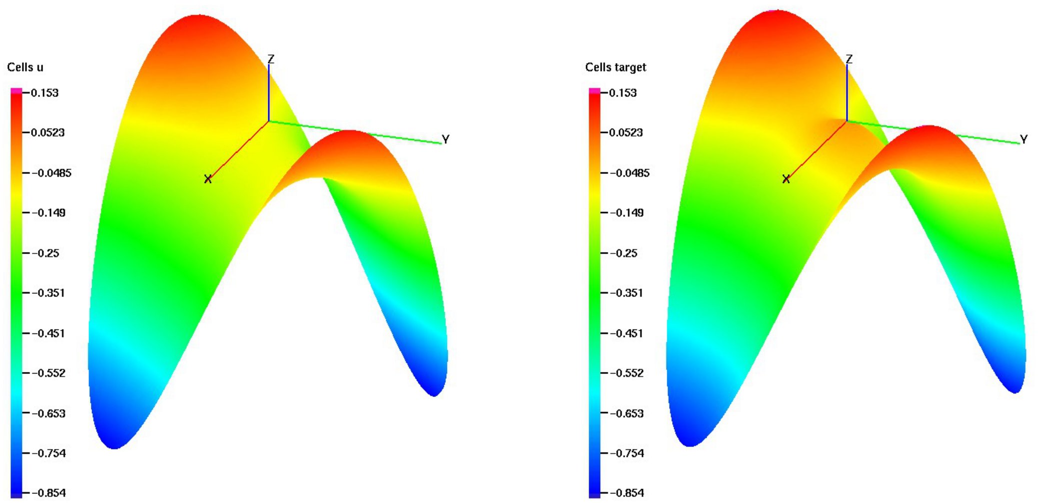

Figure 5.2: Comparison of final optimal solution (left) and target function (right).

6 CONCLUSIONS

In this work, boundary control problems governed by boundary value problems of linear second order elliptic/parabolic partial differential equations have been studied. The controls are considered in the energy spaces. The difference to the more common approach when considering $L_2(\Gamma)$ or $L_2(\Sigma)$ as control spaces is in the optimality condition. Especially, it shows the proper mapping properties which link the Dirichlet and Neumann data. This results in a higher regularity of the controls. In particular, when considering L_2 as the control spaces, for polygonal or polyhedral domains, the controls are zero at all corner points and along edges ($d = 3$).

In this thesis, we have applied the boundary element analysis for the solution of boundary control problems. We have presented here the model problems for the Poisson equation and for the heat equation. However, the approach can be applied for any linear elliptic partial differential equation if a fundamental solution is known. For the nonhomogeneous heat equations we need to compute additional related Newton potentials. The advantage of using boundary element methods is in the fact that only a boundary discretization is required. This allows to deal with the boundary control problems subject to partial differential equations in unbounded exterior domains, analogously. While the non-symmetric variational formulation which is based on the first boundary integral equation only requires to use the appropriate boundary element spaces, the use of the hypersingular operator in a symmetric formulation is stable for all standard boundary element spaces. Moreover, the Galerkin approximation results in a symmetric system. Hence the symmetric formulation seems to be the method of choice.

We have derived a priori error estimates of the Galerkin boundary element methods for general Lipschitz domains Ω. In the case of smooth data, we can prove the order $\mathcal{O}(h^2)$ of the errors in $L_2(\Gamma)$ norm for the Dirichlet control and linear order for the Neumann control. Whereas for the finite element approximation, a reduced order of $\mathcal{O}(h^{3/2})$ can be proved only, see [51] and see [19] for the L_2 setting.

This work is on the stability and error analysis of boundary element methods. Moreover, boundary element methods result in densely populated system matrices. Further work can be on studies of an efficient solution method to solve the discrete variational inequalities. In particular, further research is on the construction of efficient preconditioners and the use of fast boundary element methods as well. In addition, it is interesting to answer the open questions which appear in the thesis, e.g., the regularity of the control in parabolic boundary control problems.

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STATUTORY DECLARATION

I, Thanh Xuan Phan, declare that I have authored this thesis independently, that I have not used other than the declared sources/resources, and that I have explicitely marked all material which has been quotes either literally or by content from the used sources.

Graz, ...

(signature)